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Chapter 1

Introduction

This monogram is written with the graduate student in mind. I had in mind to write a short, crisp book that would introduce my students to the basic ideas and concepts behind many body physics. At the same time, I felt very strongly that I should like to share my excitement with this field, for without feeling the thrill of entering uncharted territory, I do not think one has the motivation to learn and to make the passage from learning to research.

Traditionally, as physicists we ask "what are the microscopic laws of nature ?", often proceeding with the brash certainty that once revealed, these laws will have such profound beauty and symmetry, that the properties of the universe at large will be self-evident. This basic philosophy can be traced from the earliest atomistic philosophies of Democritus, to the most modern quests to unify quantum mechanics and gravity.

The dreams and aspirations of many body physics interwine the atomistic approach with a complimentary philosophy- that of *emergent phenomena*. From this view, fundamentally new kinds of phenomena emerge within complex assemblies of particles which can not be anticipated from an à priori knowledge of the microscopic laws of nature. Many body physics aspires to synthesize from the microscopic laws, new principles that govern the macroscopic realm, asking

What new principles and laws emerge as we make the journey from the microscopic to the macroscopic?

This is a comparatively new scientific philosophy. Darwin was the perhaps the first to seek an understanding of emergent laws of nature. Following in his footsteps, Boltzmann was probably the first physicist to appreciate the need to understand how emergent principles are linked to microscopic physics, From Boltzmann's biography, we learn that he was strongly influenced and inspired by Darwin. In more modern times, a strong advocate of this philosophy has been Philip Anderson, who first coined the phrase "emergent phenomenon".

In an ideal world, I would hope that from this short course your knowledge of many body techniques will grow hand-in-hand with an appreciation of the motivating philsophy.

In many ways, this dual track is essential, for often, one needs both inspiration and overview to steer one lightly through the formalism, without getting bogged down in mathematical quagmires.

Here is a brief summary of what we will cover:

1. Scales and complexity, where we discuss the gulf of time (T), length-scale (L), particle number (N) and complexity that separates the microscopic from the macroscopic.
2. Second Quantization. Where make the passage from the wavefunction, to the field operator, and introduce the excitation concept.
3. Introducing the fundamental correlator of quantum fields: the Green's functions. Here we develop the tool of Feynman diagrams for visualizing and calculating many body processes.
4. Finite temperature and imaginary time. By replacing $it \longrightarrow \tau$, $e^{-iHt} \longrightarrow e^{-T\tau}$, we will see how to extend quantum field theory to finite temperature, where we will find that there is an intimate link between fluctuations and dissipation.
5. The disordered metal. Second quantized treatment of weakly disordered metals: the Drude metal, and the derivation of "Ohm's law" from first principles.
6. The concept of broken symmetry, as illustrated by superconductivity and pairing.
7. Opening the door to Path Integrals, linking the partition function and S-matrix to an integral over all possible time-evolved paths of the many-body system. $Z = \int_{PATH} e^{-S/\hbar}$.

Chapter 2

Scales and Complexity

We do infact know the microscopic physics that governs all metals, chemistry, materials and possibly life itself. In principle, all can be determined from the many-particle wavefunction

$$\Psi(\vec{x}_1, \vec{x}_2 \ldots \vec{x}_N, t), \tag{2.1}$$

which in turn, is governed by the Schödinger equation

$$\left\{ -\frac{\hbar^2}{2m}\sum_{j=1}^{N}\nabla_j^2 + \sum_{i<j} V(\vec{x}_i - \vec{x}_j) + \sum_j U(\vec{x}_j) \right\} \Psi = i\hbar\frac{\partial \Psi}{\partial t} \tag{2.2}$$

[*Schrödinger, 1926*]

There are of course many details that I have omitted- for instance, in an electromagnetic field we must gauge the derivatives $\nabla \rightarrow \nabla + i(e/\hbar)\vec{A}$, $U(x) \rightarrow U(x) - eV_{ext}(\vec{x})$. Here $V(x)$ is the Coulomb interaction potential,

$$V(\vec{x}) = \frac{e^2}{4\pi\epsilon_o}\frac{1}{|\vec{x}|}. \tag{2.3}$$

Also, to be complete, we must discuss spin, and the antisymmetry of Ψ under particle exchange. With these provisos, we have every reason to believe that this is the equation that governs the microsopic behavior of materials.

Unfortunately this knowledge does not help us! Why? At the most pragmatic level, we are defeated by the sheer complexity of the problem. Even for the chemist, the task of solving the Schrödinger equation for modest multi-electron atoms proves insurmountable without bold approximations. The problem facing the condensed matter physicist, with systems involving 10^{23} atoms, is qualitatively more severe. The amount of storage required for numerical solution of Schrodinger equation grows exponentially with the number of particles, so with a macroscopic number of interacting particles this becomes far more than a technical problem- it becomes one of principle. Indeed, we believe that the gulf between

the microscopic and the macroscopic is something qualitative and fundamental, so much so that new types of property emerge in macroscopic systems that we can not anticipate a priori by using brute-force analyses of the Schrödinger equation.

Let us dwell a little more on this gulf of complexity that separates the microscopic from the macroscopic. We can try to describe this gulf using four main catagories of scale:

- T. Time 10^{15}.
- L. Length 10^7.
- N. Number of particles. 10^{22}
- $\mathcal{C}$ Complexity.

2.1 Time scales

We can make an estimate of the characteristic quantum time scale by using the uncertainty principle $\Delta\tau\Delta E \sim \hbar$, so that

$$\Delta\tau \sim \frac{\hbar}{[1eV]} \sim \frac{\hbar}{10^{-19}J} \sim 10^{-15}s, \tag{2.4}$$

Although we know the physics on this timescale, in our macroscopic world, the the characteristic timescale $\sim 1s$, so that

$$\frac{\Delta\tau_{Macro}}{\Delta\tau_{Quantum}} \sim 10^{15}. \tag{2.5}$$

To link quantum, and macroscopic timescales, we must make a leap comparable with an extrapolation from the the timescale of a heart-beat to the age of the universe. (10 *billion yrs* $\sim 10^{17}$ *s*.)

2.2 L: Length scales

An approximate measure for the characteristic length scale in the quantum world is the de Broglie wavelength of an electron in a hydrogen atom,

$$L_{Quantum} \sim 10^{-10}m, \tag{2.6}$$

so

$$\frac{L_{Macroscopic}}{L_{Quantum}} \sim 10^8 \tag{2.7}$$

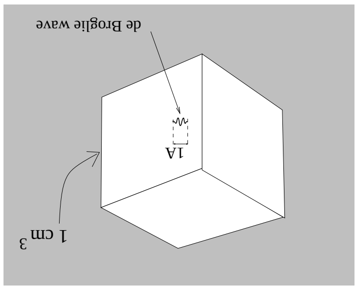

Figure 2.1: The typical size of a de Broglie wave is $10^{-10}m$, to be compared with a typical scale $1cm$ of a macroscopic crystal.

2.3 N: particle number

To visualize the number of particles in a single mole of substance, it is worth reflecting that a crystal containing a mole of atoms occupies a cube of roughly $1cm^3$. From the quantum perspective, this is a cube with approximately 100million atoms along each edge. Avagadros number

$$N_{Macroscopic} = 6 \times 10^{23} \sim (100 \text{ million})^3 \tag{2.8}$$

a number which is placed in perspective by reflecting that the number of atoms in a grain of sand is roughly comparable with the number of sand-grains in a 1 mile beach. Notice however that we are used to dealing with inert beaches, where there is no interference between the constituent particles.

2.4 C: Complexity and diversity.

Real materials are like macroscopic atoms, where the quantum interference amongst the constituent particles gives rise to a range of complexity and diversity that constitutes the largest gulf of all. We can attempt to quantify the "complexity" axis by considering the number of atoms per unit cell of a crystal. Whereas there are roughly 100 stable elements, there are roughly 100^2 stable binary compounds. The number of stable tertiary compounds

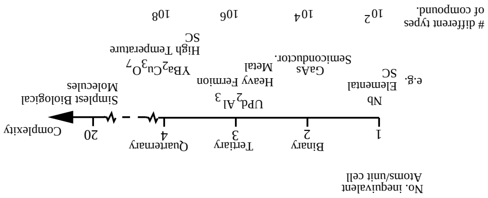

Figure 2.2: Examples of crystals of increasing complexity. As the number of inequivalent atoms per unit cell grows, the complexity of the material and the potential for new types of behavior grows.

is conservatively estimated at more than 10^6, of which still only a tiny fraction have been explored experimentally. At each step, the range of diversity increases, and there is reason to believe that at each level of complexity, new types of phenomenon begin to emerge.

When experimentalists began to explore the properties of quaternary compounds ten years ago, they came across the completely unexpected phenomenon of high temperature superconductivity. At present we have only just begun to scratch the surface of quaternary materials physics, and it seems not unreasonable to suppose that there are other similar surprises awating us. But lest you think that this is where it ends, it is worth reflecting on the fact that further out along the complexity axis we reach the most elementary molecules of life: an emergent phenomenon that is still unfolding from its inorganic origins roughly 10^{10} years ago.

Chapter 3

Quantum Fields: Overview

At the heart of quantum many body theory lies the concept of the quantum field. Like other quantum variables, the quantum field is in general a strongly fluctuating degree of freedom that only becomes sharp in certain special eigenstates; its function is to add or subtract particles to the system.

Quantum fields are intimately related to the idea of second quantization. First quantization permits us to make the jump from the classical world, to the simplest quantum systems. The classical momentum and position variables are replaced by operators, such as

$$\begin{aligned} E &\rightarrow i\hbar\partial_t, \\ p &\rightarrow \hat{p} = -i\hbar\partial_x, \end{aligned} \tag{3.1}$$

whilst the Poisson bracket which relates canonical conjugate variables is now replaced by the quantum commutator:

$$[x, p] = i\hbar. \tag{3.2}$$

The commutator is the key to first quantization, and it is the non-commuting property that leads to quantum fluctuations and the Heisenberg uncertainty principle. (See examples). Second quantization permits us to take the next step, extending quantum mechanics to

- Macroscopic numbers of particles.
- Develop an "excitation" or "quasiparticle" description of the low energy physics.
- Describe the dynamical response and internal correlations of large systems.
- To describe collective behavior and broken symmetry phase transitions.

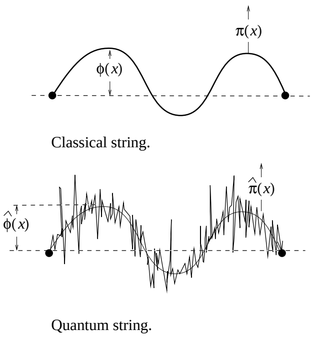

Figure 3.1: Contrasting a classical, and a quantum string.

In its simplest form, second quantization elevates classical fields to the status of operators. The simplest example, is the quantization of a classical string as shown in Fig. 3.1. Classically, the string is described by a smooth field $\phi(x)$ which measures the displacement from equilibrium, plus the conjugate field $\pi(x)$ which measures the transverse momentum per unit length. The classical Hamiltonian is

$$H = \int dx \left[\frac{T}{2}(\nabla_x\phi(x))^2 + \frac{1}{2\rho}\pi(x)^2\right] \tag{3.3}$$

where T is the tension in the string and ρ the mass per unit length. In this case, second-quantization is accomplished by imposing the canonical commutation relations

$$[\phi(x), \pi(y)] = i\hbar\delta(x-y), \qquad \textbf{Canonical commutation relation} \tag{3.4}$$

In this respect, second-quantization is no different to conventional quantization, except that the degrees of freedom are defined continuously throughout space. The basic method I have just described works for describing collective fields, such as sound vibrations, or the electromagnetic field, but we also need to know how to develop the field theory of identical particles, such as an electron gas in a metal, or a fluid of identical Helium atoms.

For particle fields, the process of second-quantization is more subtle, for here we the underlying fields have no strict classical counterpart.

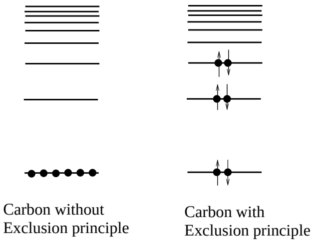

Figure 3.2: Without the exclusion principle, all electrons would occupy the same atomic orbital. There would be no chemistry, no life.

Historically, the first steps to dealing with such many particle systems were made in atomic physics. In 1925 Pauli proposed his famous "exclusion principle" to account for the diversity of chemistry, and the observation that atomic spectra could be understood only if one assumed there was no more than one electron per quantum state. (Fig. 3.2.)Shortly thereafter, Dirac and Fermi examined the consequences of this principle for a gas of particles, which today we refer to as "fermions". In 1926, Dirac realized that the two fundamental varieties of particle- fermions and bosons could be related to the parity of the many-particle wavefunction under particle exchange

$$\Psi(\text{particle at A, particle at B}) = e^{i\Theta}\Psi(\text{particle at B, particle at A}) \tag{3.5}$$

If one exchanges the particles twice, the total phase is $e^{2i\Theta}$. If we are to avoid a many-valued wavefunction, then we must have

$$e^{2i\Theta} = 1 \Rightarrow e^{i\Theta} = \pm 1 \left\{ \begin{array}{l} \text{bosons} \\ \text{fermions} \end{array} \right. \tag{3.6}$$

The choice of $e^{i\Theta} = 1$ leads to a wavefunction which is completely antisymmetric under particle exchange, which immediately prevents more than one particle in a given quantum state. [1]

In 1927, Jordan and Wigner realized that to cast physics of a many body system into a more compact form, one needs to introduce an operator for the particle itself-the field

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[1] In dimensions below three, it is possible to have wavefunctions with several Reimann sheets, which gives rise to the concept of fractional statistics and "anyons".

operator. With their innovation, it proves possible to unshackle ourselves from the many body wavefunction. The particle field

$$\hat{\psi}(x) \tag{3.7}$$

operator can be very loosely regarded as a quantization of the one-body Schrodinger wavefunction. Jordan and Wigner proposed that the particle field, and its complex conjugate are conjugate variables. With this insight, the second-quantization of bosons is achieved by introducing a non-zero commutator between the particle field, and its complex conjugate. The new quantum fields that emerge play the role of creating, and destroying particles (see below)

$$\underbrace{\psi(x), \psi^*(x)}_{\text{1 ptcle wavefunction}} \xrightarrow{[\psi(x), \psi^\dagger(y)] = \delta(x-y)} \underbrace{\hat{\psi}(x), \hat{\psi}^\dagger(x)}_{\text{destruction /creation operator}} \text{ Bosons} \tag{3.8}$$

For fermions, the existence of an antisymmetric wavefunction, means that particle fields must *anticommute*, i.e

$$\psi(x)\psi(y) = -\psi(y)\psi(x), \tag{3.9}$$

a point first noted by Jordan and Wigner. The simplest example of anticommuting operators, is provided by the Pauli matrices: we are now going to have to get used to a whole continuum of such operators! Jordan and Wigner realized that the second-quantization of fermions requires that the the non-trivial commutator between conjugate particle fields must be replaced by an anticommutator

$$\underbrace{\psi(x), \psi^*(x)}_{\text{1 ptcle wavefunction}} \xrightarrow{\{\psi(x), \psi^\dagger(y)\} = \delta(x-y)} \underbrace{\hat{\psi}(x), \hat{\psi}^\dagger(x)}_{\text{destruction /creation operator}} \text{ Fermions.} \tag{3.10}$$

The operation $\{a,\ b\} = ab + ba$ denotes the anticommutator. Remarkably, just as bosonic physics derives from commutators, fermionic physics derives from an algebra of anticommutators.

How real is a quantum field and what is its physical significance? To begin to to get a feeling of its meaning, let us look at some key properties. The transformation from wavefunction, to operator also extends to more directly observable quantities. Let us begin with Born's famous expression for the probability density in first quantization, $\rho(x) = \psi^*(x)\psi(x)$. By elevating the wavefunction to the status of a field operator, we obtain

$$\rho(x) = |\psi(x)|^2 \longrightarrow \hat{\rho}(x) = \hat{\psi}^\dagger(x)\hat{\psi}(x), \tag{3.11}$$

which is now the *operator* that represents the fluctuating particle density in the many body systems, so loosely speaking, the intensity of the quantum field represents the density of particles

Another aspect of the quantum field we have to understand, is its relationship to the many-body wavefunction. This link depends on a new concept, the "vacuum". This unique

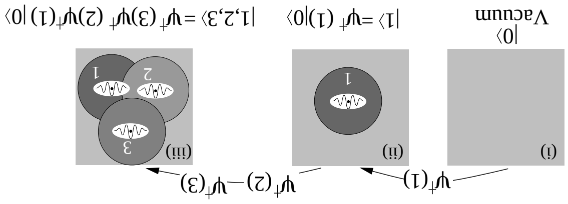


Figure 3.3: Action of creation operator on vacuum to create (i) a one particle and (ii) a three particle state

state, denoted by $|0\rangle$ is devoid of particles, and for this reason it is the only state for which there is no amplitude to destroy a particle so

$$\psi(x)|0\rangle = 0. \qquad \text{The vacuum} \tag{3.12}$$

We shall see that as a consequence of the canonical algebra, the creation operator $\hat{\psi}^\dagger(x)$ increments the number of particles by one, *creating* a particle at x, so that

$$|x_1\rangle = \psi^\dagger(x_1)|0\rangle \tag{3.13}$$

is a single particle at x_1,

$$|x_1, \ldots x_N\rangle = \psi^\dagger(x_N)\ldots\psi^\dagger(x_1)|0\rangle \tag{3.14}$$

is the N-particle state with particles located at $x_1 \ldots x_N$ and

$$\langle x_1, \ldots x_N| = \langle 0|[\psi(x_N)\ldots\psi(x_1)]^\dagger = \langle 0|\psi(x_1)\ldots\psi(x_N) \tag{3.15}$$

is its conjugate "bra" vector. The wavefunction of an N particle state, $|N\rangle$ is given by the overlap of $\langle x_1, \ldots x_N|$ with $|N\rangle$:

$$\psi(x_1, \ldots x_N) = \langle x_1, \ldots x_N|N\rangle = \langle 0|\psi(x_1)\ldots\psi(x_N)|N\rangle \tag{3.16}$$

So many body wavefunctions correspond to matrix elements of the quantum fields. From this link we can see that the exchange symmetry under particle exchange is directly linked to the exchange algebra of the field operators. For Bosons and Fermions respectively, we have

$$\langle 0|\ldots\psi(x_r)\psi(x_{r+1})\ldots|N\rangle = \pm\langle 0|\ldots\psi(x_{r+1})\psi(x_r)\ldots|N\rangle \tag{3.17}$$

(where + refers to Bosons, −to fermions), so that

$$\psi(x_r)\psi(x_{r+1}) = \pm\psi(x_{r+1})\psi(x_r) \tag{3.18}$$

From this we see that Bosonic operators commute, but fermionic operators must *anticommute*. Thus ultimately, it is the exchange symmetry of the two types of particles which dictates their commuting, or anticommuting algebra.

Unlike a classical field, quantum fields are in a state of constant fluctuation. This applies to both collective fields, as in the example of the string in Fig. 3.1, and to quantum fluids. Just as the commutator between position and momentum gives rise to the uncertainty principle: $[x, p] = i\hbar \longrightarrow \Delta x \Delta p \gtrsim \hbar$, the canonical commutation, or anticommutation relations give rise to a similar relatio between the amplitude and phase of the quantum field. Under certain conditions the fluctuations of a quantum field can be eliminated, and in these extreme limits, the quantum field begins to take on a tangible classical existence. In a bose superfluid for example, the quantum field becomes a sharp variable, and we can really ascribe a meaning to the expectation of the quantum field

$$\langle\psi(x)\rangle = \sqrt{\rho_s}e^{i\theta} \tag{3.19}$$

where ρ_s measures the density of particles in the superfluid condensate. We shall see that there is a completely parallel uncertainty relation between the phase and density of quantum fields,

$$\Delta N \Delta\theta \gtrsim 1 \tag{3.20}$$

where θ is the average phase of a condensate and N the number of particles it contains. When N is truly macroscopic, the uncertainty in the phase may be made arbitrarily small, so that in a Bose superfluid, the phase becomes sufficiently well defined that it becomes possible to observe interference phenomenon! Similar situations arise inside a Laser, where the phase of the electromagnetic field becomes well-defined, or a superconductor, where the phase of the electrons in the condensate becomes well defined.

Perhaps the greatest distinction between quantum, and classical fields, is the appearance of particles. The commutation, or anticommutation properties of quantum fields leads to an intrinsic "*graininess*" that is absent in classical fields. Quantum fields, though nominally continuous degrees of freedom, can always be decomposed in terms of a discrete particular content. The action of a collective field involves the creation of a wavepacket centered at x by both the creation, and destruction of quanta, schematically,

$$\phi(x) = \sum_{\mathbf{k}} \left[\begin{array}{c} \text{boson creation,} \\ \text{momentum -k} \end{array} + \begin{array}{c} \text{boson destruction} \\ \text{momentum k} \end{array} \right] e^{-i\mathbf{k}\cdot\mathbf{x}}, \tag{3.21}$$

Examples of such quanta, include quanta of sound, or phonons, and quanta of radiation, or photons. In a similar way, the action of a particle creation operator creates a wavepacket of particles at x, schematically,

$$\psi^\dagger(x) = \sum_{\mathbf{k}} \left[\begin{array}{c} \text{particle creation} \\ \text{momentum k} \end{array} \right] e^{-i\mathbf{k}\cdot\mathbf{x}}. \tag{3.22}$$

Chapter 4

Collective Quantum Fields

In this chapter, we will begin to familiarize ourselves with quantum fields by developing the field theory of a free, bosonic field. It is important to realize that a bosonic quantum field is fundamentally nothing more than a set of linearly coupled oscillators, and in particular, so long as the system is linear, the modes of oscillation can always be decomposed into a linear sum of independent normal modes. Each normal mode is nothing more than a simple harmonic oscillator, which provides the basic building block for bosonic field theories.

Our basic strategy for quantizing collective, bosonic fields, thus consists of two basic parts. First, we must reduce the Hamiltonian to its normal modes. For translationally invariant systems, this is just a matter of Fourier transforming the field, and its conjugate momenta. Second, we then quantize the normal mode Hamiltonian as a sum of independent Harmonic oscillators.

$$H(\phi,\pi) \xrightarrow{[F.T.]} \text{Normal Co-ords} \xrightarrow{\phi_q \sim (a_q + a^\dagger{}_{-q})} H = \sum_q \hbar\omega_q (n_q + \tfrac{1}{2}) \qquad (4.1)$$

The first part of this procedure is essentially identical for both quantum, and classical oscillators. The second-stage is nothing more than the quantization of a single Harmonic oscillator. Consider the family of lattices shown in Figure 4.1. We shall start with a single oscillator at one site. We shall then graduate to one and higher dimensional chain of oscillators, as shown in Fig 4.1.

4.1 Harmonic oscillator: a zero-dimensional field theory

Although the Schrodinger approach is most widely used in first quantization, it is the Heisenberg approach that opens the door to second-quantization. In the Schrödinger approach, one solves the wave-equation

$$\left(\frac{-\hbar^2\partial_x^2}{2m} + \frac{1}{2}m\omega^2 x^2\right)\psi_n = E_n\psi_n \qquad (4.2)$$

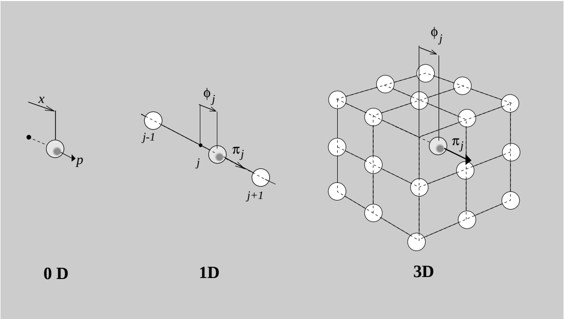


Figure 4.1: Family of zero, one and three-dimensional Harmonic crystals.

from which one finds the energy levels are evenly spaced, according to

$$E_n = (n + \frac{1}{2})\hbar\omega, \qquad (4.3)$$

where ω is the frequency of the oscillator.

The door to second-quantization is opened by re-interpreting these evenly spaced energy levels in terms of "quanta", each of energy $\hbar\omega$. The nth excited state corresponds to the addition of n quanta to the ground-state. We shall now see how we can put mathematical meat on these words by introducing an operator "$a^\dagger$" that creates these quanta, so that the n-th excited state is obtained by acting n times on the ground-state with the creation operator.

$$|n\rangle = \frac{1}{\sqrt{n!}}(a^\dagger)^n|0\rangle. \qquad (4.4)$$

Let us now see how this works. The Hamiltonian for this problem involves conjugate position and momentum operators as follows

$$\left.\begin{array}{rcl} H & = & \frac{p^2}{2m} + \frac{1}{2}m\omega^2 x^2 \\ [x,p] & = & i\hbar, \end{array}\right]. \qquad (4.5)$$

When the underlying particles develop coherence, the quantum field begins to behave classically. It is the ability of quantum fields to describe continuous classical behavior *and* discrete particulate behavior in a unified way that makes them so very special.

In the next two chapters we shall go back and see how these features appear systematically in the context of "free field theory". We shall begin with collective bosonic fields, which behave as a dense ensemble of coupled Harmonic oscillators. In the next chapter, we shall move to conserved particles, and see how the exchange symmetry of the wavefunction leads to the commutation, and anticommutation algebra of bose and Fermi fields. We shall see how this information enables us to completely solve the properties of a non-interacting Bose, or Fermi fluid.

Example. By considering the positivity of the quantity $\langle A(\lambda)^\dagger A(\lambda)\rangle$, where $\hat{A} = \hat{x} + i\lambda p$ and λ is a real number, prove the Heisenberg uncertainty relation $\Delta x \Delta p \geq \frac{\hbar}{2}$.

Example. How does the uncertainty principle prevent the collapse of the Hydrogen atom. Is the uncertainty principle enough to explain the stability of matter?

In the ground-state, the particle in the Harmonic potential undergoes zero-point motion, with an uncertainty in position and momentum Δp and Δx which satisfy $\Delta x \Delta p \sim \hbar$. Since the zero-point kinetic and potential energies are equal, $\Delta p^2/2m = m\omega^2 \Delta x^2/2$, so

$$\Delta x = \sqrt{\frac{\hbar}{m\omega}}, \ \Delta p = \sqrt{m\omega\hbar} \tag{4.6}$$

define the scale of zero-point motion. It is useful to define dimensionless position and momentum variables by factoring out the scale of zero-point motion

$$\xi = \frac{x}{\Delta x}, \qquad p_\xi = \frac{p}{\Delta p}. \tag{4.7}$$

One quickly verifies that $[\xi, p_\xi] = i$ are still canonically conjugate, and that now

$$H = \frac{\hbar\omega}{2}\Big[\xi^2 + p_\xi^2\Big]. \tag{4.8}$$

Next, introduce the "creation" and "annihilation" operators

$$\begin{aligned} a^\dagger &= \frac{1}{\sqrt{2}}(\xi - ip_\xi), && \text{"creation operator"} \\ a &= \frac{1}{\sqrt{2}}(\xi + ip_\xi), && \text{"annihilation operator".} \end{aligned} \tag{4.9}$$

Since $[a, a^\dagger] = \frac{-i}{2}([\xi, p_\xi] - [p_\xi, \xi]) = 1$, these operators satisfy the algebra

$$\left.\begin{aligned} [a, a] = [a^\dagger, a^\dagger] &= 0 \\ [a, a^\dagger] &= 1. \end{aligned}\right\} \textit{canonical commutation rules} \tag{4.10}$$

It is this algebra which lies at the heart of bosonic physics, enabling us to interpret the creation and annihilation operators as the objects which add, and remove quanta of vibration to and from the system.

To follow the trail further, we rewrite the Hamiltonian in terms of a and $a^\dagger$. Since $\xi = (a + a^\dagger)/\sqrt{2}$, $p_\xi = (a - a^\dagger)/\sqrt{2}i$, the core of the Hamiltonian can be rewritten as

$$\xi^2 + p_\xi^2 = a^\dagger a + a a^\dagger \tag{4.11}$$

But $aa^\dagger = a^\dagger a + 1$, from the commutation rules, so that

$$H = \hbar\omega[a^\dagger a + \frac{1}{2}]. \tag{4.12}$$

This has a beautifully simple interpretation. The second term is just the zero-point energy $E_0 = \hbar\omega/2$ The first term contains the "number operator"

$$\hat{n} = a^\dagger a, \qquad \textit{"number operator"} \tag{4.13}$$

which counts the number of vibrational quanta added to the ground state. Each of these quanta carries energy $\hbar\omega$.

To see this, we need to introduce the concept of the vacuum, defined as the unique state such that

$$a|0\rangle = 0. \tag{4.14}$$

From (4.12), this state is clearly an eigenstate of H, with energy $E = \hbar\omega/2$. We now assert that the state

$$|N\rangle = \frac{1}{\lambda_N}(a^\dagger)^N|0\rangle \tag{4.15}$$

where λ_N is a normalization constant, contains N quanta.

To verify that $\hat{n}$ counts the number of bosons, we use the commutation algebra to show that $[\hat{n}, a^\dagger] = a^\dagger$ and $[\hat{n}, a] = -a$, or

$$\begin{aligned} \hat{n}a^\dagger &= a^\dagger(\hat{n} + 1) \\ \hat{n}a &= a(\hat{n} - 1) \end{aligned} \tag{4.16}$$

which means that when $a^\dagger$ or a act on a state, they respectively add, or remove one quantum of energy. Suppose that

$$\hat{n}|N\rangle = N|N\rangle \tag{4.17}$$

for some N, then from (4.16),

$$\hat{n}\ a^\dagger|N\rangle = a^\dagger(\hat{n} + 1)|N\rangle = (N + 1)\ a^\dagger|N\rangle \tag{4.18}$$

so that $a^\dagger|N\rangle \equiv |N + 1\rangle$ contains $N + 1$ quanta. Since (4.17) holds for $N = 0$, it holds for all N. To complete the discussion, let us fix λ_N by noting that from the definition of $|N\rangle$,

$$\langle N - 1|aa^\dagger|N - 1\rangle = \left(\frac{\lambda_N}{\lambda_{N-1}}\right)^2 \langle N|N\rangle = \left(\frac{\lambda_N}{\lambda_{N-1}}\right)^2, \tag{4.19}$$

but since $aa^\dagger = \hat{n} + 1$, $\langle N - 1|aa^\dagger|N - 1\rangle = N\langle N - 1|N - 1\rangle = N$. Comparing these two expressions, it follows that $\lambda_N/\lambda_{N-1} = \sqrt{N}$, and since $\lambda_0 = 1$, $\lambda_N = \sqrt{N!}$.

Summarizing the discussion

$$\boxed{\begin{aligned} H &= \hbar\omega(\hat{n} + \tfrac{1}{2}) \\ \hat{n} &= a^\dagger a, && \textit{"number operator"} \\ |N\rangle &= \tfrac{1}{\sqrt{N!}}(a^\dagger)^N|0\rangle && \textit{N-Boson state} \end{aligned}} \tag{4.20}$$

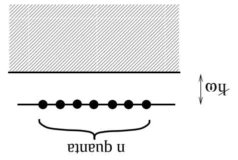


Figure 4.2: Illustrating the excitation picture for a single harmonic oscillator.

Using these results, we can quickly learn many things about the quantum fields a and $a^\dagger$. Let us look at a few examples. First, we can transform all time dependence from the states to the operators by moving to a Heisenberg representation, writing

$$a(t) = e^{iHt/\hbar} a e^{-iHt/\hbar} \qquad \textbf{Heisenberg representation} \tag{4.21}$$

This transformation preserves the canonical commutation algebra, and the form of H. The equation of motion of $a(t)$ is given by

$$\frac{da}{dt} = \frac{i}{\hbar}[H, a(t)] = -i\omega a(t) \tag{4.22}$$

so that the Heisenberg operators are given by

$$\begin{aligned} a(t) &= e^{-i\omega t}a, \\ a^\dagger(t) &= e^{i\omega t}a^\dagger \end{aligned} \tag{4.23}$$

Using these results, we can decompose the original momentum and displacement operators as follows

$$\begin{aligned} \hat{x}(t) &= \Delta x \xi(t) = \frac{\Delta x}{\sqrt{2}}(a(t) + a^\dagger(t)) = \sqrt{\frac{\hbar}{2m\omega}}(ae^{-i\omega t} + a^\dagger e^{i\omega t}) \\ \hat{p}(t) &= \Delta p p_\xi(t) = -i\sqrt{\frac{m\hbar\omega}{2}}(ae^{-i\omega t} - a^\dagger e^{i\omega t}) \end{aligned} \tag{4.24}$$

Notice how the displacement operator- a priori a continuous variable, has the action of creating and destroying discrete quanta.

We can use this result to compute the correlation functions of the displacement.

Example 1. *Calculate the autocorrelation function $S(t-t') = \frac{1}{2}\langle 0|\{x(t), x(t')\}|0\rangle$ and the "response" function $R(t-t') = -(i/\hbar)\langle 0|[x(t), x(t')]|0\rangle$ in the ground-state of the quantum Harmonic oscillator.*

Solution We may expand the correlation function and response function as follows

$$\begin{aligned} S(t_1 - t_2) &= \frac{1}{2}\langle 0|x(t_1)x(t_2) + x(t_2)x(t_1)|0\rangle \\ R(t_1 - t_2) &= -(i/\hbar)\langle 0|x(t_1)x(t_2) - x(t_2)x(t_1)|0\rangle \end{aligned} \tag{4.25}$$

But we may expand $x(t)$ as given in (4.24). The only term which survives in the ground-state, is the term proportional to $aa^\dagger$, so that

$$\langle 0|x(t)x(t')|0\rangle = \frac{\hbar}{2m\omega}\langle 0|aa^\dagger|0\rangle e^{-i\omega(t_1 - t_2)} \tag{4.26}$$

Now using (4.25) we obtain

$$\begin{aligned} \frac{1}{2}\langle 0|\{x(t), x(t')\}|0\rangle &= \frac{\hbar}{2m\omega}\cos[\omega(t - t')] && \text{"Correlation function"} \\ -i\langle 0|[x(t), x(t')]|0\rangle &= \frac{1}{m\omega}\sin[\omega(t - t')] && \text{"Response function"} \end{aligned}$$

- We shall later see that $R(t-t')$ gives the response of the ground-state to an applied force $F(t')$, so that at a time t, the displacement is given by

$$\langle x(t)\rangle = \int_{-\infty}^{t} R(t - t')F(t')dt' \tag{4.27}$$

Remarkably, the response function is identical with a classical Harmonic oscillator.

Example 2. *Calculate the number of quanta present in a Harmonic oscillator with characteristic frequency ω, at temperature T.*

To calculate the expectation value of any operator at temperature T, we need to consider an ensemble of systems in different quantum states $|\Psi\rangle = \sum_n c_n|n\rangle$. The expectation value of operator $\hat{A}$ in state $|\Psi\rangle$ is then

$$\langle \hat{A}\rangle = \langle\Psi|\Psi\rangle = \sum_{m,n} c_m^* c_n \langle m|\hat{A}|n\rangle \tag{4.28}$$

In a position basis, this would be

$$\langle \hat{A}\rangle = \sum_{m,n} c_m^* c_n \int dx \psi_m^*(x) A(x) \psi_m(x) \tag{4.29}$$

But now we have to average over the typical state $|\Psi\rangle$ in the ensemble, which gives

$$\overline{\langle\hat{A}\rangle} = \sum_{m,n}\overline{c^*_m c_n}\langle m|\hat{A}|n\rangle = \sum_{m,n}\rho_{mn}\langle m|\hat{A}|n\rangle \tag{4.30}$$

where $\rho_{mn} = \overline{c^*_m c_n}$ is the "density matrix". If the ensemble is in equilibrium with an incoherent heat bath, at temperature T, quantum statistical mechanics asserts that there are no residual phase correlations between the different energy levels, which acquires a Boltzmann distribution

$$\rho_{mn} = \overline{c^*_m c_n} = p_n\delta_{n,m} \tag{4.31}$$

where $p_n = e^{-\beta E_n}/Z$ is the Boltzman distribution, with $\beta = 1/k_BT$, and k_B is Boltzmann's constant. Let us now apply this to our problem, where

$$\hat{A} = \hat{n} = a^\dagger a \tag{4.32}$$

is the number operator. In this case,

$$\langle\hat{n}\rangle = \sum_n(e^{-\beta E_n}/Z)\langle n|\hat{n}|n\rangle = \frac{1}{Z}\sum_n ne^{-\beta E_n} \tag{4.33}$$

To normalize the distribution, we must have $\sum_n p_n = 1$, so that

$$Z = \sum_n e^{-\beta E_n} \tag{4.34}$$

Finally, since $E_n = \hbar\omega(n+\frac{1}{2})$,

$$\langle\hat{n}\rangle = \frac{\sum_n e^{-\beta\hbar\omega(n+\frac{1}{2})}n}{\sum_n e^{-\beta\hbar\omega(n+\frac{1}{2})}} = \frac{\sum_n e^{-\lambda n}n}{\sum_n e^{-\lambda n}}, \qquad \lambda = \beta\hbar\omega. \tag{4.35}$$

The sum in the denominator is a geometric series

$$\sum_n e^{-\lambda n} = \frac{1}{1-e^{-\lambda}}, \tag{4.36}$$

and the numerator is given by

$$\sum_n e^{-\lambda n}n = -\frac{\partial}{\partial\lambda}\sum_n e^{-\lambda n} = \frac{e^{-\lambda}}{(1-e^{-\lambda})^2} \tag{4.37}$$

so that

$$\langle\hat{n}\rangle = \frac{1}{e^{\lambda}-1} = \frac{1}{e^{\beta\hbar\omega}-1} \tag{4.38}$$

which is the famous Bose-Einstein distribution function.

Example 3. (Boguilubov transformation)*Calculate the spectrum of the Harmonic oscillator with a pairing term:*

$$H = \omega(a^\dagger a + \frac{1}{2}) + \frac{1}{2}\Delta(a^\dagger a^\dagger + a\ a) \tag{4.39}$$

Hint: show that the transformation $b = ua + va^\dagger$ preserves the canonical commutation alegbra when $u^2 - v^2 = 1$. By assuming that $H = \tilde{\omega}(b^\dagger b + \frac{1}{2})$, obtain an expression for $\tilde{\omega}$, u and v.

4.2 Collective modes: phonons

We now extend the discussion of the last section from zero to higher dimensions. Let us go back to the lattice shown in Fig 4.1 . To simplify our discussion, let imagine that at each site there is a single elastic degree of freedom. For simplicity, let us imagine we are discussing the longitundinal displacement of an atom along a one-dimensional chain that runs in the x-direction. For the j-th atom,

$$x_j = x^0_j + \phi_j. \tag{4.40}$$

If π_j is the conjugate momentum to x_j, then the two variables must satisfy canonical commutation relations

$$[\phi_i,\ \pi_j] = i\hbar\delta_{ij}. \tag{4.41}$$

Notice how variables at different sites are fully independent. We'll imagine that our one-dimensional lattice has N_s sites, and we shall make life easier by working with periodic boundary conditions, so that $\phi_{j+N_s} \equiv \phi_j$ and $\pi_j \equiv \pi_{j+N_s}$. Suppose nearest neighbors are connected by a "spring", in which case, the total total energy is then a sum of kinetic and potential energy

$$\hat{H} = \sum_{j=1,N_s}\left[\frac{\pi_j^2}{2m} + \frac{m\omega^2}{2}(\phi_j - \phi_{j+1})^2\right] \tag{4.42}$$

where m is the mass of an atom.

Now the great simplifying feature of this model, is that that it possesses *translational symmetry*, so that under the translation

$$\pi_j \rightarrow \pi_{j+1}, \qquad \phi_j \rightarrow \phi_{j+1} \tag{4.43}$$

the Hamiltonian and commutation relations remain unchanged. If we shrink the size of the lattice to zero, this symmetry will become a continuous translational symmetry. The generator of these translations is the *crystal momentum* operator, which must therefore commute with the Hamiltonian. Because of this symmetry, it makes sense to transform to operators that are diagonal in momentum space, so we'll Fourier transform all fields as follows:

$$\left.\begin{array}{ll} \phi_j & = \frac{1}{\sqrt{N_s}}\sum_q e^{iqR_j}\phi_q, \\ \pi_j & = \frac{1}{\sqrt{N_s}}\sum_q e^{iqR_j}\pi_q, \end{array}\right\} \qquad R_j = ja. \tag{4.44}$$

The periodic boundary conditions, $\phi_j = \phi_{j+N_s}$, $\pi_j = \pi_{j+N_s}$ mean that the values of q entering in this sum must satisfy $qL = 2\pi n$, where $L = N_s a$ is the length of the chain and n is an integer, thus

$$q = \frac{2\pi}{L}n, \qquad (n \in [1, N_s]) \tag{4.45}$$

Notice that $q \in [0,\ 2\pi/a]$ defines the range of q. As in any periodic structure, the crystal momentum is only defined modulo a reciprocal lattice vector, which in this case is $2\pi/a$, so

that $q + \frac{2\pi}{a} \equiv q$, (you may verify that $(q + \frac{2\pi}{a})R_j = qR_j + 2\pi m$, which is why we restrict $n \in [1, N_s]$. The functions $\frac{1}{\sqrt{N_s}}e^{iqR_j} \equiv \langle j|q\rangle$ form a complete orthogonal basis, so that in particular

$$\sum_j\langle q'|j\rangle\langle j|q'\rangle \equiv \frac{1}{N_s}\sum_j e^{i(q-q')R_j} = \langle q|q'\rangle \equiv \delta_{q,q'}. \qquad \text{orthogonality} \tag{4.46}$$

is only unity if $q = q'$. This relationship (which extends to any number of dimensions) is immensely useful, and we shall use it time and time again. Using the orthogonality relation, we can check that the inverse transformations are

$$\begin{array}{ll} \phi_q & = \frac{1}{\sqrt{N_s}}\sum_j e^{-iqR_j}\phi_j \\ \pi_q & = \frac{1}{\sqrt{N_s}}\sum_q e^{-iqR_j}\pi_j \end{array} \tag{4.47}$$

Notice that since ϕ_j and π_j are Hermitian operators, it follows that $\phi^\dagger(q) = \phi(-q)$ and $\pi^\dagger(q) = \pi(-q)$. Using the orthogonality, we can verify the transformed commutation relations are

$$\begin{aligned} [\phi(-q), \pi(q')] &= \frac{1}{N_s}\sum_{i,j}e^{i(qR_i - q'R_j)}\overbrace{[\phi_i, \pi_j]}^{i\hbar\delta_{ij}} \\ &= \frac{i\hbar}{N_s}\sum_j e^{i(q-q')R_j} = i\hbar\delta_{qq'} \end{aligned} \tag{4.48}$$

We shall now see that π_q and ϕ_q are quantized version of "normal co-ordinates" which bring the Hamiltonian back into the standard Harmonic oscillator form. To check that the Hamiltonian is truly diagonal in these variables we

1. expand ϕ_j and π_j in terms of their Fourier components,
2. regroup the sums so that the summation over momenta is on the outside,
3. Eliminate all but one summation over momentum by carrying out the internal sum over site variables. This will involve terms like $N_s^{-1}\sum_j e^{i(q+q')R_j} = \delta_{q+q'}$, which constrains $q' = -q$ and eliminates the sum over q'.

With a bit of practice, these steps can be carried out very quickly. In transforming the potential energy, it is useful to rewrite it in the form

$$V = \frac{m\omega^2}{2}\sum_j\phi_j(2\phi_j - \phi_{j+1} - \phi_{j-1}). \tag{4.49}$$

The term in brackets can be Fourier transformed as follows:

$$(2\phi_j - \phi_{j+1} - \phi_{j-1}) = \frac{1}{\sqrt{N_s}}\sum_q\phi_q e^{iqR_j}\overbrace{[2 - e^{iqa} - e^{-iqa}]}^{4\sin^2(qa/2)} \tag{4.50}$$

so that

$$\begin{aligned} V &= \frac{m}{2}\sum_{q,q'}\phi_{-q}\phi_{q'}\omega_q^2\overbrace{N_s^{-1}\sum_j e^{i(q'-q)R_j}}^{\delta_{q,q'}} \\ &= \sum_q\frac{m\omega_q^2}{2}\phi_{-q}\phi_q \end{aligned} \tag{4.51}$$

where we have defined $\omega_q^2 = 4\omega\sin^2(qa/2)$. Carrying out the same procedure on the kinetic energy, we obtain

$$H = \sum_q\left(\frac{1}{2m}\pi_q\pi_{-q} + \frac{m\omega_q^2}{2}\phi_q\phi_{-q}\right) \tag{4.52}$$

which expresses the Hamiltonian in terms of "normal co-ordinates", ϕ_q and π_q. So far, all of the transformations we have preserved the ordering of the operators, so it is no surprise that the quantum and classical expressions for the Hamiltonian in terms of normal co-ordinates are formally identical. Notice that we have essentially reduced the problem to a single harmonic oscillator- one set of oscillators for each momentum

The next step merely repeats the procedure carried out for the single harmonic oscillator. We define a set of conjugate creation and annihilation operators

$$\left.\begin{array}{ll} a_q & = \sqrt{\frac{m\omega_q}{2\hbar}}(\phi_q + \frac{i}{m\omega_q}\pi_q) \\ a^\dagger{}_q & = \sqrt{\frac{m\omega_q}{2\hbar}}(\phi_{-q} - \frac{i}{m\omega_q}\pi_{-q}) \end{array}\right\} \qquad [a_q,\ a^\dagger{}_{q'}] = \frac{-i}{2\hbar}\Big[[\phi_q, \pi_{-q'}] - [\pi_q, \phi_{-q'}]\Big] = \delta_{q,q'} \tag{4.53}$$

Note that the second expression for $a^\dagger{}_q$ is obtained by taking the complex conjugate of a_q, and remembering that $\phi^\dagger{}_q = \phi_{-q}$ and $\pi^\dagger{}_q = \pi_{-q}$, since the underlying fields are real.

The inversion of these expressions is

$$\left.\begin{array}{ll} \pi_q & = -i\sqrt{\frac{m\omega_q\hbar}{2}}(a_q - a^\dagger{}_{-q}) \\ \phi_a & = \sqrt{\frac{\hbar}{2m\omega_q}}(a_q + a^\dagger{}_{-q}) \end{array}\right\} \tag{4.54}$$

Notice how the Fourier component of the field at wavevector q either destroys a phonon of momentum q or creates a phonon of momentum $-q$. Both have reduce the total momentum by q.

From these expressions, it follows that

$$\begin{aligned} \pi_q\pi_{-q} &= \frac{m\omega_q\hbar}{2}(a^\dagger{}_{-q}a_{-q} + a_q a^\dagger{}_q - a^\dagger{}_{-q}a^\dagger{}_q - a_q a_{-q}) \\ \phi_q\phi_{-q} &= \frac{\hbar}{2m\omega_q}(a^\dagger{}_{-q}a_{-q} + a_q a^\dagger{}_q + a^\dagger{}_{-q}a^\dagger{}_q + a_q a_{-q}) \end{aligned} \tag{4.55}$$

Adding the two terms inside the Hamiltonian then gives

$$H = \frac{1}{2}\sum_q\hbar\omega_q(a^\dagger{}_q a_q + a_q a^\dagger{}_q), \tag{4.56}$$

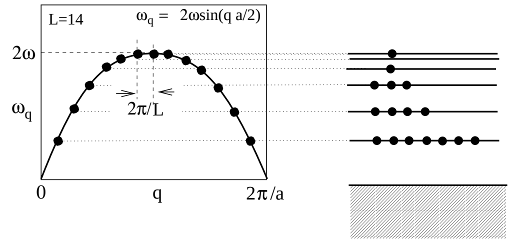


Figure 4.3: Illustrating the excitation picture for a chain of coupled oscillators, length L=14.

or using the commutation relations,

$$H = \sum_q \hbar\omega_q ({a^\dagger}_q a_q + \frac{1}{2}) \tag{4.57}$$

Since each set of a_q and ${a^\dagger}_q$ obey canonical commutation relations, we can immediately identify $n_q = {a^\dagger}_q a_q$ as the number operator for quanta in the q-th momentum state. Remarkably, the system of coupled oscillators can be reduced to a sum of independent Harmonic oscillators, with characteristic frequency ω_q, energy $\hbar\omega_q$ and momentum q. Each normal mode of the original classical system corresponds to particular phonon excitation.

We can immediately generalize all of our results from a single Harmonic oscillator. For example, the general state of the system will now be an eigenstate of the phonon occupancies,

$$|\Psi\rangle = |n_{q_1},\ n_{q_2} \dots n_{q_N}\rangle = \prod_{\otimes} |n_{q_i}\rangle = \left[\prod_i \frac{({a^\dagger}_{q_i})^{n_{q_i}}}{\sqrt{n_{q_i}!}}\right] |0\rangle \tag{4.58}$$

where the vacuum is the unique state that is annihilated by all of the a_q. In this state, the occupation numbers n_q are diagonal, so this is an energy eigenstate with energy

$$E = E_o + \sum_q n_q \hbar\omega_q \tag{4.59}$$

where $E_o = \frac{1}{2}\sum_q \hbar\omega_q$ is the zero-point energy.

Remarks

- The quantized displacements of a crystal are called phonons. Quantized fluctuations of magnetization in a magnet are "magnons".
- We can easily transform to a Heisenberg representation, whereapon $a_q(t) = a_q e^{-i\omega_q t}$.
- We can expand the local field entirely in terms of phonons. Using (4.54), we obtain

$$\begin{aligned} \phi_j(t) &= \frac{1}{\sqrt{N_s}} \sum_q \phi_q e^{iqR_j} \\ &= \frac{1}{\sqrt{N_s}} \sum_q \sqrt{\frac{\hbar}{2m\omega_q}} (a_q(t) + {a^\dagger}_{-q}(t)) e^{iqR_j}. \end{aligned} \tag{4.60}$$

- The transverse displacements of the atoms can be readily included by simply upgrading the displacement and momentum ϕ_j and π_j to vectors. For "springs", the energy associated with transverse and longitudinal displacements is not the same because the stiffness associated with transverse displacements depends on the tension. Nevertheless, the Hamiltonian has an identical form for the one longitudinal and two transverse modes, provided one inserts a different stiffness for the transverse modes. The initial Hamiltonian is then simply a sum over three degenerate polarizations $\lambda \in [1,3]$

$$\hat{H} = \sum_{\lambda=1,3} \sum_{j=1,N_s} \left[\frac{\pi_{j\lambda}^2}{2m} + \frac{m\omega_\lambda^2}{2} (\phi_{j\lambda} - \phi_{j+1\lambda})^2\right] \tag{4.61}$$

where $\omega_1^2 = \omega^2$ for the longitudinal mode, and $\omega_{2,3}^2 = T/a$, where T is the tension in the spring, for the two transverse modes. By applying the same procedure to all three modes, the final Hamiltonian then becomes

$$H = \sum_{\lambda=1,3} \sum_q \hbar\omega_{q\lambda} ({a^\dagger}_{q\lambda} a_{q\lambda} + \frac{1}{2}).$$

where $\omega_{q\lambda} = 2\omega_\lambda sin(qa/2)$. Of course, in more realistic crystal structures, the energies of the three modes will no longer be degenerate.

- We can generalize all of this discussion to a 2 or 3 dimensional square lattice, by noting that the orthogonality relation becomes

$$N_s^{-1} \sum_j e^{-i(\mathbf{q}-\mathbf{q}')\cdot R_j} = \delta_{\mathbf{q}-\mathbf{q}'} \tag{4.62}$$

where now,

$$\mathbf{q} = \frac{2\pi}{L}(i_i, i_2 \dots i_D) \tag{4.63}$$

and $\mathbf{R_j}$ is a site on the lattice. The general form for the potential energy is slightly more complicated, but one can still cast the final Hamiltonian in terms of a sum over longitudinal and transverse modes.

- The zero-point energy $E_o = \frac{1}{2}\sum_q \hbar\omega_q$ is very important in $He-4$ and $He-3$ crystals, where the lightness of the atoms gives rise to such large phonon frequencies that the crystalline phase is unstable, except at high pressures.

4.3 The Thermodynamic Limit

In the last section, we examined a system of coupled oscillators on a finite lattice. By restricting a system to a finite lattice, we impose a restriction on the *maximium* wavelength, and hence, the excitation spectrum. This is known as an "infra-red" cut-off. When we take $L \to \infty$, the allowed momentum states become closer and closer together, and we now have a continuum in momentum space.

What happens to the various momentum summations in the thermodynamic limit, $L \to \infty$? When the allowed momenta become arbitrarily close together, the discrete summations over momentum must be replaced by continuous integrals. For each dimension, the increment in momentum appearing inside the discrete summations is

$$\Delta q = \frac{2\pi}{L} \tag{4.64}$$

so that $L\frac{\Delta q}{2\pi} = 1$. Thus in one dimension, the summation over the discrete values of q can be formally rewritten as

$$\sum_{q_j} \{\dots\} = L \sum_{q_j} \frac{\Delta q}{2\pi} \{\dots\} \tag{4.65}$$

where $q_j = 2\pi\frac{j}{L}$, and $j \in [1, N_s]$. When we take $L \to \infty$, q becomes a continuous variable $q \in [0, 2\pi/a]$, where $a = L/N_s$ is the lattice spacing, so that the summation can now be replaced by a continuous integral:

$$\sum_q \{\dots\} \longrightarrow L \int_0^{2\pi/a} \frac{dq}{2\pi} \{\dots\} \tag{4.66}$$

Similarly, in in D-dimensions, we can regard the D-dimensional sum over momentum as a sum over tiny hypercubes, each of volume

$$(\Delta q)^D = \frac{(2\pi)^D}{L^D} \tag{4.67}$$

so that $L^D\frac{(\Delta q)^D}{(2\pi)^D} = 1$ and

$$\sum_q \{\dots\} = L^D \sum_q \frac{(\Delta q)^D}{(2\pi)^D} \{\dots\} \longrightarrow L^D \int_{0<q_i<2\pi/a} \frac{d^D q}{(2\pi)^D} \{\dots\} \tag{4.68}$$

where the integral is over a hypercube in momentum space, with sides of length $2\pi/a$.

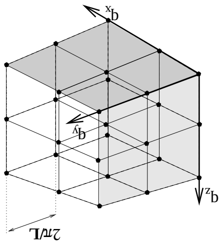


Figure 4.4: Illustrating the grid of allowed momenta for a three-dimensional crystal of dimensions L^3. In the limit $L \to \infty$, the grid becomes a continuum, with $(L/2\pi)^3$ points per unit volume of momentum space.

Once the momentum sums become continuous, we need to change the normalization of our states. By convention, we now normalize our plane wave basis per unit volume, writing

$$\langle\vec{x}|\vec{k}\rangle \longrightarrow e^{i\vec{x}\cdot\vec{k}} \tag{4.69}$$

In a finite volume, this means that the orthogonality condition on these plane waves is

$$\langle\vec{k}'|\vec{k}\rangle = \int d^D x e^{i(\vec{k}-\vec{k}')\cdot\vec{x}} = L^D \delta_{\vec{k}-\vec{k}'}, \tag{4.70}$$

where $\delta_{\vec{k}-\vec{k}'}$ is the discrete delta function on the grid of allowed wavevectors. In the thermodynamic limit, this becomes

$$\int d^D x e^{i(\vec{k}-\vec{k}')\cdot\vec{x}} = (2\pi)^D \delta^D(\vec{k}-\vec{k}') \tag{4.71}$$

so that the continuum limit of the discrete delta-function is given by

$$L^D \delta_{\vec{k}\vec{k}'} \longrightarrow (2\pi)^D \delta^D(\vec{k}-\vec{k}') \tag{4.72}$$

Example 4.*Re-express the Hamiltonian $\hat{H}$ of a simplified three-dimensional Harmonic crystal in terms of phonon number operators and calculate the zero-point energy, where*

$$H = \sum_j \frac{\pi_j^2}{2m} + \sum_{j,\vec{a}=(\hat{x},\hat{y},\hat{z})} \frac{m\omega_o^2}{2} (\Phi_j - \Phi_{j+\vec{a}})^2 \tag{4.73}$$

where $\phi_j \equiv \phi(x_j)$ and $\pi_j \equiv \pi(x_j)$ denote canonically conjugate (scalar) displacement, and momenta at site j, and $\hat{a} = (\hat{x}, \hat{y}, \hat{z})$ denotes the unit vector separating nearest neigbor atoms.

Solution First we must Fourier transform the co-ordinates and the Harmonic potential. The potential can be re-written as

$$\hat{V} = \frac{1}{2}\sum_{i,j} V_{i-j}\phi_i\phi_j \tag{4.74}$$

where

$$V_{\mathbf{R}} = m\omega_o^2 \sum_{\vec{a}=(\hat{x},\hat{y},\hat{z})} (2\delta_{\mathbf{R}} - \delta_{\mathbf{R}-\vec{a}} - \delta_{\mathbf{R}+\vec{a}}) \tag{4.75}$$

The Fourier transform of this expression is

$$\begin{aligned} V_{\mathbf{q}} &= \sum_{\mathbf{R}} V_{\mathbf{R}} e^{-i\mathbf{q}\cdot\mathbf{R}} \\ &= m\omega_o^2 \sum_{\vec{a}=(\hat{x},\hat{y},\hat{z})} (2 - e^{-i\mathbf{q}\cdot\mathbf{a}} - e^{i\mathbf{q}\cdot\mathbf{a}}) \\ &= m\omega_o^2 \sum_{l=x,y,z} [2 - \cos(q_l a)] \end{aligned} \tag{4.76}$$

so that writing $V_{\mathbf{q}} = m(\omega_{\mathbf{q}})^2$, it follows that the normal mode frequency are given by

$$\omega_{\mathbf{q}} = 2\omega_o[\sin^2(q_x a/2) + \sin^2(q_y a/2) + \sin^2(q_z a/2)]^{\frac{1}{2}} \tag{4.77}$$

Fourier transforming the fields

$$\begin{aligned} \phi_j &= \frac{1}{\sqrt{N_s}}\sum_{\mathbf{q}} \phi_{\mathbf{q}} e^{i\mathbf{q}\cdot\mathbf{x}} \\ \pi_j &= \frac{1}{\sqrt{N_s}}\sum_{\mathbf{q}} \pi_{\mathbf{q}} e^{i\mathbf{q}\cdot\mathbf{x}} \end{aligned} \tag{4.78}$$

where $\mathbf{q} = \frac{2\pi}{L}(i, j, k)$ are the discrete momenta of a cubic crystal of volume L^3, with periodic boundary conditions, we find

$$H = \sum_{\mathbf{q}} \left[\frac{\pi_{\mathbf{q}}\pi_{-\mathbf{q}}}{2m} + \frac{m\omega_{\mathbf{q}}^2}{2}\phi_{\mathbf{q}}\phi_{-\mathbf{q}}\right] \tag{4.79}$$

Defining the creation and annihilation operator

$$b_{\mathbf{q}} = \sqrt{\frac{m\omega_{\mathbf{q}}}{2\hbar}}(\phi_{\mathbf{q}} + \frac{i}{m\omega_{\mathbf{q}}}\pi_{\mathbf{q}}), \qquad b^{\dagger}{}_{\mathbf{q}} = \sqrt{\frac{m\omega_{\mathbf{q}}}{2\hbar}}(\phi_{-\mathbf{q}} - \frac{i}{m\omega_{\mathbf{q}}}\pi_{-\mathbf{q}}), \tag{4.80}$$

we reduce the Hamiltonian to its standard form

$$H = \sum_{\mathbf{q}} \hbar\omega_{\mathbf{q}}(\hat{n}_{\mathbf{q}} + \frac{1}{2}) \tag{4.81}$$

where $\hat{n}_{\mathbf{q}} = b^{\dagger}{}_{\mathbf{q}} b_{\mathbf{q}}$ is the phonon number operator.

In the ground-state, $n_{\mathbf{q}} = 0$, so that the zero-point energy is

$$E_o = \sum_{\mathbf{q}} \frac{\hbar\omega_{\mathbf{q}}}{2} \longrightarrow V\int \frac{d^3q}{(2\pi)^3}\frac{\hbar\omega_{\mathbf{q}}}{2} \tag{4.82}$$

where $V = L^3$. Substituting for $\omega_{\mathbf{q}}$, we obtain

$$\begin{aligned} E_o &= V\prod_{l=1,3}\int_0^{2\pi/a}\frac{dq_l}{2\pi}\hbar\omega_o\sqrt{\sum_{l=1,3}\sin^2(q_l a/2)} \\ &= N_s\hbar\omega_o I_3 \end{aligned} \tag{4.83}$$

where

$$I_3 = \int_{0<u_1,u_2,u_3<\pi}\frac{d^3u}{\pi^3}\sqrt{\sum_{l=1,3}\sin^2(u_l)} = 1.19 \tag{4.84}$$

and N_s is the number of sites.

Remarks

- The zero point energy per unit cell of the crystal is $\hbar\omega_o(I_3/\pi^3)$, a finite number.
- Were we to take the "continuum limit", taking the lattice separation to zero, the zero-point energy would diverge, due to the profusion of ultraviolet modes.

4.4 Continuum Limit

In contrast to the thermodynamic limit, when we take the continuum limit we remove the discrete character of the problem, allowing fluctuations of arbitrarily small wavelength, and hence arbitrarily large energy. For a discrete system with periodic boundary conditions, the momentum in any one direction can not exceed $2\pi/a$. By taking a to zero, we remove the ultra-violet cut-off in momentum.

As a simple example, we shall consider a one-dimensional string. The important lesson that we shall learn, is that both the discrete model, and the continuum model have the same long-wavelength physics. Their behavior will only differ on very short distances, at high frequencies and short times. This is a very simple example of the concept of renormalization. Provided we are interested in low energy properties, the details of the string at short-distances- whether it is discrete, or continuous don't matter.

Of course, in many respects, the continuum model is more satisfying and elegant. We shall see however, that we always have to be careful in going to the continuum limit, because this introduces quantum fluctuations on arbitrarily short length scales. These fluctuations don't affect the low energy excitations, but they do mean that the zero-point fluctuations of the field become arbitrarily large.

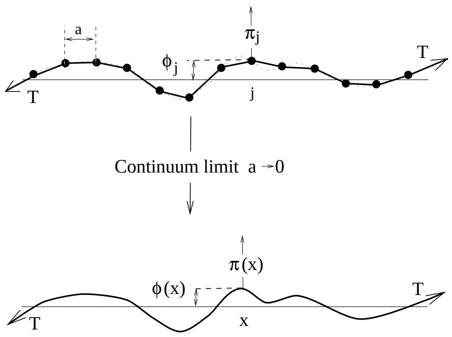


Figure 4.5: Illustrating a (a) discrete and a (b) continuous string. By taking the length between units in the string to zero, maintaining the density per unit length and the tension, we arrive at the continuum limit.

Let us start out with a discrete string, as shown in fig 4.5. For small displacements, the Hamiltonian for this discrete string is identical to that of the last section, as we can see by the following argument. If a string is made up of point particles of mass m, separated by a distance a, with a tensile force T acting between them, then for small transverse displacements ϕ_j, the link between the j th and $j+1$th particle is expanded by an amount $\Delta s_j = (\phi_j - \phi_{j+1})^2/2a$, raising the potential energy by an amount $T\Delta s_j$. The Hamiltonian is then

$$\hat{H} = \sum_{j=1,N_s}\left[\frac{\pi_j^2}{2m} + \frac{T}{2a}(\phi_j - \phi_{j+1})^2\right] \tag{4.85}$$

which reverts to (4.42) with the replacement $T/a \rightarrow m\omega^2$.

To take the continuum limit, we let $a \rightarrow 0$, preserving $\rho = m/a$. In this limit, we may replace

$$\begin{aligned} a\sum_j &\rightarrow \int dx, \\ \frac{(\phi_j - \phi_{j+1})^2}{a^2} &\rightarrow (\nabla_x\phi(x))^2, \end{aligned} \tag{4.86}$$

Making the replacement

$$\pi_j/a \rightarrow \tilde{\pi}(x) \tag{4.87}$$

we obtain

$$H = \int dx\left[\frac{T}{2}(\nabla_x\phi)^2 + \frac{1}{2\rho}\tilde{\pi}(x)^2\right] \tag{4.88}$$

On the discrete lattice, the commutation relations

$$[\phi_i, \tilde{\pi}_j] = i\hbar\tilde{\delta}(x_i - x_j), \tag{4.89}$$

where $\tilde{\delta}(x_i - x_j) = a^{-1}\delta_{ij}$. In the limit $a \rightarrow 0$, $\tilde{\delta}(x_i - x_j)$ behaves as a Dirac delta function, so that in this limit,

$$[\phi(x), \tilde{\pi}(y)] = i\hbar\delta(x - y) \tag{4.90}$$

We now make the jump to Fourier space, writing

$$\phi(x) = \int\frac{dq}{2\pi}\phi_q e^{iqx}e^{-\epsilon|q|/2} \tag{4.91}$$

with a similar relation between $\pi(x)$ and π_q. In the continuum limit, q is no longer bounded by the cut-off $2\pi/a$. To control the wild fluctuations that arise at high momentum we still need some kind of cut-off, and this is why we introduce the small exponential convergence factor into the inverse Fourier transform. Now it is just a question of repeating the same steps of the last section, but for the continuous fields ϕ_q and π_q. We may confirm that in the canonical commutation relation, we must now replace $\langle q|q'\rangle = \delta_{qq'}$ by $\langle q|q'\rangle = 2\pi\delta(q - q')$, so that

$$[\phi_q, \pi_{-q'}] = i\hbar 2\pi\delta(q - q') \tag{4.92}$$

When we transform the Hamiltonian, we obtain

$$H = \int\frac{dq}{2\pi}\left[\frac{\pi_{\mathbf{q}}\pi_{-\mathbf{q}}}{2\rho} + \frac{\rho\omega_{\mathbf{q}}^2}{2}\phi_{\mathbf{q}}\phi_{-\mathbf{q}}\right]e^{-\epsilon|q|} \tag{4.93}$$

where now $\omega_q = c|q|$, and $c = \sqrt{T/\rho}$ is the velocity of the phonons. Notice how this has almost exactly the same form as the the discrete lattice. Defining the creation and annihilation operator by the relations

$$\begin{aligned} \phi_q &= \sqrt{\frac{\hbar}{2\rho\omega_q}}[a_q + a^{\dagger}{}_{-q}] \\ \pi_q &= -i\sqrt{\frac{\hbar\rho\omega_q}{2}}[a_q - a^{\dagger}{}_{-q}] \end{aligned} \tag{4.94}$$

we find that the creation and annihilation operators satisfy

$$[a_q, a^{\dagger}{}_{q'}] = 2\pi\delta(q - q'). \tag{4.95}$$

We may now rewrite the Hamiltonian as

$$H = \int_{-\infty}^{\infty} \frac{dq}{2\pi} \frac{\hbar\omega_{\mathbf{q}}}{2} (a^\dagger{}_q a_q + a_{-q} a^\dagger{}_{-q}) e^{-\epsilon|q|} \tag{4.96}$$

If we re-order the Boson operators, we obtain

$$H = \int_{\infty}^{\infty} \frac{dq}{2\pi} \hbar\omega_{\mathbf{q}} (a^\dagger{}_q a_q + \overbrace{2\pi\delta(0)}^{``L''} \frac{1}{2}) e^{-|\epsilon q|/2} \tag{4.97}$$

The first terms corresponds to the excitations of string, and we recognize the last term as the zero-point energy of the string. Had we been less ambitious, and started out on a finite, but lattice long , the term 2 $\pi\delta(0)$ would be replaced by L, which is merely the statement that the zero-point energy scales with the length,

$$E_{ZP} = L \int \frac{dq}{2\pi} \hbar c|q||e^{-\epsilon|q|\epsilon} = L\hbar(\frac{c}{\epsilon}) \tag{4.98}$$

is the total zero-point energy. Once we remove the momentum cut-off, the momentum sum is unbounded and the zero-point energy per unit length becomes infinite in the continuum limit. It often proves convenient to remove this nasty infinity by introducing the concept of *"normal ordering"*. If we take any operator A, then we denote its normal ordered count-part by the symbol $: A :$. The operator $: A :$ is the same as A, excepting that all the creation operators have been ordered to the left of all of the annihilation operators. All commutators associated with the ordering are neglected, so that the normal ordered Hamiltonian is

$$: H := \hbar c \int_{-\infty}^{\infty} |q| \hat{n}_q \tag{4.99}$$

measures the excitation energy above the ground-state.

Finally, let us look at the field correlations in the continuum string. The fields in real space are given by

$$\phi(x,t) = \int \frac{dq}{2\pi} \sqrt{\frac{\hbar}{2\rho\omega_q}} [a_q(t) + a_{-q}(t)] e^{iqx} e^{-\epsilon|q|/2} \tag{4.100}$$

where, as in the case of the Harmonic oscillator

$$a_q(t) = a_q e^{-i\omega_q t}, \qquad a^\dagger{}_q(t) = a_q e^{i\omega_q t}, \tag{4.101}$$

Example 5. *Calculate the the equal-time ground-state correlation function*

$$S(x) = \frac{1}{2} \langle 0|(\phi(x) - \phi(0))^2|0\rangle. \tag{4.102}$$

for a one-dimensional string.

<u>*Solution:*</u> Let us begin by rewriting

$$S(x) = \langle 0|(\phi(x)\phi(0) - \phi(0)^2)|0\rangle \tag{4.103}$$

where we have used translational invariance to replace the expectation value of $\phi(x)^2$ by the expectation value of $\phi(0)^2$. When we expand $\phi(x)$ and $\phi(0)$ in terms of creation and annihilation operators, only the terms of the form $\langle 0|a_q a^\dagger{}_{-q'}|o\rangle = \langle 0|[a_q, a^\dagger{}_{-q'}]|o\rangle = (2\pi)\delta(q - q')$ will survive. Let us write this out explicitly:

$$\begin{aligned} S(x) &= \int \frac{dqdq'}{(2\pi)^2} \frac{\hbar}{2\rho c\sqrt{|q||q'|}} \langle 0|[a_q + a^\dagger{}_{-q}][a_{-q'} + a^\dagger{}_{q'}]|0\rangle (e^{iqx} - 1) e^{-|q|\epsilon} \\ &= \frac{\hbar}{2\rho c} \int \frac{dq}{2\pi} e^{-|q|\epsilon} \left(\frac{e^{iqx} - 1}{|q|} \right) \\ &= \left(\frac{\hbar}{\rho c} \right) \left[\frac{1}{4\pi} \ln(\frac{\epsilon^2}{\epsilon^2 + x^2}) \right] \end{aligned} \tag{4.104}$$

where to obtain the last step, we first calculate

$$\frac{dS}{dx} = -\frac{\hbar}{\rho c} \int_0^{\infty} \frac{dq}{2\pi} e^{-|q|\epsilon} \sin(qx) = -\left(\frac{\hbar}{2\pi\rho c} \right) \frac{x}{x^2 + \epsilon^2} \tag{4.105}$$

and then integrate the answer on x, noting $S(0) = 0$.

<u>*Remarks*</u>

- Note that at small distances the fluctuations in the string displacement grow as $\ln(|x|)$. This is because the number of short-wavelength fluctuations is unbounded.
- Note also that we could have obtained this result by working with a discrete string, and taking $a \to 0$ at the end of the calculation. Had we done this, we would have found that

  $$S(x) = \frac{a\hbar}{2\rho} \int \frac{dq}{2\pi} \left(\frac{e^{iqx} - 1}{\omega_q} \right) \tag{4.106}$$

  which has the same long-wavelength behavior.
- Had we repeated this calculation in D dimensions, the integral over q becomes a d-dimensional integral. In this case,

  $$S(x) \sim \int d^D q \left(\frac{e^{iqx} - 1}{|q|} \right) \sim \frac{1}{x^{D-1}} \tag{4.107}$$

  In higher dimensions, the phase space for number of short-wavelength fluctuations grows as q^D, which leads to stronger fluctuations at short-distances.

4.5 Exercises for chapter 4

1. For the Harmonic oscillator $H = \hbar\omega[a^\dagger a + \frac{1}{2}]$, we know that

   $$\langle \hat{n} \rangle = n(\omega) = \frac{1}{e^{\beta\hbar\omega} - 1}, \tag{4.108}$$

   where $\beta = 1/(k_B T)$ and $\hat{n} = a^\dagger a$ is the number operator. In the ground-state, using the equations of motion for the creation and annihilation operators, we showed that the zero-point fluctuations in position were described by the correlation function

   $$\frac{1}{2} \langle \{x(t),\ x(0)\} \rangle = \frac{\hbar}{2m\omega} \cos\omega t. \tag{4.109}$$

   Generalize this result to finite temperatures. You should find that there are two terms in the correlation function. *Please* give them a physical interpretation.

2. (a) Show that if a is a canonical bose operator, the canonical transformation

   $$\begin{aligned} b &= ua + va^\dagger, \\ b^\dagger &= ua^\dagger + va, \end{aligned} \tag{4.110}$$

   (where u and v are real), preserves the canonical commutation relations, provided $u^2 - v^2 = 1$.

   (b) Using the results of (a), diagonalize the Hamiltonian

   $$H = \omega(a^\dagger a + \frac{1}{2}) + \frac{1}{2}\Delta(a^\dagger a^\dagger + aa), \tag{4.111}$$

   by transforming it into the form $H = \tilde{\omega}(b^\dagger b + \frac{1}{2})$. Find $\tilde{\omega}$, u and v in terms of ω and Δ. What happens when $\Delta = \omega$?

3. (Harder) Find the classical normal mode frequencies and normal co-ordinates for the one dimensional chain with Hamiltonian

   $$H = \sum_j \left[\frac{p_j^2}{2m_j} + \frac{k}{2}(\phi_j - \phi_{j-1})^2 \right] \tag{4.112}$$

   where at even sites $m_{2j} = m$ and at odd sites $m_{2j+1} = M$. Please sketch the dispersion curves.

   (ii) What is the gap in the excitation spectrum?

   (iii)Write the diagonalized Hamiltonian in second quantized form and discuss how you might arrive at your final answer. You will now need two types of creation operator.

4. (Harder) According to the "Lindeman" criterion, a crystal melts when the rms displacement of its atoms exceeds a third of the average separation of the atoms. Consider a three dimensional crystal with separation a, atoms of mass m and a nearest neigbor quadratic interaction $V = (m\omega^2/2)(\vec{\Phi}_{\mathbf{R}} - \vec{\Phi}_{\mathbf{R+a}})^2$.

   (i) Using strictly physical arguments, show that if

   $$\frac{\hbar}{m\omega a^2} > \zeta_c \tag{4.113}$$

   the crystal will melt due to zero-point fluctuations. (Hint... what would the answer be for a simple harmonic oscillator?)

   (ii)Calculate ζ_c. If you like, to start out, imagine that the atoms only move in one direction, so that Φ is a scalar displacement at the site with equilibrium position $\mathbf{R}$. Calculate the rms zero-point displacement of an atom $\sqrt{\langle 0|\Phi(x)^2|0\rangle}$. Now generalize your result to take account of the fluctuations in three orthogonal directions.

   (iii)Suppose $\hbar\omega/k_B = 300K$, and the atom is a Helium atom. Estimate the maximum atomic separation at which the solid will be stable against quantum fluctuations.

5. (Harder) Find the transformation that diagonalizes the Hamiltonian

   $$H = \sum_j \left\{ J_1(a^\dagger{}_{i+1} a_i + H.c) + J_2(a^\dagger{}_{i+1} a^\dagger{}_i + H.c) \right\} \tag{4.114}$$

   where the ith site is located at $R_j = aj$. You may find it helpful to (i) transform to momentum space, writing $a_j = \frac{1}{N^{1/2}} \sum_q e^{iqR_j} a_q$ and (ii) carrying out a canonical transformation of the form $b_q = u_q a_q + v_q a^\dagger{}_{-q}$, where $u^2 - v^2 = 1$. What happens when $J_1 = J_2$?

Chapter 5

Conserved Particles

The method we have just examined is fine for "collective excitations" of a medium, but it does not make it self-evident how we should proceed for systems of conserved particles, such as a gas of Helium-4 atoms, or an electron gas inside a metal. Now we shall return to discuss conserved particles.

First quantized quantum mechanics *can* deal with many body physics, through the introduction of a many particle wavefunction. This is the approach favored in fields such as quantum chemistry, where the number of electrons is large, but not macroscopic. The quantum chemistry approach revolves around the many-body wavefunction. For N particles, this a function of $3N$ variables and N spins. The Hamiltonian is then an operator expressed in terms of these co-ordinates:

$$\begin{aligned}\psi &\longrightarrow \psi(x_1, x_2 \ldots x_N, t)\\ H &\longrightarrow \sum_j\left[-\frac{\hbar^2}{2m}\nabla_j^2 + U(x_j)\right] + \frac{1}{2}\sum_{i<j}V(x_i - x_j)\end{aligned} \tag{5.1}$$

With a few famous exceptions this method is cumbersome, and ill-suited to macroscopically large systems. The most notable exceptions occur in low dimensional problems, where wavefunctions of macroscopically large ensembles of interacting particles have been obtained. Examples include

- Bethe Ansatz solutions to interacting one, and zero-dimensional problems.
- Laughlin's wavefunction for interacting electrons in high magnetic fields, at commensurate filling factors.

Second-quantization provides a general way of approaching many body systems in which the wavefunction plays a minor role. As we mentioned in chapter 3, the essence of second-quantization is a process of raising the Schrodinger wavefunction to the level of an operator which satisfies certain "canonical commutation" or "canonical anticommutation" algebras".

In first quantized physics physical properties of a quantum particle, such as its density, Kinetic energy, potential energy can be expressed in terms of the one-particle wavefunction. Second quantization elevates each of these quantities to the status of an operator by replacing the one-particle wavefuncion by its corresponding field operator:

$$\left.\begin{array}{ccc}\psi(x,t) & \longrightarrow & \hat\psi(x,t)\\ \text{one particle wavefunction} & & \text{Field operator}\\ & & \\ O(\psi^*,\psi) & \longrightarrow & \hat O(\hat\psi^\dagger,\hat\psi)\end{array}\right\}\text{2nd Quantization} \tag{5.2}$$

For example, Born's famous expression for the one-particle (probability) density becems an operator as follows:

$$\rho(x) = |\psi(x)|^2 \longrightarrow \hat\rho(x) = \hat\psi^\dagger(x)\hat\psi(x), \tag{5.3}$$

so that the potential energy associated with an external potential is

$$\hat V = \int d^3x U(x)\hat\rho(x). \tag{5.4}$$

Similarly, the Kinetic energy in first-quantization

$$T[\psi^*,\ \psi] = \int d^3x\psi^*(x)\left[-\frac{\hbar^2}{2m}\nabla^2\right]\psi(x) \tag{5.5}$$

becomes the operator

$$\hat T = \int d^3x\hat\psi^\dagger(x)\left[-\frac{\hbar^2}{2m}\nabla^2\right]\hat\psi(x). \tag{5.6}$$

Finally

$$H = \int d^3x\hat\psi^\dagger(x)\left[-\frac{\hbar^2}{2m}\nabla^2 + U(x)\right]\psi + \frac{1}{2}\int d^3xd^3x'V(x-x') : \hat\rho(x)\hat\rho(x') : \tag{5.7}$$

is the complete many-body Hamiltonian in second-quantized form. Here $V(x-x')$ is the interaction potential between the particles, and the symbol ":" reflects the fact that order of the operators counts. ": ...:" is the normal ordering operator denotes that all creation operators between the two colons must be ordered to lie to the left of all destruction operators.

5.1 Commutation and Anticommutation Algebras

In 1927, Jordan and Wigner proposed that the microscopic field operators describing identical particles divide up into two types. These are axioms of quantum field theory. For identical bosons, field operators satisfy a commutation algebra, whereas for Fermions, the

field operators satisfy an *anticommutation* algebra. Since we will be dealing with many of their properties in parallel, it useful to introduce the notation

$$[a,b]_\pm = ab \pm ba, \qquad \text{fermions/bosons} \tag{5.8}$$

to denote commutators $(-)$ for bosons or anticommutators $(+)$ for fermions . The algebra of field operators is then

$$\left.\begin{aligned}[][\psi(1),\psi(2)]_\pm = [\psi^\dagger(2),\psi^\dagger(1)]_\pm &= 0\\ [\psi(1),\psi^\dagger(2)]_\pm &= \delta(1-2)\end{aligned}\right\}\textbf{Fermions/ Bosons} \tag{5.9}$$

When spin is involved, $1 \equiv (x_1,\sigma_1)$ and $\delta(1-2) = \delta^{(D)}(x_1 - x_2)\delta_{\sigma_1\sigma_2}$. We shall motivate these axioms in two ways: (i) by showing, in the case of Bosons, that they are a natural result of trying to quantize the one-particle wavefunction. ; (ii) by showing that they lead to the first quantized formulation of many-body physics, naturally building the particle exchange statistics into the mathematical framework.

5.1.1 Heuristic Derivation for Bosons

The name second-quantization derives from the notion that many body physics can be obtained by quantizing the one-particle wavefunction. Philosophically, this is very tricky, for surely, the wavefunction is already a quantum object? Let us imagine however, a thought experiment, when we prepare a huge number of non-interacting particles, prepared in such a way that they are all in precisely the same quantum state. The feasibility of this does not worry us here, but note that it can actually be done for a large ensemble of bosons, by condensing them into a single quantum state. In this circumstance, every single particle lies in the same one-particle state. If we time evolve the system we can begin to think of the single-particle wavefunction as if it is a classical variable.

Let us briefly recall one-particle quantum mechanics. If the particle is in a state $|\psi\rangle$, then we can always expand the state in terms of a complete basis $\{|n\rangle\}$, as follows:

$$|\psi(t)\rangle = \sum_n |n\rangle\overbrace{\langle n|\psi(t)\rangle}^{\psi_n(t)} = \sum_n |n\rangle\psi_n(t) \tag{5.10}$$

so that $|\psi_n(t)|^2 = p_n(t)$ gives the probability of being in state n. Now applying Schrodinger's equation, $\hat H|\psi\rangle = i\hbar\partial_t|\psi\rangle$ gives

$$\begin{aligned}i\hbar\dot\psi_n(t) &= \sum_m\langle n|H|m\rangle\psi_m(t)\\ i\hbar\dot\psi_n^*(t) &= -\sum_m\langle m|H|n\rangle\psi_m^*(t)\end{aligned} \tag{5.11}$$

Now if we write the ground-state energy as a functional of the $b_m(t)$, we get

$$H(\psi,\psi^*) = \langle H\rangle = \sum_{m,n}\psi_m^*\psi_n\langle m|H|n\rangle \tag{5.12}$$

we see that the equations of motion can be written in Hamiltonian form

$$\begin{aligned}\dot\psi_m &= \frac{\partial H(\psi,\psi^*)}{i\hbar\partial\psi_m^*}, &\qquad (\text{c.f } \dot q = \frac{\partial H}{\partial p})\\ i\hbar\dot\psi_m^* &= -\frac{\partial H(\psi,\psi^*)}{\partial\psi_m}, &\qquad (\text{c.f } \dot p = -\frac{\partial H}{\partial q})\end{aligned} \tag{5.13}$$

so we can identify

$$\{\psi_n, i\hbar\psi_n^*\} \equiv \{q_n, p_n\} \tag{5.14}$$

as the canonical position and momentum co-ordinates.

But suppose we don't have a macroscopic number of particles in a single state. In this case, the amplitudes $\psi_n(t)$ are expected to undergo quantum fluctuations. Let us examine what happens if we "second-quantize" these variables, making the replacement

$$[q_n,\ p_m] = i\hbar\delta_{nm} = i\hbar[\psi_n, \psi^\dagger{}_m] \tag{5.15}$$

or

$$\boxed{\begin{aligned}[][\psi_n,\psi_m] &= [\psi^\dagger{}_n,\psi^\dagger{}_m] = 0,\\ [\psi_n,\psi^\dagger{}_m] &= \delta_{nm}\end{aligned}} \tag{5.16}$$

In terms of these operators, our second quantized Hamiltonian becomes

$$H = \sum_{m,l}\hat\psi^\dagger{}_m\hat\psi_l\langle m|H|l\rangle \tag{5.17}$$

If we now use this to calculate the time-evolution of the quantum fields we obtain

$$-i\hbar\partial_t\psi_j = [\hat H,\ \psi_j] = \sum_{m,l}\langle m|H|l\rangle\overbrace{[\psi^\dagger{}_m\psi_l,\psi_j]}^{-\delta_{mj}\psi_l} \tag{5.18}$$

Eliminating the sum over m, we obtain

$$\begin{aligned}-i\hbar\partial_t\psi_j &= -\sum_l\langle j|H|l\rangle\psi_l\\ -i\hbar\partial_t\psi^\dagger{}_j &= [\hat H,\ \psi^\dagger{}_j] = \sum_l\psi^\dagger{}_l\langle l|H|j\rangle,\end{aligned} \tag{5.19}$$

where the complex conjugated expression gives the time evolution of $\psi^\dagger{}_l$. Remarkably, the equations of motion of the operators match the time evolution of the one-particle amplitudes. But now we have operators, we have all the new physics associated with quantum fluctuations of the particle fields.

5.2 What about Fermions?

Remarkably, as Jordan and Wigner first realized, we recover precisely the same time-evolution if second-quantize the operators using anticommutators, rather than commutators, and it this is what gives rise to fermions and the exclusion principle. But for fermions, we can not offer a heurtistic argument, because they don't condense: as far as we know, there is no situation in which individual fermi field operators behave semi-classically. although of course, in a superconductor, pairs of fermions that behave semi-classically.

In fact, all of the operations we carried out above work equally well with either canonical commutation or canonical *anticomutation* relations:

$$\boxed{\begin{aligned}[][\psi_n,\psi_m]_\pm &= [\psi^\dagger{}_n,\psi^\dagger{}_m]_\pm = 0,\\ [\psi_n,\psi^\dagger{}_m]_\pm &= \delta_{nm}\end{aligned}} \qquad (5.20)$$

where the ± refers to fermions/bosons respectively. To evaluate the equation of motion of the field operators, we need to know the commutator $[H,\psi_n]$. Using the relation

$$[ab,c]_\pm = a[b,c]_\pm \mp [a,c]_\pm \qquad (5.21)$$

we may verify that

$$\begin{aligned}[][\psi^\dagger{}_m\psi_l,\psi_j] &= \psi^\dagger{}_m\overbrace{[\psi_l,\psi_j]_\pm}^{0} \overbrace{\mp[\psi^\dagger{}_m,\psi_j]_\pm}^{-\delta_{mj}}\psi_l\\ &= -\delta_{mj}\psi_l \qquad (5.22)\end{aligned}$$

so that

$$\begin{aligned}-i\hbar\partial_t\psi_j &= [\hat{H},\ \psi_j] = \sum_{m,l}\langle m|H|l\rangle\overbrace{[\psi^\dagger{}_m\psi_l,\psi_j]}^{-\delta_{mj}\psi_l}\\ &= -\sum_l\langle j|H|l\rangle\psi_l \qquad (5.23)\end{aligned}$$

independently of whether we use an anticommuting, or commuting algebra.

Let us now go on, and look at some general properties of second-quantized operators that hold for both bosons and fermions.

5.3 Field operators in different bases

Let us first check that our results don't depend on the one-particle basis we use. To do this, we must confirm that the commutation or anticommutation algebra of bosons or fermions

is basis independent. Suppose we have two bases of one-particle states: the $\{|r\rangle\}$ basis, and a new $\{|\tilde{s}\rangle\}$ basis, where

$$|\psi\rangle = \sum_r |r\rangle\psi_r = \sum_s |\tilde{s}\rangle a_s \qquad (5.24)$$

where $\langle\tilde{s}|\psi\rangle = a_s, \qquad \langle r|\psi\rangle = \psi_r$. Introducing the completeness relation $1 = \sum_r |r\rangle\langle r|$ into the first expression, we obtain

$$\overbrace{\langle\tilde{s}|\psi\rangle}^{a_s} = \sum_r\langle\tilde{s}|r\rangle\overbrace{\langle r|\psi\rangle}^{\psi_s} \qquad (5.25)$$

If this is how the one-particle states transform between the two bases, then we must use the same unitary transformation to relate the field operators that destroy particles in the two bases

$$\hat{a}_s = \sum_r\langle\tilde{s}|r\rangle\hat{\psi}_r \qquad (5.26)$$

The commutation algebra of the new operators is now

$$[\hat{a}_s,\hat{a}^\dagger{}_p]_\pm = \sum_{l,m}\langle\tilde{s}|l\rangle\overbrace{[\hat{\psi}_l,\hat{\psi}^\dagger{}_m]_\pm}^{\delta_{lm}}\langle m|\tilde{p}\rangle \qquad (5.27)$$

This is just the pre- and post-multiplication of a unit operator by the unitary matrix $U_{sl}\langle\tilde{s}|l\rangle$ and its conjugate $U^\dagger{}_{mp} = \langle m|\tilde{p}\rangle$. The final result, is unity, as expected:

$$[\hat{a}_s,\hat{a}^\dagger{}_p]_\pm = \sum_r\langle\tilde{s}|r\rangle\langle r|\tilde{p}\rangle = \langle\tilde{s}|\tilde{p}\rangle = \delta_{sp} \qquad (5.28)$$

In other words, the canonical commutation algebra is preserved by unitary transformations of basis.

A basis of particular importance, is the position basis. The one-particle wavefunction can always be decomposed in a discrete basis, as follows

$$\psi(x) = \langle x|\psi(t)\rangle = \sum_n\langle x|n\rangle\psi_n \qquad (5.29)$$

where $\langle x|n\rangle = \phi_n(x)$ is the wavefunction of the nth state. We now define the corresponding destruction operator

$$\hat{\psi}(x) = \sum_n\langle x|n\rangle\hat{\psi}_n \qquad (5.30)$$

which defines the field operator in real space. and we can also use the orthogonality relation

$$\text{“}\sum_x\text{”}\langle n|x\rangle\langle x|m\rangle = \delta_{nm}, \qquad (\text{“}\sum_x\text{”} = \int d^Dx) \qquad (5.31)$$

to invert these relations:

$$\psi_n = \int d^Dx\langle n|x\rangle\psi, \qquad \psi^\dagger{}_n = \int d^Dx\psi^\dagger(x)\langle x|n\rangle \qquad (5.32)$$

You can see by now, that so far as transformation laws are concerned, ψ_n and $\psi(x)$ transforms like "bra" vectors, whilst their conjugates transform like "kets".

By moving to a real-space representation, we have traded in a discrete basis, for a continuous basis. The corresponding "unit" operator appearing in the commutation algebra now becomes a delta-function.

$$\begin{aligned}[][\psi(x),\psi^\dagger(y)]_\pm &= \sum_{n,m}\langle x|n\rangle\langle m|y\rangle\overbrace{[\psi_n,\ \psi^\dagger{}_m]_\pm}^{\delta_{nm}}\\ &= \sum_n\langle x|n\rangle\langle n|y\rangle = \langle x|y\rangle\\ &= \delta^3(x-y) \qquad (5.33)\end{aligned}$$

where we have assumed a three-dimensional system.

Another basis of importance, is the basis provided by the one-particle energy eigenstates. In this basis $\langle l|H|m\rangle = E_l\delta_{lm}$, so the Hamiltonian becomes diagonal

$$H = \sum_l E_l\psi^\dagger{}_l\psi_l = \sum E_l\hat{n}_l \qquad (5.34)$$

The Hamiltonian of the non-interacting many-body system thus divides up into a set of individual components, each one describing the energy associated with the occupancy of a given one-particle eigenstate. The eigenstates of the many-body Hamiltonian are thus labelled by the occupancy of the lth one-particle state. Of course, in a real-space basis the Hamiltonian becomes more complicated. Formally, if we transform this back to the real-space basis, we find that

$$H = \int d^Dxd^Dx'\psi^\dagger(x)\langle x|H|x'\rangle\psi(x') \qquad (5.35)$$

For free particles in space, the one-particle Hamiltonian is

$$\langle x|H|x'\rangle = \Big[-\frac{\hbar^2}{2m}\nabla^2 + U(x)\Big]\delta^D(x-x') \qquad (5.36)$$

so that the Hamiltonian becomes

$$H = \int d^Dx\psi^\dagger(x)\Big[-\frac{\hbar^2}{2m}\nabla^2 + U(x)\Big]\psi(x) \qquad (5.37)$$

which despite its formidable appearance, is just a a transformed version of the diagonalized Hamiltonian (5.34).

5.4 Fields as particle creation and annihilation operators.

By analogy with collective fields, we now interpret the quantity $\hat{n}_l = \psi^\dagger{}_l\psi_l$ as the number number operator, counting the number of particles in the one-particle state l. The total particle number operator is then

$$N = \sum_l\psi^\dagger{}_l\psi_l \qquad (5.38)$$

Using relation (5.21), it is easy to verify that for both fermions and bosons,

$$[\hat{N},\psi_l] = [\hat{n}_l,\psi_l] = -\psi_l, \qquad [\hat{N},\psi^\dagger{}_l] = [\hat{n}_l,\psi^\dagger{}_l] = \psi^\dagger{}_l. \qquad (5.39)$$

In other words, $\hat{N}\psi^\dagger{}_l = \psi^\dagger{}_l(\hat{N}+1)$ so that $\psi^\dagger{}_l$ adds a particle to state l. Similarly, since $\hat{N}\psi_l = \psi_l(\hat{N}-1)$, ψ_l *destroys* a particle from state l.

There is however a vital and essential difference between bosons and fermions. For bosons, the number of particles n_l in the *lth* state is unbounded, but for fermions, since

$$\psi^{\dagger 2}_l = \frac{1}{2}\{\psi^\dagger{}_l,\ \psi^\dagger{}_l\} = 0 \qquad (5.40)$$

the amplitude to add more than one particle to a given state is always zero. We can never add more than one particle to a given state: in otherwords, the *exclusion principle* follows from the algebra! The occupation number bases for bosons and fermions are given by

$$\boxed{\begin{aligned}|n_1,n_2\dots n_l\dots\rangle &= \textstyle\prod_l\frac{(\psi^\dagger{}_l)^{n_l}}{\sqrt{n_l!}}|0\rangle, && (n_r = 0,1,2\dots) \quad \textbf{bosons}\\ |n_1,n_2\dots n_r\rangle &= (\psi^\dagger{}_r)^{n_r}\dots(\psi^\dagger{}_1)^{n_1}|0\rangle, && (n_r = 0,1) \quad \textbf{fermions}\end{aligned}} \qquad (5.41)$$

A specific example for fermions, is

$$|\overset{1\,2\,3\,4\,5\,6}{101101}\rangle = \psi^\dagger{}_6\psi^\dagger{}_4\psi^\dagger{}_3\psi^\dagger{}_1|0\rangle \qquad (5.42)$$

which contains particles in the 1st, 3rd, 4th and 6th one-particle states. Notice how the *order* in which we add the particles affects the sign of the wavefunction, so exchanging particles 4 and 6 gives

$$\psi^\dagger{}_4\psi^\dagger{}_6\psi^\dagger{}_3\psi^\dagger{}_1|0\rangle = -\psi^\dagger{}_6\psi^\dagger{}_4\psi^\dagger{}_3\psi^\dagger{}_1|0\rangle = -|\overset{1\,2\,3\,4\,5\,6}{101101}\rangle \qquad (5.43)$$

By contrast, a bosonic state is symmetric, for example

$$|\overset{1\,2\,3\,4\,5\,6}{805241}\rangle = \frac{1}{\sqrt{4!2!5!8!}}\psi^\dagger{}_6(\psi^\dagger{}_5)^4(\psi^\dagger{}_4)^2(\psi^\dagger{}_3)^5(\psi^\dagger{}_1)^8|0\rangle \qquad (5.44)$$

To get further insight, let us transform the number operator to a real-space basis by writing

$$\hat{N} = \int d^Dxd^Dy\sum_l\psi^\dagger(x)\overbrace{\langle x|l\rangle\langle l|y\rangle}^{\delta^D(x-y)}\psi(y) \qquad (5.45)$$

so that

$$\hat{N} = \int d^Dx\psi^\dagger(x)\psi(x) \qquad (5.46)$$

From this expression, we are immediately led to identify

$$\rho(x) = \psi^\dagger(x)\psi(x) \tag{5.47}$$

as the density operator. Furthermore, since

$$[\rho(y), \psi(x)] = \mp[\psi^\dagger(y), \psi(x)] \pm \psi(y) = -\delta^3(x-y)\psi(y). \tag{5.48}$$

we can we can identify $\psi(x)$ as the operator which annihilates a particle at x.

Example Using the result (5.48) that if

$$\hat{N}_{\mathcal{R}} = \int_{\vec{y}\in\mathcal{R}} d^3y\rho(\vec{y}) \tag{5.49}$$

measures the number of particles in some region $\mathcal{R}$, that

$$[\hat{N}_{\mathcal{R}}, \psi(x)] = \left\{ \begin{array}{rl} -\psi(x), & (x \in \mathcal{R}) \\ 0 & (x \notin \mathcal{R}) \end{array} \right. \tag{5.50}$$

By localizing region $\mathcal{R}$ around x, use this to prove that $\psi(x)$ annihilates a particle at position x.

Example Suppose $b_{\vec{q}}$ destroys a boson in a cubic box of side length L,where $\vec{q} = \frac{2\pi}{L}(i,j,k)$ is the momentum of the boson. Express the field operator in real space, and show they satisfy canonical commutation relations. Write down the Hamiltonian in both bases.

Solution The field operators in momentum space satisfy $[b_{\vec{q}}, b^\dagger{}_{\vec{q}'}] = \delta_{\vec{q}\vec{q}'}$. We may expand the field operator in real space as follows

$$\psi(x) = \sum_{\mathbf{q}} \langle\vec{x}|\vec{q}\rangle b_{\vec{q}} \tag{5.51}$$

Now

$$\langle\vec{x}|\vec{q}\rangle = \frac{1}{L^{3/2}}e^{i\vec{q}\cdot\vec{x}} \tag{5.52}$$

is the one-particle wavefunction of a boson with momentum $\vec{q}$. Calculating the commutator between the fields in real space, we obtain

$$\begin{aligned} [\psi(\vec{x}), \psi^\dagger(\vec{y})] &= \sum_{\vec{q},\vec{q}'} \langle\vec{x}|\vec{q}\rangle\langle\vec{q}'|\vec{y}\rangle \overbrace{[b_{\vec{q}}, b^\dagger{}_{\vec{q}'}]}^{\delta_{\vec{q}\vec{q}'}} = \sum_{\vec{q}} \langle\vec{x}|\vec{q}\rangle\langle\vec{q}|\vec{y}\rangle \\ &= \frac{1}{L^3}\sum_{\mathbf{q}} e^{i\vec{q}\cdot(\vec{x}-\vec{y})} = \delta^{(3)}(\vec{x}-\vec{y}). \end{aligned} \tag{5.53}$$

The last two steps could have been carried out by noting that $\sum_q |q\rangle\langle q| = 1$, so that $[\psi(\vec{x}), \psi^\dagger(\vec{y})] = \langle x|y\rangle = \delta^3(x-y)$.

The Hamiltonian for the bosons in a box is

$$H = -\frac{\hbar^2}{2m}\int d^3x\psi^\dagger(x)\nabla^2\psi(x) \tag{5.54}$$

We now Fourier transform this, writing

$$\begin{aligned} \psi^\dagger(x) &= \frac{1}{L^{3/2}}\sum_{\mathbf{q}} e^{-i\vec{q}\cdot\vec{x}} b^\dagger{}_{\mathbf{q}} \\ \nabla^2\psi(x) &= -\frac{1}{L^{3/2}}\sum_{\mathbf{q}} q^2 e^{i\vec{q}\cdot\vec{x}} b_{\mathbf{q}} \end{aligned} \tag{5.55}$$

Substituting into the Hamiltonian, we obtain

$$H = \frac{1}{L^3}\sum_{\mathbf{q},\ \mathbf{q}'} \epsilon_{\mathbf{q}} b^\dagger{}_{\mathbf{q}'} b_{\mathbf{q}} \int d^3x\, \overbrace{e^{i\mathbf{q}-\mathbf{q}'\cdot\mathbf{x}}}^{L^3\delta_{q-q'}} = \sum_{\mathbf{q}} \epsilon_{\mathbf{q}} b^\dagger{}_{\mathbf{q}} b_{\mathbf{q}}, \tag{5.56}$$

where

$$\epsilon_{\mathbf{q}} = \left(\frac{\hbar^2 q^2}{2m}\right). \tag{5.57}$$

is the one-particle energy.

5.5 The vacuum and the many body wavefunction

We are now in a position to build up the many-body wavefunction. Once again, of fundamental importance here, is the notion of the vacuum, the unique state $|0\rangle$ which is annihilated by all field operators. If we work in the position basis, we can add a particle at site x to make the one-particle state

$$|x\rangle = \psi^\dagger(x)|0\rangle, \tag{5.58}$$

Notice that the overlap between two one-particle states is

$$\langle x|x'\rangle = \langle 0|\psi(x)\psi^\dagger(x')|0\rangle. \tag{5.59}$$

By using the (anti) commutation algebra to move the creation operator in the above expression to the right-hand side, where it annihilates the vacuum, we obtain

$$\langle 0|\psi(x)\psi^\dagger(x')|0\rangle = \langle 0|\overbrace{[\psi(x),\ \psi^\dagger(x')]_\pm}^{\delta^{(3)}(x-x')}|0\rangle = \delta^{(3)}(x-x'). \tag{5.60}$$

We can equally well add many particles, forming the N-particle state:

$$|x_1, x_2 \dots x_N\rangle = \psi^\dagger(x_N)\dots\psi^\dagger(x_2)\psi^\dagger(x_1)|0\rangle \tag{5.61}$$

Now the corresponding "bra" state is given by

$$\langle x_1, x_2 \dots x_N| = \langle 0|\psi(x_1)\psi(x_2)\dots\psi(x_N) \tag{5.62}$$

The wavefunction of the N-particle state Ψ is the overlap with this state

$$\boxed{\Psi(x_1, x_2, \dots x_N) = \langle x_1, x_2 \dots x_N|\Psi\rangle = \langle 0|\psi(x_1)\psi(x_2)\dots\psi(x_N)|\Psi\rangle} \tag{5.63}$$

The commutation/ anticommutation algebra guarantees that the symmetry of this wavefunction under particle exchange is positive for bosons, and negative for fermions, so that if we permute the particles, $(12\dots N) \to (P_1P_2\dots P_N)$

$$\langle 0|\psi(x_{P_1})\psi(x_{P_2})\dots\psi(x_{P_N})|\Psi\rangle = (\mp 1)^P\langle 0|\psi^\dagger(x_1)\psi(x_2)\dots\psi(x_N)|\Psi\rangle \tag{5.64}$$

where P is the number of pairwise permutations involved in making the permutation. Notice that for fermions, this guarantees that the wavefunction vanishes if any two co-ordinates are the same.

Example Two spinless fermions are added to a cubic box with sides of length L, in momentum states k_1 and k_2, forming the state

$$|\Psi\rangle = |\mathbf{k}_1, \mathbf{k}_2\rangle = c^\dagger{}_{\mathbf{k}_2}c^\dagger{}_{\mathbf{k}_1}|0\rangle \tag{5.65}$$

Calculate the two-particle wavefunction

$$\Psi(x_1, x_2) = \langle x_1, x_2|\Psi\rangle \tag{5.66}$$

Solution Written out explicitly, the wavefunction is

$$\Psi(x_1, x_2) = \langle 0|\psi(x_1)\psi(x_2)c^\dagger{}_{\mathbf{k}_2}c^\dagger{}_{\mathbf{k}_1}|0\rangle \tag{5.67}$$

To evaluate this quantity, we commute the two destruction operators to the right, until they annihilate the vacuum. Each time a destruction operator passes a creation operator, we generate a "contraction" term

$$\{\psi(x), c^\dagger{}_{\mathbf{k}}\} = \int d^3y\, \overbrace{\{\psi(x), \psi^\dagger(y)\}}^{\delta^3(x-y)}\langle y|\mathbf{k}\rangle = \langle x|\mathbf{k}\rangle = L^{-3/2}e^{i\mathbf{k}\cdot\mathbf{x}} \tag{5.68}$$

Carrying out this procedure, we generate a sum of pairwise contractions, as follows:

$$\begin{aligned} \langle 0|\psi(x_1)\psi(x_2)c^\dagger{}_{\mathbf{k}_2}c^\dagger{}_{\mathbf{k}_1}|0\rangle &= \langle x_1|\mathbf{k}_1\rangle\langle x_2|\mathbf{k}_2\rangle - \langle x_1|\mathbf{k}_2\rangle\langle x_2|\mathbf{k}_1\rangle \\ &= \frac{1}{L^3}\left[e^{i(\mathbf{k}_1\cdot\mathbf{x}_1+\mathbf{k}_2\cdot\mathbf{x}_2)} - e^{i(\mathbf{k}_1\cdot\mathbf{x}_2+\mathbf{k}_2\cdot\mathbf{x}_1)}\right] \end{aligned}$$

5.6 Interactions

Second-quantization is easily extended to incorporate interactions. Classically, the interaction potential energy between particles is given by

$$V = \frac{1}{2}\int d^3xV(x-x')\rho(x)\rho(x') \tag{5.69}$$

so we might expect that the corresponding second-quantized expression is

$$\frac{1}{2}\int d^3xV(x-x')\hat{\rho}(x)\hat{\rho}(x') \tag{5.70}$$

This is wrong, because we have not been careful about the ordering of operators. Were we to use (5.70), then a one-particle state would interact with itself! We require that the action of the potential on the vacuum, or a one-particle state, gives zero

$$\hat{V}|0\rangle = \hat{V}|x\rangle = 0 \tag{5.71}$$

To guarantee this, we need to be careful that we "normal-order" the field operators, by permuting them so that all destruction operators are on the right-hand-side. All additional terms that are generated by permuting the operators are removed, but the sign associated with the permutation process is preserved. We denote the normal ordering process by two semi-colons. Thus

$$\begin{aligned} :\rho(x)\rho(y): &= :\psi^\dagger(x)\psi(x)\psi^\dagger(y)\psi(y): \\ &= \mp :\psi^\dagger(x)\psi^\dagger(y)\psi^\dagger(x)\psi(y) :=: \psi^\dagger(y)\psi^\dagger(x)\psi(x)\psi(y): \end{aligned} \tag{5.72}$$

and the correct expression for the interaction potential is then

$$\begin{aligned} V &= \frac{1}{2}\int d^3xV(x-x') :\hat{\rho}(x)\hat{\rho}(x'): \\ &= \sum_{\sigma,\sigma'}\frac{1}{2}\int d^3xV(x-x')\psi_\sigma{}^\dagger(y)\psi_{\sigma'}{}^\dagger(x)\psi_{\sigma'}(x)\psi_\sigma(y) \end{aligned} \tag{5.73}$$

where we have written a more general expression for fields with spin.

Example. Show that the action of the operator V on the many body state $|x_1, \dots x_N\rangle$ is given by

$$\hat{V}|x_1, x_2, \dots x_N\rangle = \sum_{i<j} V(x_i - x_j)|x_1, x_2, \dots x_N\rangle \tag{5.74}$$

Solution: To prove this, we need the intermediate result

$$[V, \psi^\dagger(x)] = \int d^3yV(x-y)\psi^\dagger(x)\rho(y). \tag{5.75}$$

We now calulate

$$V|x_1, \dots x_N\rangle = V\psi^\dagger(x_N)\dots\psi^\dagger(x_1)|0\rangle \tag{5.76}$$

by commuting V successively to the right until it annihilates with the vacuum. At each stage, we generate a "remainder term". When we commute it between the "jth" and the "j-1st" creation operator, we obtain

$$\psi^\dagger(x_N)\dots V\psi^\dagger(x_j)\dots\psi^\dagger(x_1)|0\rangle = \psi^\dagger(x_N)\dots\psi^\dagger(x_j)V\dots\psi^\dagger(x_1)|0\rangle + \mathcal{R}_j$$

where the remainder is

$$\mathcal{R}_j = \int d^3y V(y-x_j)\psi^\dagger(x_N)\dots\psi^\dagger(x_j)\rho(y)\dots\psi^\dagger(x_1)|0\rangle \tag{5.77}$$

By commuting the density operator to the right until it annihilates the vacuum, the remainder term can be written

$$\mathcal{R}_j = \sum_{i<j} V(x_i-x_j)\psi^\dagger(x_N)\dots\psi^\dagger(x_1)|0\rangle. \qquad \text{(no sum on j)} \tag{5.78}$$

When we commute V all the way from the right until it annihilates the vacuum, our final answer is the sum of all these remainder terms,

$$\begin{aligned} V\psi^\dagger(x_N)\dots\psi^\dagger(x_1)|0\rangle &= \sum_{j=2,N}\mathcal{R}_j \\ &= \sum_{i<j} V(x_i-x_j)|x_1,x_2\dots x_N\rangle. \end{aligned} \tag{5.79}$$

In otherwords, the state $|x_1\dots x_N\rangle$ is an eigenstate of the interaction operator, with eigenvalue given by the classical interaction potential energy.

To get another insight into the interaction, we shall now rewrite it in the momentum basis. This is very useful in translationally invariant systems, where momentum is conserved in collisions. Let us imagine we are treating fermions, with spin. The transformation to a momentum basis is then Writing

$$\begin{aligned} \psi_\sigma(x) &= \text{“}\sum_{\mathbf{k}}\text{”}\langle\mathbf{x}|\mathbf{k}\rangle c_{\mathbf{k}\sigma} = \int_{\mathbf{k}} c_{\mathbf{k}\sigma}e^{i(\mathbf{k}\cdot\mathbf{x})} \\ \psi_\sigma(x) &= \text{“}\sum_{\mathbf{k}}\text{”}c^\dagger{}_{\mathbf{k}\sigma}\langle\mathbf{k}|\mathbf{x}\rangle = \int_{\mathbf{k}} c^\dagger{}_{\mathbf{k}\sigma}e^{-i(\mathbf{k}\cdot\mathbf{x})} \end{aligned} \tag{5.80}$$

where $\{c_{\mathbf{k}\sigma}, c^\dagger{}_{\mathbf{k}'\sigma'}\} = (2\pi)^3\delta^3(\mathbf{k}-\mathbf{k}')\delta_{\sigma\sigma'}$ are canonical fermion operators and we have used the short-hand notation

$$\int_{\mathbf{k}} = \int\frac{d^3k}{(2\pi)^3}. \tag{5.81}$$

We shall also Fourier transform the interaction

$$V(x-x') = \int_{\mathbf{q}} V(\mathbf{q})e^{i\mathbf{q}\cdot(\mathbf{x}-\mathbf{x}')}. \tag{5.82}$$

When we substitute these expressions into the interaction, we need to regroup the Fourier terms so that the momentum integrals are on the outside, and the spatial integrals are on the inside. Doing this, we obtain

$$\hat{V} = \frac{1}{2}\sum_{\sigma\sigma'}\int_{\mathbf{k}_{1,2,3,4}} V(\mathbf{q})\times c^\dagger{}_{\mathbf{k}_4\sigma}c^\dagger{}_{\mathbf{k}_3\sigma'}c_{\mathbf{k}_2\sigma'}c_{\mathbf{k}_1\sigma}\times\text{spatial integrals} \tag{5.83}$$

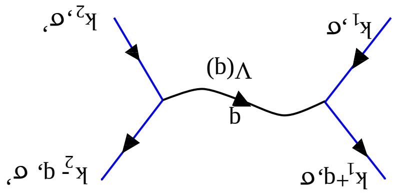


Figure 5.1: Scattering of two particles, showing transfer of momentum. **q**.

where the spatial integrals take the form

$$\int d^3xd^3x'e^{i(\mathbf{k}_1-\mathbf{k}_4+\mathbf{q})\cdot\mathbf{x}}e^{i(\mathbf{k}_2-\mathbf{k}_3-\mathbf{q})\cdot\mathbf{x}'} = (2\pi)^6\delta^{(3)}(\mathbf{k}_4-\mathbf{k}_1-\mathbf{q})\delta^{(3)}(\mathbf{k}_3-\mathbf{k}_2+\mathbf{q}) \tag{5.84}$$

which impose momentum conservation at each scattering event. Using the spatial integrals to eliminate the integrals over $\mathbf{k}_3$ and $\mathbf{k}_4$, the final result is

$$\hat{V} = \frac{1}{2}\sum_{\sigma\sigma'}\int_{\mathbf{k}_{1,2},\mathbf{q}}\frac{d^3q}{(2\pi)^3}V(\mathbf{q})c^\dagger{}_{\mathbf{k}_1+\mathbf{q}\sigma}c^\dagger{}_{\mathbf{k}_2-\mathbf{q}\sigma'}c_{\mathbf{k}_2\sigma'}c_{\mathbf{k}_1\sigma} \tag{5.85}$$

In other words, when the particles scatter at positions x and x', momentum is conserved. Particle 1 comes in with momentum $\mathbf{k}_1$, and transfers momentum $\mathbf{q}$ to particle 2. Particle 2 comes in with momentum $\mathbf{k}_2$, and thereby gains momentum $\mathbf{q}$:

$$\begin{array}{lccc} \text{particle 1} & \mathbf{k}_1 & \longrightarrow & \mathbf{k}_1+\mathbf{q} \\ \text{particle 2} & \mathbf{k}_2 & \longrightarrow & \mathbf{k}_2-\mathbf{q} \end{array} \tag{5.86}$$

as illustrated in Fig. 5.1. The matrix element associated with this scattering process is merely the Fourier transform of the potential $V(\mathbf{q})$.

Example: Particles interact via a delta-function interaction $V(x) = Ua^3\delta^{(3)}(x)$. Write down the second-quantized interaction in a momentum space representation.

Solution: The Fourier transform of the interaction is

$$V(q) = \int d^3xUa^3\delta(x)e^{-i\mathbf{q}\cdot\mathbf{x}} = Ua^3 \tag{5.87}$$

so the interaction in momentum space is

$$\hat{V} = \sum_{\sigma\sigma'}\frac{Ua^3}{2}\int_{\mathbf{k}_{1,2},\mathbf{q}}\frac{d^3q}{(2\pi)^3}c^\dagger{}_{\mathbf{k}_1-\mathbf{q}\sigma}c^\dagger{}_{\mathbf{k}_2+\mathbf{q}\sigma'}c_{\mathbf{k}_2\sigma'}c_{\mathbf{k}_1\sigma} \tag{5.88}$$

Example: A set of fermions interact via a screened Coulomb (Yukawa) potential

$$V(r) = \frac{Ae^{-\lambda r}}{r} \tag{5.89}$$

Write down the interaction in momentum space.

Solution: The interaction in momentum space is given by

$$\hat{V} = \frac{1}{2}\sum_{\sigma\sigma'}\int_{\mathbf{k}_{1,2},\mathbf{q}}\frac{d^3q}{(2\pi)^3}V(\mathbf{q})c^\dagger{}_{\mathbf{k}_1+\mathbf{q}\sigma}c^\dagger{}_{\mathbf{k}_2-\mathbf{q}\sigma'}c_{\mathbf{k}_2\sigma'}c_{\mathbf{k}_1\sigma} \tag{5.90}$$

where

$$V(\mathbf{q}) = \int d^3x\frac{Ae^{-\lambda r}}{r}e^{-i\mathbf{q}\cdot\mathbf{x}} \tag{5.91}$$

To carry out this integral, we use Polar co-ordinates with the z-axis aligned along the direction $\hat{\mathbf{q}}$. Writing $\mathbf{q}\cdot\mathbf{x} = qr\cos\theta$, then $d^3x = r^2d\phi d\cos\theta \to 2\pi r^2d\cos\theta$, so that

$$V(\mathbf{q}) = \int 4\pi r^2drV(r)\underbrace{\frac{1}{2}\int_{-1}^{1}d\cos\theta\, e^{-iqr\cos\theta}}_{\langle e^{-i\mathbf{q}\cdot\mathbf{x}}\rangle = \frac{\sin qr}{qr}} \tag{5.92}$$

so that for an arbitrary spherically symmetric potential

$$V(q) = \int_0^\infty 4\pi r^2drV(r)\left(\frac{\sin qr}{qr}\right) \tag{5.93}$$

In this case,

$$V(q) = \frac{4\pi A}{q}\int_0^\infty dre^{-\lambda r}\sin(qr) = \frac{4\pi A}{q^2+\lambda^2}, \tag{5.94}$$

Notice that the Coulomb interaction,

$$V(r) = \frac{e^2}{4\pi\epsilon_0 r}, \tag{5.95}$$

is the infinite range limit of the Yukawa potential, with $\lambda = 0$, $A = e^2/4\pi\epsilon_o$, so that for the Coulomb interaction,

$$V(q) = \frac{e^2}{q^2\epsilon_o}. \tag{5.96}$$

Example: If one transforms to a new one particle basis, writing $\psi(x) = \sum_s \Phi_s(x)c_s$, show that the interaction becomes

$$\hat{V} = \frac{1}{2}\sum_{lmnp}c^\dagger{}_lc^\dagger{}_mc_nc_p\langle lm|V|pn\rangle \tag{5.97}$$

where

$$\langle lm|V|pn\rangle = \int_{x,x'}\Phi^*_l(x)\Phi_p(x)\Phi^*_m(x')\Phi^*_n(x')V(x-x') \tag{5.98}$$

is the matrix element of the interaction between the two particle states $|lm\rangle$ and $|pn\rangle$.

Table. 5.1. First and Second Quantization .

	First Quantization	Second Quantization
Wavefn ⟶ Field Operator	$\psi(x) = \langle x\|\psi\rangle$	$\hat{\psi}(x)$
Commutator	$[x,p] = i\hbar$	$[\psi(x),\psi(x')]_\mp = \delta^D(x-x'$
Density	$\rho(x) = \|\psi(x)\|^2$	$\hat{\rho}(x) = \hat{\psi}^\dagger(x)\hat{\psi}(x)$
Arbitrary Basis	$\psi_\lambda = \langle\lambda\|\psi\rangle$	$\hat{\psi}_\lambda$
Change of Basis	$\langle\tilde{s}\|\psi\rangle = \sum_\lambda\langle\tilde{s}\|\lambda\rangle\langle\lambda\|\psi\rangle$	$\hat{a}_s = \sum_\lambda\langle\tilde{s}\|\lambda\rangle\hat{\psi}_\lambda$
Orthogonality	$\langle\lambda\|\lambda'\rangle = \delta_{\lambda\lambda'}$	$[\psi_\lambda,\psi^\dagger{}_{\lambda'}]_\mp = \delta_{\lambda\lambda'}$
One ptcle Energy	$\frac{p^2}{2m}+U$	$\psi^\dagger\left(-\frac{\hbar^2}{2m}+U(x)\right)\psi$
Interaction	$\sum_{i<j}V(x_i-x_j)$	$\hat{V} = \frac{1}{2}\int_{x,x'}V(x-x'):\hat{\rho}(x)\hat{\rho}($ $= \frac{1}{2}\sum V(\mathbf{q})c^\dagger{}_{\mathbf{k}+\mathbf{q}}c^\dagger{}_{\mathbf{k}'-\mathbf{q}}c_{\mathbf{k}'}c$
Many Body Wavefunction	$\Psi(x_1,x_2\dots x_N)$	$\langle 0\|\hat{\psi}(x_1)\dots\hat{\psi}(x_N)\|0\rangle$
Schrodinger Eqn	$\left(\sum\mathcal{H}_i+\sum_{i<j}V_{ij}\right)\Psi = i\hbar\dot{\Psi}$	$[\mathcal{H}^{(0)}+\int_{x'}\rho(x')V(x'-x)]\psi(x) =$

Table 5.1 summarizes the main points of second-quantization.

5.7 Identical Conserved Particles in Thermal Equilibrium

5.7.1 Generalities

By quantizing the particle field, we have been led to a version of quantum mechanics with a vastly expanded Hilbert space which includes the vacuum and all possible states with an arbitrary number of particles. An exactly parallel development occurs in statistical thermodynamics, in making the passage from a canonical, to a grand canonical ensemble,

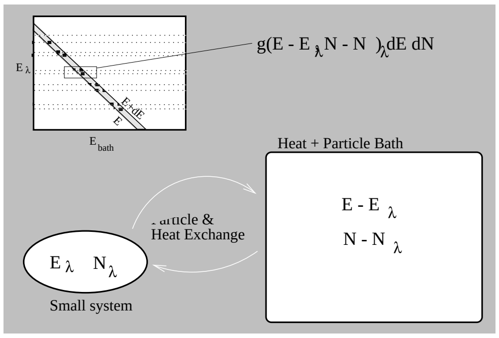


Figure 5.2: Illustrating equilibrium between a small system and a large heat bath. Inset illustrates how the number of states with energy E_λ, particle number N_λ is proportional to the density of states in the big system.

where systems are considered to be in equilibrium with a heat and particle bath. Not surprisingly then, second quantization provides a beautiful way of treating a grand canonical ensemble of identical particles.

When we come to treat conserved particles in thermal equilibrium, we have to take into the account the conservation of two independent quantities

- Energy. E
- Particle number. N

When we consider an ensemble of small systems, in equilibrium with a heat bath, we must now consider the possibility of an exchange of both energy, and particles with the heat bath, as shown in Fig. 5.2. Suppose our system of interest is in equilibrium with a huge heat and particle bath. In the huge heat and particle bath, the energy levels are so close together, that they behave almost as a continuum. The density of states per unit energy and particle number is taken to be $g(E,N)$, where E is the energy and N the number of particles in the bath. Suppose that the total number of particles and energy are E and N respectively.

When the system is in a quantum state $|\lambda\rangle$ with energy E_λ, particle number N_λ, the large system has energy $E - E_\lambda$, particle number $N - N_\lambda$.

The probability that the small system is in state $|\lambda\rangle$ is then given by

$$p(E_\lambda, N_\lambda) \propto g(E - E_\lambda, N - N_\lambda) = e^{\ln g(E-E_\lambda, N-N_\lambda)} \tag{5.99}$$

In the heat bath, we assum that the logarithm of the density of states is a smoothly varying function of energy and particle number, so that we may expand it around E and N, writing

$$\ln g(E - E_\lambda, N - N_\lambda) = \ln g(E, N) - E_\lambda \frac{\partial \ln g}{\partial E} - N_\lambda \frac{\partial \ln g}{\partial N} + \dots \tag{5.100}$$

We define the two quantities

$$\frac{\partial \ln g}{\partial E} = \beta = \frac{1}{k_B T}, \qquad \frac{\partial \ln g}{\partial N} = -\frac{\mu}{k_B T}. \tag{5.101}$$

These are the two Lagrange multipliers associated with the conservation of energy and particle number. It is only later, after calculating some physical quantities, that one can physically identify T as the temperature, and μ as the chemical potential. Once we have made this expansion, it follows that the probability to be in state $|\lambda\rangle$ is

$$p_\lambda = \frac{1}{Z} e^{-\beta(E_\lambda - \mu N_\lambda)} \tag{5.102}$$

where now the normalizing partition function can be written

$$\begin{aligned} Z &= \sum_\lambda e^{-\beta(E_\lambda - \mu N_\lambda)} \\ &= \sum_\lambda \langle\lambda| e^{-\beta(\hat{H} - \mu\hat{N})} |\lambda\rangle = \mathrm{Tr}[e^{-\beta(\hat{H} - \mu\hat{N})}] \end{aligned} \tag{5.103}$$

Finally, we can go to a position independent basis by noting that if A is a quantity that is diagonal in the state $|\lambda\rangle$, then the expectation value of A in the ensemble is

$$\langle A\rangle = \sum_\lambda p_\lambda \langle\lambda|\hat{A}|\lambda\rangle = \mathrm{Tr}[\hat{\rho}\hat{A}] \tag{5.104}$$

where we have elevated the probability distribution p_λ to an operator- the density matrix:

$$\boxed{\hat{\rho} = \sum_\lambda |\lambda\rangle p_\lambda \langle\lambda| = Z^{-1} e^{-\beta(\hat{H} - \mu\hat{N})}} \tag{5.105}$$

A central assumption of quantum statistical mechanics , is that (5.104) holds for all observable quantities represented by an operator $\hat{A}$, whether or not the quantity is diagonal in the basis of energy and particle number eigenstates.

5.7.2 Identification of the Free energy: Key Thermodynamic Properties

There are a number of key thermodynamic quantities of great interest: the energy E, the particle number N, the entropy S and the Free energy $F = E - ST - \mu N$. One of the key relations from elementary thermodynamics is that

$$dE = TdS - \mu dN - PdV \tag{5.106}$$

By putting $F = E - TS - \mu N$, $dF = dE - dTS - SdT - \mu dN - Nd\mu$, one can also derive

$$dF = -SdT - Nd\mu - PdV \tag{5.107}$$

a relationship of great importance.

The energy and particle number can be easily written in the language of second-quantization as

$$\begin{aligned} E &= \mathrm{Tr}[\hat{H}\hat{\rho}], \\ N &= \mathrm{Tr}[\hat{N}\hat{\rho}], \end{aligned} \tag{5.108}$$

but what about the entropy? From statistical mechanics, we know that the general expression for the entropy is given by

$$S = -k_B \sum_\lambda p_\lambda \ln p_\lambda \tag{5.109}$$

Now since the diagonal elements of the density matrix are p_λ, we can rewrite this expression as

$$S = -k_B \mathrm{Tr}[\hat{\rho}\ln\hat{\rho}] \tag{5.110}$$

If we substitute $\ln\hat{\rho} = -\beta(\hat{H} - \mu\hat{N}) - \ln Z$ into this expression, we obtain

$$\begin{aligned} S &= \frac{1}{T}\mathrm{Tr}\hat{\rho}(H - \mu N) - k_B T \ln Z \\ &= \frac{1}{T}(E - \mu N) + k_B \ln Z \end{aligned} \tag{5.111}$$

i.e $-k_B T\ln Z = E - ST - \mu N$, from which we identify

$$F = -k_B T \ln Z \tag{5.112}$$

as the Free energy. Summarizing these key relationships all together, we have

Thermodynamic Relations

$$\boxed{\begin{array}{rcll} F &=& -k_B T\ln \mathrm{Z}, & \textbf{Free energy} \\ Z &=& \mathrm{Tr}[e^{-\beta(\hat{H}-\mu\hat{N})}], & \textbf{Partition function} \\ \hat{\rho} &=& \dfrac{e^{-\beta(\hat{H}-\mu\hat{N})}}{Z}, & \textbf{Density Matrix} \\ N &=& \mathrm{Tr}[\hat{N}\hat{\rho}] = -\frac{\partial F}{\partial \mu} & \text{Particle number} \\ S &=& -k_B \mathrm{Tr}[\hat{\rho}\ln\hat{\rho}] = -\frac{\partial F}{\partial T} & \text{Entropy} \\ P &=& -\frac{\partial F}{\partial V}, & \text{Pressure} \\ E - \mu N &=& \mathrm{Tr}[(\hat{H} - \mu\hat{N})\hat{\rho}], = -\frac{\partial Z}{\partial \beta} & \text{Energy} \end{array}} \tag{5.113}$$

Notice how, in this way, all the key thermodynamic properties can be written as appropriate derivatives of Free energy.

Example (i) Enumerate the energy eigenstates of a single fermion Hamiltonian.

$$H = \epsilon c^\dagger c \tag{5.114}$$

where $\{c, c^\dagger\} = 1$, $\{c,\ c\} = \{c^\dagger,\ c^\dagger\} = 0$. (ii) Calculate the number of fermions at temperature T.

Solution (i) The states of this problem are the vacuum state and the one-particle state

$$\begin{array}{lrcl} |0\rangle & E &=& 0, \\ |1\rangle = c^\dagger|0\rangle, & E &=& \epsilon. \end{array} \tag{5.115}$$

(ii) The number of fermions at temperature T is given by

$$\langle\hat{n}\rangle = \mathrm{Tr}[\hat{\rho}\hat{n}] \tag{5.116}$$

where $\hat{n} = c^\dagger c$,

$$\rho = e^{-\beta(\hat{H}-\mu\hat{N})}/Z \tag{5.117}$$

is the density matrix, and where

$$Z = \mathrm{Tr}[e^{-\beta(H-\mu N)}] \tag{5.118}$$

is the "partition function". For this problem, we can write out the matrices explicitly.

$$e^{-\beta H} = \begin{bmatrix} 1 & 0 \\ 0 & e^{-\beta(\epsilon-\mu)} \end{bmatrix}, \qquad \hat{n} = \begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix} \tag{5.119}$$

so that

$$Z = 1 + e^{-\beta(\epsilon-\mu)} \tag{5.120}$$

and

$$\mathrm{Tr}[\hat{n}e^{-\beta H}] = e^{-\beta(\epsilon-\mu)} \tag{5.121}$$

The final result is thus

$$\langle \hat{n} \rangle = \frac{e^{-\beta(\epsilon-\mu)}}{1+e^{-\beta(\epsilon-\mu)}} = \frac{1}{e^{\beta(\epsilon-\mu)}+1} \tag{5.122}$$

which is the famous Fermi-Dirac function for the number of fermions in a state of energy ϵ, chemical potential μ.

Example: (i) Show that for a general system of conserved particles at chemical potential, the total particle number in thermal equilibrium can be written as

$$N = -\partial F/\partial \mu \tag{5.123}$$

where

$$\begin{aligned} F &= -k_BT\ln Z \\ Z &= \mathrm{Tr}[e^{-\beta(\hat{H}-\mu N)}]. \end{aligned} \tag{5.124}$$

(ii) Apply this to a single bosonic energy level, where

$$H - \mu N = (\epsilon - \mu)a^\dagger a \tag{5.125}$$

and $\hat{a}^\dagger$ creates either a Fermion, or a boson, to show that

$$\langle \hat{n} \rangle = \frac{1}{e^{\beta(\epsilon-\mu)}-1} \tag{5.126}$$

Why does μ have to be negative positive for bosons?

5.7.3 Independent Particles

In a system of independent particles with many energy levels, ϵ_λ each energy level can be regarded as an independent member of a microcanonical ensemble. Formally, this is because the Hamiltonian is a sum of independent Hamiltonians

$$H - \mu N = \sum_\lambda (\epsilon_\lambda - \mu)\hat{n}_\lambda \tag{5.127}$$

so that the partition function is then a product of the individual partition functions:

$$Z = \mathrm{Tr}[\prod_{\lambda\,\otimes} e^{-\beta(\epsilon_\lambda-\mu)\hat{n}_\lambda}] \tag{5.128}$$

and since the trace of an (exterior) product of matrices, is equal to the product of their individual traces, $(\mathrm{Tr}\prod_{\lambda\otimes} = \prod_\lambda \mathrm{Tr})$,

$$Z = \prod_\lambda \mathrm{Tr}[e^{-\beta(\epsilon_\lambda-\mu)\hat{n}_\lambda}] = \prod_\lambda Z_\lambda \tag{5.129}$$

Since

$$Z_\lambda = \begin{cases} 1+e^{-\beta(\epsilon_\lambda-\mu)} & \mathit{Fermions} \\ 1+e^{-\beta(\epsilon_\lambda-\mu)}+e^{-2\beta(\epsilon_\lambda-\mu)}+\ldots = (1-e^{-\beta(\epsilon_\lambda-\mu)})^{-1} & \mathit{Bosons} \end{cases} \tag{5.130}$$

The corresponding Free energy is given by

$$\boxed{F = \mp k_BT\sum_\lambda \ln[1 \pm e^{-\beta(\epsilon_\lambda-\mu)}], \qquad \left\{ \begin{array}{l} \mathit{fermions} \\ \mathit{bosons} \end{array} \right.} \tag{5.131}$$

The occupancy of the l th level is independent of all the other levels, and given by

$$\begin{aligned} \langle \hat{n}_l \rangle = \mathrm{Tr}[\hat{\rho}\hat{n}_l] &= \mathrm{Tr}[(\prod_\otimes \hat{\rho}_\lambda)\hat{n}_l] \\ &= \prod_{\lambda\neq l} \overbrace{\mathrm{Tr}[\rho_\lambda]}^{=1} \times \mathrm{Tr}[\rho_l\hat{n}_l] = \frac{1}{e^{\beta(\epsilon_l-\mu)}\pm 1} \end{aligned} \tag{5.132}$$

where (+) refers to Fermions and (−) to bosons.

In the next chapter, we shall examine the consequences of these relationships.

5.8 Exercises for chapter 5

1. In this question $c_i{}^\dagger$ and c_i are fermion creation and annihilation operators and the states are fermion states. Use the convention $|11111000\ldots\rangle = c_5{}^\dagger c_4{}^\dagger c_3{}^\dagger c_2{}^\dagger c_1{}^\dagger|\mathrm{vacuum}\rangle$.

   (i) Evaluate $c_3{}^\dagger c_6 c_4 c_6{}^\dagger c_3|111111000\ldots\rangle$.

   (ii) Write $|1101100100\ldots\rangle$ in terms of excitations about the "filled Fermi sea" $|1111100000\ldots\rangle$. Interpret your answer in terms of electron and hole excitations.

   (iii) Find $\langle\psi|\hat{N}|\psi\rangle$ where $|\psi\rangle = A|100\rangle + B|111000\rangle$, $\hat{N} = \sum_i c_i{}^\dagger c_i$.

2. (a) Consider two fermions, a_1 and a_2. Show that the Boguilubov transformation

$$\begin{aligned} c_1 &= ua_1 + va^\dagger{}_2 \\ c^\dagger{}_2 &= -va_1 + ua^\dagger{}_2 \end{aligned} \tag{5.133}$$

   where u and v are real, preserves the canonical anti-commutation relations if $u^2 + v^2 = 1$.

   (b) Use this result to show that the Hamiltonian

$$H = \epsilon(a^\dagger{}_1 a_1 - a_2 a_2{}^\dagger) + \Delta(a^\dagger{}_1 a^\dagger{}_2 + \mathrm{H.c.}) \tag{5.134}$$

   can be diagonalized in the form

$$H = \sqrt{\epsilon^2+\Delta^2}(c^\dagger{}_1 c_1 + c^\dagger{}_2 c_2 - 1) \tag{5.135}$$

   (c) What is the ground-state energy of this Hamiltonian?

---

3. Show that for a general system of conserved particles at chemical potential, the total particle number in thermal equilibrium can be written as

$$N = -\partial F/\partial \mu \tag{5.136}$$

   where

$$\begin{aligned} F &= -k_BT\ln Z \\ Z &= \mathrm{Tr}[e^{-\beta(\hat{H}-\mu N)}]. \end{aligned} \tag{5.137}$$

   (ii) Apply this to a single bosonic energy level, where

$$H - \mu N = (\epsilon - \mu)a^\dagger a \tag{5.138}$$

   and $\hat{a}^\dagger$ creates either a Fermion, or a boson, to show that

$$\begin{aligned} F &= \pm k_BT\ln[1 \mp e^{-\beta(\epsilon-\mu)}] \\ \langle \hat{n} \rangle &= \frac{1}{e^{\beta(\epsilon-\mu)}\mp 1} \end{aligned} \tag{5.139}$$

   where the upper sign refers to bosons, the lower, to fermions. Sketch the occupancy as a function of ϵ for the case of fermions and bosons. Why does μ have to be negative for bosons?

4. Consider a system of fermions or bosons, created by the field $\psi^\dagger(\vec{r})$ interacting under the potential

$$V(r) = \begin{cases} U, & (r < R), \\ 0, & (r > R), \end{cases} \tag{5.140}$$

   (i) Write the interaction in second quantized form.

   (ii) Switch to the momentum basis, where $\psi(\vec{r}) = \int \frac{d^3k}{(2\pi)^3} c_{\vec{k}} e^{i\vec{k}\cdot\vec{r}}$. Verify that $[c_{\vec{k}},\ c^\dagger{}_{\vec{k}'}]_\pm = (2\pi)^3\delta^{(3)}(\vec{k}-\vec{k}')$, and write the interaction in this new basis. Please sketch the form of the interaction in momentum space.

Chapter 6

Simple Examples of Second-quantization

In this section, we give three examples of the application of second quantization, mainly to non-interacting systems.

6.1 Jordan Wigner Transformation

A "non-interacting" gas of Fermions is still highly correlated: the exclusion principle introduces a "hard-core" interaction between fermions in the same quantum state. This feature is exploited in the Jordan -Wigner representation of spins. A classical spin is represented by a vector pointing in a specific direction. Such a representation is fine for quantum spins with extremely large spin S, but once the spin S becomes small, spins behave as very new kinds of object. Now their spin becomes a quantum variable, subject to its own zero-point motions. Furthermore, the spectrum of excitations becomes discrete or grainy.

Quantum spins are notoriously difficult objects to deal with in many-body physics, because they do not behave as canonical fermions or bosons. In one dimension however, it turns out that spins with $S = 1/2$ actually behave like fermions. We shall show this by writing the quantum spin-1/2 Heisenberg chain as an interacting one dimensional gas of fermions, and we shall actually solve the limiting case of the one-dimensional spin-1/2 x-y model.

Jordan and Wigner noticed that the down and up state of a single spin can be thought of as an empty or singly occupied fermion state, (Fig. 6.1.) enabling them to make the mapping

$$| \uparrow\rangle \equiv f^\dagger|0\rangle, \qquad | \downarrow\rangle \equiv |0\rangle. \tag{6.1}$$

.

An explicit representation of the spin raising and lowering operators is then

$$S^+ \quad = \quad f^\dagger = \begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix}$$

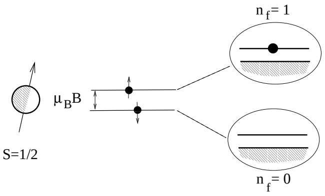


Figure 6.1: Showing how the "up" and "down" states of a spin-1/2 can be treated as a one particle state which is either full, or empty.

$$S^- \quad = \quad f \equiv \begin{bmatrix} 0 & 0 \\ 1 & 0 \end{bmatrix} \tag{6.2}$$

The z component of the spin operator can be written

$$S_z = \frac{1}{2}\Big[| \uparrow\rangle\langle\uparrow | - | \downarrow\rangle\langle\downarrow |\Big] \equiv f^\dagger f - \frac{1}{2} \tag{6.3}$$

We can also reconstruct the transverse spin operators,

$$\begin{aligned} S_x &= \frac{1}{2}(S^+ + S^-) = \frac{1}{2}(f^\dagger + f), \\ S_y &= \frac{1}{2i}(S^+ - S^-) = \frac{1}{2i}(f^\dagger - f), \end{aligned} \tag{6.4}$$

The explicit matrix representation of these operators makes it clear that they satisfy the same algebra

$$[S_a, S_b] = i\epsilon_{abc}S_c. \tag{6.5}$$

Curiously, due to a hidden supersymmetry, they also satisfy an anti-commuting algebra

$$\{S_a, S_b\} = \frac{1}{4}\{\sigma_a, \sigma_b\} = \frac{1}{2}\delta_{ab}, \tag{6.6}$$

and in this way, the Pauli spin operators provided Jordan and Wigner with an elementary model of a fermion.

Unfortunately the represeentation needs to be modified if there is more than one spin, for independent spin operators commute, but independent fermions anticommute! Jordan and Wigner discovered a way to fix up this difficulty in one dimension by attaching a phase

factor called a "string" to the fermions. For a chain of spins in one dimension, the Jordan Wigner representation of the spin operator at site j is defined as

$$S^+_j = f_j{}^\dagger e^{i\phi_j} \tag{6.7}$$

where the phase operator ϕ_j contains the sum over all fermion occupancies at sites to the left of j,

$$\phi_j = \pi\sum_{l<j} n_j \tag{6.8}$$

The complete transformation is then

$$\boxed{\left.\begin{aligned} S^z_j &= f^\dagger{}_j f_j - \tfrac{1}{2}, \\ S^+_j &= f^\dagger{}_j e^{i\pi\sum_{l<j} n_j}, \\ S^+_j &= f_j e^{i\pi\sum_{l<j} n_j} \end{aligned}\right\} \textbf{Jordan Wigner transformation}} \tag{6.9}$$

Notice how the sign infront of the phase factor does not matter. The important point in this representation, is that the operator $e^{i\pi n_j}$ anticommutes with the fermion operators at the same site:

$$\{e^{i\pi n_j}, f^{(\dagger)}_j\} = e^{i\pi n_j}f^{(\dagger)}_j + f^{(\dagger)}_j e^{i\pi n_j} = (-)[f^{(\dagger)}_j - f^{(\dagger)}_j] = 0 \tag{6.10}$$

so that by multiplying a fermion by the string operator, one changes it from a fermion, into a boson. We can verify that the transverse spin operators now satisfy the correct commutation algebra. Suppose $j < k$, then $e^{i\phi_j}$ commutes with both f_j and f_k. $e^{i\phi_k}$ commutes with f_k, but it contains $e^{i\pi n_j}$, which does not commute with f_j or $f^\dagger{}_j$. Thus we may write

$$\begin{aligned} [S^{(\pm)}_j, S^{(\pm)}_k] &= [f^{(\dagger)}_j e^{i\phi_j}, f^{(\dagger)}_k e^{i\phi_k}] \\ &= [f^{(\dagger)}_j, f^{(\dagger)}_k e^{i\pi n_j}] \\ &= \{f^{(\dagger)}_j, f^{(\dagger)}_k\}e^{i\pi n_j} - f^{(\dagger)}_k\{f^{(\dagger)}_j, e^{i\pi n_j}\} = 0. \end{aligned} \tag{6.11}$$

To see how this works, we shall now discuss the one-dimensional Heisenberg model

$$H = -J\sum[S^x_j S^x_{j+1} + S^y_j S^y_{j+1}] - J_z\sum_j S^z_j S^z_{j+1} \tag{6.12}$$

In real magnetic systems, local moments can interact via ferromagnetic, or antiferromagnetic interactions. Ferromagnetic interactions generally arise as a result of "direct exchange", whereby the Coulomb repulsion energy is lowered when electrons are in a triplet state, because the wavefunction is then spatially antisymmetric. Antiferromagnetic interactions are generally produced by the mechanism of "double exchange", whereby electrons in antiparallel spin states can lower their energy by undergoing virtual fluctuations into high energy states where two electrons occupy the same orbital. Here we have written the model as if the interactions are ferromagnetic.

For convenience, the model can be rewritten as

$$H = -\frac{J}{2}\sum[S^+_{j+1}S^-_j + \text{H.c}] - J_z\sum_j S^z_j S^z_{j+1} \tag{6.13}$$

To fermionize the first term, we note that all terms in the strings cancel, except for a $e^{i\pi n_j}$ which has no effect,

$$\frac{J}{2}\sum_j S^+_{j+1}S^-_j = \frac{J}{2}\sum_j f_{j+1}{}^\dagger e^{i\pi n_j} f_j = \frac{J}{2}\sum_j f_{j+1}{}^\dagger f_j \tag{6.14}$$

so that the transverse component of the interaction induces a "hopping" term in the fermionized Hamiltonian. Notice that the string terms would enter if the spin interaction involved next-nearest neighbors. The z-component of the Hamiltonian becomes

$$-J_z\sum_j S^z_{j+1}S^z_j \quad = \quad -J_z\sum_j(n_{j+1} - \frac{1}{2})(n_j - \frac{1}{2}) \tag{6.15}$$

Notice how the Ferromagnetic interaction means that spin-fermions attract one-another. The transformed Hamiltonian is then

$$H = -\frac{J}{2}\sum_j(f^\dagger{}_{j+1}f_j + f^\dagger{}_j f_{j+1}) + J_z\sum_j n_j - J_z\sum_j n_j n_{j+1}. \tag{6.16}$$

Interestingly enough, the pure x-y model has no interaction term in it, so we can solve this case as a non-interacting fermion problem.

To write out the fermionized Hamiltonian in its most compact form, let us transform to momentum space, writing

$$f_j = \frac{1}{\sqrt{N}}\sum_k s_k e^{ikR_j} \tag{6.17}$$

where $s^\dagger{}_k$ creates a spin excitation in momentum space, with momentum k. In this case, the one-particle terms become

$$\begin{aligned} J_z\sum_j n_j &= J_z\sum_k s^\dagger{}_k s_k. \\ -\frac{J}{2}\sum_j(f^\dagger{}_{j+1}f_j + \text{H.c}) &= -\frac{J}{2N}\sum_k(e^{-ika} + e^{ika})s^\dagger{}_k s_{k'}\overbrace{\sum_j e^{-i(k-k')R_j}}^{N\delta_{kk'}} \\ &= -J\sum_k\cos(ka)s^\dagger{}_k s_k. \end{aligned} \tag{6.18}$$

The Heisenberg Hamiltonian can thus be written

$$H = \sum_k \omega_k s^\dagger{}_k s_k - J_z\sum_j n_j n_{j+1} \tag{6.19}$$

where

$$\omega_k = (J_z - J\cos ka) \tag{6.20}$$

defines a magnon excitation energy, and the second interaction term is still written in the position basis. We can easily cast the second-term in momentum space, by noticing that the interaction is a function of $i-j$ which is $-J_z/2$ for $i-j=\pm 1$ but zero otherwise.The Fourier transform of this short-range interaction is $V(q) = -J_z \cos qa$, so that Fourier transforming the interaction term gives

$$H = \sum_k \omega_k s^\dagger{}_k s_k - \frac{J_z}{N_s}\sum_{k,k',q} \cos(qa)\ s^\dagger{}_{k-q} s^\dagger{}_{k'+q} s_{k'} s_k. \tag{6.21}$$

This transformation holds for both the ferromagnet and antiferromagnet. In the former case, the fermionic spin excitations corrrespond to the magnons of the ferromagnet. In the latter case, the fermionic spin excitations are often called "spinons".

To see what this Hamiltonian means, let us first neglect the interactions. This is a reasonable thing to do in the limiting cases of (i) the Heisenberg Ferromagnet, $J_z = J$ and (ii) the x-y model $J_z = 0$.

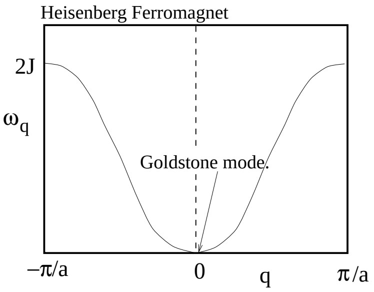


Figure 6.2: Excitation spectrum of the one dimensional Heisenberg Ferromagnet.

- *Heisenberg Ferromagnet.* $J_z = J$

  In this case, the spectrum

$$\omega_k = 2J\sin^2(ka/2) \tag{6.22}$$

is always positive, so that there are no magnons present in the ground-state. The ground-state thus contains no magnons, and can be written

$$|0\rangle = |\downarrow\downarrow\downarrow \ldots\rangle \tag{6.23}$$

corresponding to a state with a spontaneous magnetization $M = -N_s/2$.

Curiously, since $\omega_{k=0} = 0$, it costs no energy to add a magnon of arbitrarily long wavelength. This is an example of a Goldstone mode, and the reason it arises, is because the spontaneous magnetization could actually point in any direction. Suppose we want to rotate the magnetization through an infinitesimal angle $\delta\theta$ about the x axis, then the new state is given by

$$\begin{aligned} |\psi\rangle' &= e^{i\delta\theta S_x}|\downarrow\downarrow\ldots\rangle \\ &= |\downarrow\downarrow\ldots\rangle + i\frac{\delta\theta}{2}\sum_j S^+_j|\downarrow\downarrow\ldots\rangle + O(\delta\theta^2) \end{aligned} \tag{6.24}$$

The change in the wavefunction is proportional to the state

$$\begin{aligned} S^+_{TOT}|\downarrow\downarrow\ldots\rangle &\equiv \sum_j f_j{}^\dagger e^{i\phi_j}|0\rangle \\ &= \sum_j f_j{}^\dagger|0\rangle = \sqrt{N_s}s^\dagger{}_{k=0}|0\rangle \end{aligned} \tag{6.25}$$

In otherwords, the action of adding a single magnon at $q=0$, rotates the magnetization infinitesimally upwards. Rotating the magnetization should cost no energy, and this is the reason why the $k=0$ magnon is a zero energy excitation.

- *x-y Ferromagnet* As J_z is reduced from J, the spectrum develops a negative part, and magnon states with negative energy will become occupied. For the pure $x-y$ model, where $J_z = 0$, the interaction identically vanishes, and the excitation spectrum of the magnons is given by $\omega_k = -J\cos ka$ as sketched in Fig. 6.3. All the negative energy fermion states with $|k| < \pi/2a$ are occupied, so the ground-state is given by

$$|\Psi_g\rangle = \prod_{|k|<\pi/2a} s^\dagger{}_k|0\rangle \tag{6.26}$$

The band of magnon states is thus precisely half-filled, so that

$$\langle S_z\rangle = \langle n_f - \frac{1}{2}\rangle = 0 \tag{6.27}$$

so that remarkably, there is no ground-state magnetization. We may interpret this loss of ground-state magnetization as a consequence of the growth of quantum spin fluctuations in going from the Heisenberg, to the x-y ferromagnet.

Excitations of the ground-state can be made, either by adding a magnon at wavevectors $|k| > \pi/2a$, or by annihilating a magnon at wavevectors $|k| < \pi/2a$, to form a

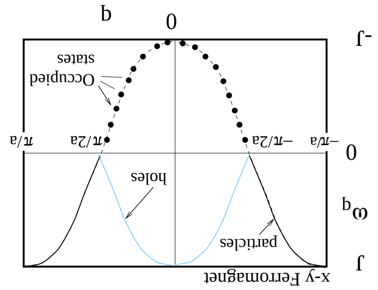


Figure 6.3: Excitation spectrum of the one dimensional x-y Ferromagnet, showing how the negative energy states are filled, the negative energy dispersion curve is "folded over" to describe the positive hole excitation energy.

"hole". The energy to form a hole is $-\omega_k$. To represent the hole excitations, we make a "particle-hole" transformation for the occupied states, writing

$$\tilde{s}_k = \begin{cases} s_k, & (|k| > \pi/2a), \\ s^\dagger{}_{-k}, & (|k| < \pi/2a) \end{cases} \tag{6.28}$$

These are the "physical" excitation operators. Since $s^\dagger{}_k s_k = 1 - s_k s^\dagger{}_k$, the Hamiltonian of the pure x-y ferromagnet can be written

$$H_{xy} = \sum_k J|\cos ka|(\tilde{s}^\dagger{}_k\tilde{s}_k - \frac{1}{2}) \tag{6.29}$$

Notice that unlike the pure Ferromagnet, the magnon excitation spectrum is now linear. The ground-state energy is evidently

$$\begin{aligned} E_g &= -\frac{1}{2}\sum_k J|\cos ka| \\ &= -a\frac{1}{2})\int_{-\pi/2a}^{\pi/2a}\frac{dk}{2\pi}J\cos(ka) = -\frac{J}{\pi} \end{aligned} \tag{6.30}$$

But if there is no magnetization, why are there zero-energy magnon modes at $q = \pm\pi/a$? It turns out that although there is no true long-range order, the spin-correlations

in the x-y model display power-law correlations with an infinite spin correlation length which correspond to the excitation of magnons in the vicinity of the gapless nodes at $q = \pm\pi/a$.

6.2 The Hubbard Model

In a real electronic systems, such as a metallic crystal at first sight it might appear to be a task of hopeless complexity to model the behavior of the electron fluid. Fortunately, even in complex systems, at low energies only a certain subset of the electronic degrees of freedom are excited. This philosophy is closely tied up with the idea of renormalization- the idea that the high energy degrees of freedom in a system can be successively eliminated or "integrated out" to reveal an effective Hamiltonian that describes the important low energy physics. One such model, which has enjoyed great success, is the Hubbard model, first introduced in the early sixties.

Suppose we have a lattice of atoms where electrons are almost localized in atomic orbitals at each site. In this case, we can use a basis of atomic orbitals. The operator which creates a particle at site j is

$$c^\dagger{}_{j\sigma} = \int d^3x\Phi(\mathbf{x}-\mathbf{R}_j)\psi^\dagger(x)_\sigma \tag{6.31}$$

where $\Phi(\mathbf{x})$ is the wavefunction of a particle in the localized atomic orbital. In this basis, the Hamiltonian governing the motion, and interactions between the particles can be written quite generally as

$$H = \sum_{i,j}\langle i|H_o|j\rangle c^\dagger{}_{i\sigma}c_{j\sigma} + \frac{1}{2}\sum_{lmnp}\langle lm|V|pn\rangle c^\dagger{}_{l\sigma}c^\dagger{}_{m\sigma'}c_{n\sigma'}c_{p\sigma} \tag{6.32}$$

where $\langle i|H_o|j\rangle c^\dagger{}_{i\sigma}$ is the one-particle matrix element between states i and j, and $\langle lm|V|pn\rangle$ is the interaction matrix element between two-particle states $|lm\rangle$ and $|pn\rangle$.

Let us suppose that the energy of an electron in this state is ϵ. If this orbital is highly localized, then the amplitude for it to tunnel or "hop" between sites will decay exponentially with distance between sites, and to a good approximation, we can eliminate all but the nearest neighbor hopping. In this case, the one-particle matrix elements which govern the motion of electrons between sites are then

$$\langle j|H^(o)|i\rangle = \begin{cases} \epsilon & j = i \\ -t & \text{i, j nearest neighbors} \\ 0 & \text{otherwise} \end{cases} \tag{6.33}$$

The hopping matrix element between neigboring states will generally be given by an overlap integral of the wavefunctions with the negative crystalline potential, and for this reason, it is taken to be be negative. Now the matrix element of the interaction between electrons at different sites will be given by

$$\langle lm|V|pn\rangle = \int_{x,x'}\Phi^*_l(x)\Phi_p(x)\Phi^*_m(x')\Phi^*_n(x')V(x-x'), \tag{6.34}$$

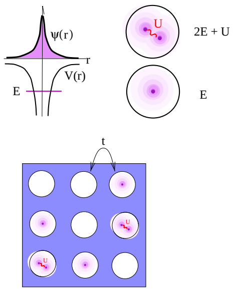


Figure 6.4: Illustrating the Hubbard Model. When two electrons of opposite spin occupy a single atom, this gives rise to a Coulomb repulsion energy U. The amplitude to hop from site to site in the crystal is t.

but in practice, if the states are well localized, this will be dominated by the onsite interaction between two electrons in a single orbital, so that we may approximate

$$\langle lm|V|pn\rangle = \begin{cases} U & i=j=m=n \\ 0 & \text{otherwise} \end{cases} \tag{6.35}$$

In this situation, the interaction between the interaction term in (6.32) simplifies to

$$\frac{U}{2}\sum_{j,\sigma\sigma'} c^\dagger{}_{j\sigma}c^\dagger{}_{j\sigma'}c_{j\sigma'}c_{j\sigma} = U\sum_j n_{j\uparrow}n_{j\downarrow}, \tag{6.36}$$

where the exclusion principle ($c_{j\sigma}^2 = 0$) means that the interaction term vanishes unless σ σ' are opposite spins. The Hubbard model can be thus be written

$$H = -t\sum_{j,\hat{a},\sigma}[c^\dagger{}_{j+\hat{a}\sigma}c_{j\sigma} + \mathrm{H.c}] + \epsilon\sum_{j\sigma}c^\dagger{}_{j\sigma}c_{j\sigma} + U\sum_j n_{j\uparrow}n_{j\downarrow}, \tag{6.37}$$

where $n_{j\sigma} = c^\dagger{}_{j\sigma}c_{j\sigma}$ represents the number of electrons of spin σ at site j. For completeness, let us rewrite this in momentum space, putting

$$c_{j\sigma} = \frac{1}{\sqrt{N_s}}\sum_{\mathbf{k}} c_{\mathbf{k}\sigma}e^{i\mathbf{k}\cdot\mathbf{R}_j} \tag{6.38}$$

whereupon

$$\boxed{H = \sum_{\mathbf{k}\sigma}\epsilon_{\mathbf{k}}c^\dagger{}_{\mathbf{k}\sigma}c_{\mathbf{k}\sigma} + \frac{U}{N_s}\sum_{\mathbf{q},\mathbf{k},\mathbf{k}'} c^\dagger{}_{\mathbf{k}-\mathbf{q}\uparrow}c^\dagger{}_{\mathbf{k}'+\mathbf{q}\downarrow}c^\dagger{}_{\mathbf{k}'\downarrow}c^\dagger{}_{\mathbf{k}\uparrow}} \tag{6.39}$$

Hubbard model

where

$$\begin{aligned}\epsilon_{\mathbf{k}} &= \sum_i \langle j+\mathbf{R}_i|H_o|j\rangle e^{i\mathbf{k}\cdot\mathbf{R}_i} \\ &= -2t(\cos k_x + \cos k_y + \cos k_z) + \epsilon \end{aligned} \tag{6.40}$$

is recognized as the kinetic energy of the electron excitations which results from their *coherent* hopping motion from site to site. We see that the Hubbard model describes a band of electrons with kinetic energy $\epsilon_{\mathbf{k}}$, and a momentum independent "point" interaction of strength U between particles of opposite spin.

Remark

- This model has played a central part in the theory of magnetism, metal-insulator transitions, and most recently, in the description of electron motion in high temperature superconductors. With the exception of one dimensional physics, we do not, as yet have a complete understanding of the physics that this model can give rise to. One prediction of the Hubbard model which is established, is that under certain circumstance, if interactions become too large the electrons become localized to form what is called "Mott insulator". This typically occurs when the interactions are large and the number of electrons per site is close to one. What is very unclear at the present time, is what happens to the Mott insulator when it is doped, and there are many who believe that a complete understanding of the doped Mott insulator will enable us to understand high temperature superconductivity.

6.3 Gas of charged particles

6.3.1 Link with first quantization

As a final example, we should like to briefly consider an interacting gas of charged particles. The second-quantized Hamiltonian for this case is

$$\boxed{H - \mu N = \overbrace{\sum_\sigma\int_x \psi_\sigma{}^\dagger\left[-\frac{\hbar^2\nabla^2}{2m} + U(x) - \mu\right]\psi_\sigma(x)}^{H_o} + \overbrace{\frac{1}{2}\sum_{\sigma\sigma'}\int_{x,x'} V(x-x') : \hat{\rho}(x)\hat{\rho}(x') :}^{\hat{V}}.(6.41)}$$

where $\int_x \equiv \int d^3x$. For a Coulomb interaction

$$V(x-x') = \frac{e^2}{4\pi\epsilon_o|x-x'|} \tag{6.42}$$

but the interaction might have a more general form, as in the case of a fluid of $He-3$ fermions or $He-4$ bosons. One can not underestimate the hidden subtleties behind this Hamiltonian! As far as we know for example, it essentially complete many body description of the electronic motions of electrons in any electronic medium, even your mind!

Let us now develop the equations of motion for this Hamiltonian, and confirm that using it, we can fully recover the first quantized approach to many body physics. The equation of motion for the Fermi field is given by

$$i\hbar\frac{\partial\psi_\sigma}{\partial t} = -[H,\psi_\sigma] \tag{6.43}$$

Now we can divide the Hamiltonian up into a one-particle part and an interaction. Using the general relations

$$\begin{aligned}[\psi_{\sigma'}{}^\dagger(x')O_{x'}\psi_{\sigma'}(x'),\psi_\sigma(x)] &= -\delta_{\sigma\sigma'}\delta^3(x-x')O_x\psi_\sigma(x), \\ :[\rho(x_1)\rho(x_2),\psi_\sigma(x)]: &= :[\rho(x_1),\psi_\sigma(x)]\rho(x_2):+:\rho(x_1)[\rho(x_2),\psi_\sigma(x)]: \\ &= -\delta^3(x_1-x)\rho(x_2)\psi_\sigma(x) - \delta^3(x_2-x)\rho(x_1)\psi_\sigma(x)\end{aligned}$$

we can see that the comutators of the one- and two-particle parts of the Hamiltonian with the field operators are

$$\begin{aligned}-[H_o,\psi_\sigma(x)] &= \left[-\frac{\hbar^2\nabla^2}{2m} + U(x) - \mu\right]\psi_\sigma(x) \\ -[V,\psi_\sigma(x)] &= \int d^3x' V(x'-x)\rho(x')\psi_\sigma(x)\end{aligned} \tag{6.44}$$

The final equation of motion of the field operator thus resembles a one-particle Schrodinger equation.

$$i\hbar\frac{\partial\psi_\sigma}{\partial t} = \left[-\frac{\hbar^2\nabla^2}{2m} + U(x) - \mu\right]\psi_\sigma(x) + \int d^3x' V(x'-x)\rho(x')\psi_\sigma(x) \tag{6.45}$$

If we now apply this to the many body wavefunction, we obtain

$$\begin{aligned}i\hbar\frac{\partial\Psi(1,2,\dots N)}{\partial t} &= i\hbar\sum_{r=1,2S}\langle 0|\psi(1)\dots\partial_t\psi(r)\dots\psi(N)|\Psi\rangle \\ &= \sum_j\left[-\frac{\hbar^2\nabla_j^2}{2m} + U(x_j) - \mu\right]\Psi\end{aligned}$$

$$+ \sum_j\int d^3x' V(x'-x_j)\langle 0|\psi(1)\dots\rho(x')\psi_\sigma(x_j)\dots\psi(N)|\Psi\rangle$$

By commuting the density operator to the left, until it annihilates with the vacuum, we find that

$$\langle 0|\psi(1)\dots\rho(x')\psi_\sigma(x_j)\dots\psi(N)|\Psi\rangle = \sum_{l<j}\delta^3(x'-x_l)\langle 0|\psi(1)\dots\psi(N)|\Psi\rangle \tag{6.46}$$

so that the final expression for the time evolution of the many body wavefunction is precisely the same as we obtain in a first quantized approach.

$$i\hbar\frac{\partial\Psi}{\partial t} = \left(\sum_j\mathcal{H}_j^{(o)} + \sum_{l<j}V_{jl}\right)\Psi \tag{6.47}$$

Our second-quantized approach has many advantages- it builds in the exchange statistics, and it does not need to make an explicit reference to the cumbersome many body wavefunction.

6.4 Non-interacting particles in thermal equilibrium

Before we start to consider the physics of the interacting problem, let us go back and look at the ground-state properties of free particles. What is not commonly recognized, is that the ground-state of non-interacting, but identical particles is in fact, a highly correlated many body state, and for this reason, the non-interacting ground-state has a robustness that does not exist in its classical counterpart. In the next chapter, we shall embody some of these thoughts in by considering turnign on the interactions on adiabatically. For the moment however, we shall content ourselves with looking at a few of the ground-state properties of non-interacting gases of identical particles.

In practice, quantum effects will influence a fluid of identical particles at the point where their characteristic wavelength is comparable with the separation between particles. At a temperature T the rms momentum of particles is given by $p_{RMS}^2 = 3mk_BT$, so that characteristic de Broglie wavelength is given by

$$\lambda_T = \frac{h}{\sqrt{p_{RMS}^2}} = \frac{h}{\sqrt{3mk_BT}} \tag{6.48}$$

so that when $\lambda_T \sim \rho^{-1/3}$, the characteristic temperature is of order

$$k_BT^* \sim \frac{\hbar^2\rho^{2/3}}{2m} \tag{6.49}$$

Below this temperature, identical particles start to interfere with one-another, and a quantum-mechanical treatment of the fluid becomes necessary. In a Fermi fluid, exclusion statistics

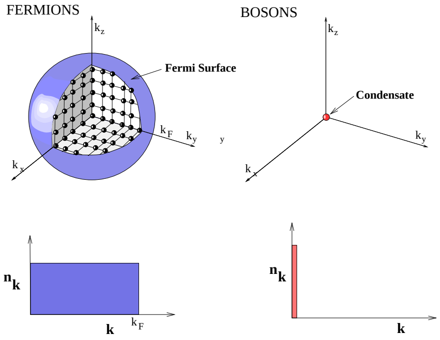


Figure 6.5: Contrasting the ground-states of non-interacting Fermions and non-interacting Bosons. Fermions form a degenerate Fermi gas, with all one-particle states below the Fermi energy individually occupied. Bosons form a Bose Einstein condensate, with a macroscopic number of bosons in the zero momentum state.

tends to keep particles apart, enhancing the pressure, whereas for a Bose fluid, the correlated motion of particles in the condensate tends to lower the pressure, ultimately causing it to vanish at the Bose Einstein condensation temperature. In electron fluids inside materials, this characteristic temperature is two orders of magnitude larger than room temperature, which makes the electricity one of the most dramatic examples of quantum physics in everyday phenomena!

6.4.1 Fluid of Fermions

The thermodynamics of a fluid of fermions leads to the concept of a "degenerate Fermi liquid", and it is important in a wide range of physical situations, such as

- The ground-state and excitations of metals.
- The low energy physics of liquid Helium 3.
- The degenerate Fermi gas of neutrons, electrons and protons that lies within a neutron

star.

The basic physics of each of these cases, can to a first approximation be described by a fluid of non-interacting Fermions, with Hamiltonian

$$H - \mu N = \sum_{\sigma} (\epsilon_{\mathbf{k}} - \mu) c^{\dagger}{}_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} \tag{6.50}$$

Following the general discussion of the last section, the Free energy of such a fluid of fermions is is described by a single Free energy functional

$$\begin{aligned} F &= -k_B T \sum_{\mathbf{k}\sigma} \ln[1 + e^{-\beta(\epsilon_{\mathbf{k}} - \mu)}] \\ &= -2k_B T V \int_{\mathbf{k}} \ln[1 + e^{-\beta(\epsilon_{\mathbf{k}} - \mu)}] \end{aligned} \tag{6.51}$$

where we have taken the thermodnamic limit, replacing $\sum_{\mathbf{k}\sigma} \rightarrow 2V \int_{\mathbf{k}}$. By differentiating F with respect to volume, temperature and chemical potential, we can immediately derive the pressure, entropy and particle density of this fluid. Let us however, begin with a more physical discussion.

In thermal equilibrium the number of fermions in a given momentum state is

$$n_{\mathbf{p}} = f(\epsilon_{\mathbf{p}} - \mu) \tag{6.52}$$

where

$$f(x) = \frac{1}{e^{\beta x} + 1} \tag{6.53}$$

is the Fermi-Dirac function. At low temperatures, this function resembles a step, with a jump in occupancy spread over an energy range of order $k_B T$ around the chemical potential. At absolute zero $f(x) \rightarrow \theta(-x)$, so that the occupancy of each state is given by

$$n_{\mathbf{p}} = \theta(\mu - \epsilon_{\mathbf{p}}) \tag{6.54}$$

is a step function with an abrupt change in occupation when $\epsilon = \mu$, corresponding to the fact that states with $\epsilon < \mu$, are completely occupied, and states above this energy are empty. The zero-temperature value of the chemical potential is often called the "Fermi energy". In momentum space, the occupied states form a sphere, whose radius in momentum space, k_F is often refered to as the Fermi momentum.

The ground-state corresponds to a state where all fermion states with momentum $k < k_F$ are occupied:

$$|\psi_g\rangle = \prod_{\mathbf{k}\sigma} c^{\dagger}{}_{\mathbf{k}\sigma}|0\rangle \tag{6.55}$$

Excitations above this ground-state are produced by the addition of particles at energies above the Fermi wavevector, or the creation of *holes* beneath the Fermi wavevector. To describe these excitations, we make the following *particle-hole* transformation

$$a^{\dagger}{}_{\mathbf{k}\sigma} = \left\{ \begin{array}{lll} c^{\dagger}{}_{\mathbf{k}\sigma} & (k > k_F) & \text{particle} \\ \sigma c_{-\mathbf{k}-\sigma} & (k > k_F) & \text{hole} \end{array} \right. \tag{6.56}$$

Beneath the Fermi surface, we must replace $c^{\dagger}{}_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} \rightarrow 1 - a^{\dagger}{}_{\mathbf{k}\sigma} a_{\mathbf{k}\sigma}$, so that in terms of particle and hole excitations, the Hamiltonian can be re-written

$$H - \mu N = \sum_{\sigma} |(\epsilon_{\mathbf{k}} - \mu)| a^{\dagger}{}_{\mathbf{k}\sigma} a_{\mathbf{k}\sigma} + F_g \tag{6.57}$$

where respectively,

$$F_g = \sum_{|bfk| < k_F, \sigma} (\epsilon_{\mathbf{k}} - \mu) = 2V \int_{|\mathbf{k}| < k_F} (\epsilon_{\mathbf{k}} - \mu), \tag{6.58}$$

is the ground-state Free energy, and E_g and N are the ground-state energy and particle number Notice that

- To create a hole with momentum $\mathbf{k}$ and spin σ, we must destroy a fermion with momentum $-\mathbf{k}$ and spin $-\sigma$. (The additional multiplying factor of σ in the hole definition is a technical feature, required so that the particle and holes have the same spin operators.)
- The excitation energy of a particle or hole is given by $\epsilon^*_{\mathbf{k}} = (\epsilon_{\mathbf{k}} - \mu)$, corresponding to "reflecting" the excitation spectrum of the negative energy fermions about the Fermi energy.

The ground-state density of a Fermi gas is given by the volume of the Fermi surface, as follows

$$\langle \hat{\rho} \rangle = \frac{1}{V} \sum_{\mathbf{k}\sigma} \langle c^{\dagger}{}_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} \rangle = 2 \int_{k < k_F} \frac{d^3 k}{2\pi} = \frac{2}{(2\pi)^3} V_{\rm FS} \tag{6.59}$$

where

$$V_{\rm FS} = \frac{4\pi}{3} k_F^3 = \left(\frac{4\pi}{3}\right) \left(\frac{2m\epsilon_F}{\hbar^2}\right)^{3/2} \tag{6.60}$$

is the volume of the Fermi surface. The relationship between the density of particles, the Fermi wavevector and the Fermi energy is thus

$$\boxed{\langle \frac{\hat{N}}{V} \rangle = \frac{1}{3\pi^2} k_F^3 = \frac{1}{3\pi^2} \left(\frac{2m\epsilon_F}{\hbar^2}\right)^{3/2}} \tag{6.61}$$

In an electron gas, where the characteristic density is $N/V \sim 10^{29} m^{-3}$ the characteristic Fermi energy is of order $1eV \sim 10,000K$. In other words, the characteristic energy of an electron is two orders of magnitude larger than would be expected classically. This is a stark and dramatic consequence of the exchange interference between identical particles, and it is one of the great early triumphs of quantum mechanics to have understood this basic piece of physics.

Let us briefly look at finite temperatures. Here, by differentiating the Free energy with respect to volume and chemical potential, we obtain

$$\begin{aligned} P &= -\frac{\partial F}{\partial V} = \frac{-F}{V} = 2 \int_{\mathbf{k}} \ln[1 + e^{-\beta(\epsilon_{\mathbf{k}} - \mu)}] \\ N &= -\frac{\partial F}{\partial \mu} = 2 \int_{\mathbf{k}} f(\epsilon_{\mathbf{k}} - \mu) \end{aligned} \tag{6.62}$$

The second equation *defines* the chemical potential in terms of the particle density at a given temperature. The first equation shows that, since the Free energy is an extensive function of volume, the pressure is simply the $-1\times$ the Free energy density per unit volume. These two equations can be solved parametrically as a function of chemical potential. At high temperatures the pressure reverts to the ideal gas law $PV = Nk_B T$, but at low temperatures, the pressure is given by $-1\times$ the ground-state Free energy per unit volume

$$P = 2 \int_{|\mathbf{k} < \mathbf{K_F}} (\mu - \epsilon_{\mathbf{k}})| = \frac{2N}{5V} \epsilon_F \tag{6.63}$$

The final result is obtained by noting that the first term in this expression is $\mu(N/V)$. The first term contains an integral over $d^3k \sim k^2 \rightarrow k_F^3/3$, whereas the second term contains an integral over $\epsilon_k d^3 k \sim k^4 \rightarrow k_F^5/5$, so the second term is 3/5 of the first term. Not surprisingly, this quantity is basically the density of fermions times the Fermi energy- a pressure that is hundreds of times larger than the classical pressure in a room temperature electron gas.

Remarks

- At first sight, it might seem very doubtful as to whether the remarkable features of the degenerate Fermi gas would survive once interactions are present. In particular, one would be tempted to wonder whether the Fermi surface would be blurred out by particle-particle interactions. Remarkably, for modest repulsive interactions, the Fermi surface is believed to be stable in dimensions bigger than one. This is because electrons at the Fermi surface have no phase space for scattering. This is the basis of Landau's *Fermi liquid Theory* of interacting Fermions.
- In a remarkable result, due to Luttinger and Ward, the jump in the occupancy at the Fermi wavevector remains finite, though reduced from unity, in the non-interacting Fermi liquid to a finite $Z_{\mathbf{k_F}} < 1$.

6.4.2 Fluid of Bosons: Bose Einstein Condensation

Bose Einstein condensation was predicted in 1924- the outcome of Einstein extending Bose's new calculations on the statistics of a gas of identical bosons. However, it was not until seventy years later- in 1995, that the groups of Cornell and Wieman and independently that of Ketterle, succeeded in cooling a low density gas of atoms - initially rubidium and sodium atoms - through the Bose Einstein transition temperature. The closely related phenomenon

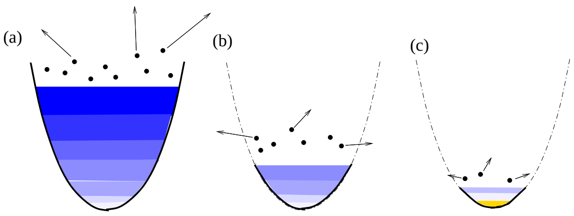


Figure 6.6: Illustrating evaporative cooling in an atom trap. (a) Atoms are held within a magnetic potential. (b) As the height of the potential well is dropped, the most energetic atoms "evaporate" from the well, progressively reducing the temperature. (c) A Bose Einstein condensate, with a finite fraction of the gas in a single momentum state, forms when the temperature drops blow the condensation temperature.

of superfluidity was first observed in the late 30's by Kapitza. Superfluidity results from a kind of Bose-Einstein condensation, in a dense quantum fluid, where interactions between the particles become important. In the modern context, ultra cold, ultra-dilute gases of alkali atoms are produced using lasers to contain a small quantity of atoms inside a magnetic trap. The most energetic atoms are allowed to evaporate out of the well and as the height of the well is reduced, the temperature of the gas reduces. Temperatures in the nano-Kelvin range are required to produce Bose-Einstein condensation in these materials.

To understand the phenomenon of BEC, conside the density of gas of bosons, which at a finite temperature takes almost precisely the same form as for fermions

$$\rho = \int_{\mathbf{k}} \frac{1}{e^{\beta(\epsilon_{\mathbf{k}}-\mu)}-1} \tag{6.64}$$

where we have written the expression for spinless bosons, as would be the case for a gas of liquid Helium-4, or ultra-dilute Potassium atoms, for instance. But there is a whole world of physics in the innocent minus sign in the denominator! Whereas for fermions, the chemical potential is positive, the chemical potential for bosons is negative. For a gas at fixed volume , the above expression (6.64) thus defines the chemical potential $\mu(T)$. By changing variables, writing

$$x \quad = \quad \beta\epsilon_{\mathbf{k}} = \beta\frac{\hbar^2k^2}{2m}, \qquad \left(\frac{m}{\beta\hbar^2}\right)dx = kdk$$

$$\frac{d^3k}{(2\pi)^3} \quad\rightarrow\quad \frac{4\pi k^2dk}{(2\pi)^3} = \frac{1}{\sqrt{2}\pi^2}\left(\frac{m}{\beta\hbar^2}\right)^{3/2}\sqrt{x}dx \tag{6.65}$$

we can rewrite the Boson density in the form

$$\rho = \frac{2}{\sqrt{\pi}\tilde{\lambda}_T^3}\int_0^\infty dx\sqrt{x}\frac{1}{e^{x-\beta\mu}-1} \tag{6.66}$$

where

$$\tilde{\lambda}_T = \left(\frac{2\pi\hbar^2}{mk_BT}\right)^{1/2} \tag{6.67}$$

is a convenient definition of the thermal de Broglie wavelength In order to maintain a fixed density, as one lowers the temperature, the chemical potential $\mu(T)$ must rise. At a certain temperature, the chemical potential becomes zero, $\rho(T,\mu=0)=N/V$ At this temperature,

$$\left(\frac{\tilde{\lambda}_T}{a}\right)^3 = \frac{2}{\sqrt{\pi}}\int_0^\infty dx\sqrt{x}\frac{1}{e^x-1} = \zeta(\frac{3}{2}) = 2.61 \tag{6.68}$$

where $a=\rho^{-1/3}$ is the interparticle spacing. The corresponding temperature

$$k_BT_o = 3.31\left(\frac{\hbar^2}{ma^2}\right) \tag{6.69}$$

is the Bose-Einstein condensation temperature.

Below this temperature, the number of Bosons in the $\mathbf{k}=0$ state becomes macroscopic, i.e.

$$n_{\epsilon=0} = \frac{1}{e^{-\beta\mu}-1} = N_o(T) \tag{6.70}$$

becomes a finite fraction of the total particle number. Since $N_o(T)$ is macroscopic, it follows that

$$\frac{\mu}{k_BT} = -\frac{1}{N_o(T)} \tag{6.71}$$

is infinitesimally close to zero. For this reason, we must be careful to split off the $\mathbf{k}=0$ contribution to the particle density, writing

$$N = N_o(T) + \sum_{\mathbf{k}\neq\mathbf{0}} n_{\mathbf{k}} \tag{6.72}$$

and *then* taking the thermodynamic limit of the second term. For the density, this gives

$$\rho = \frac{N}{V} = \rho_0(T) + \int_{\mathbf{k}}\frac{1}{e^{\beta(\epsilon_{\mathbf{k}})}-1} \tag{6.73}$$

The the second term is proportional to $\tilde{\lambda}_T{-}3 \propto T^{3/2}$. Since the first term vanishes at $T=T_o$, it follows that below the Bose Einstein condensation temperature, the density of bosons in the condensate is thus given by

$$\rho_o(T) = \rho\left[1-\left(\frac{T}{T_o}\right)^{3/2}\right] \tag{6.74}$$

Remarks

- The Bose Einstein Condensation is an elementary example of a second-order phase transition.
- Bose Einstein condensation is an example of a broken symmetry phase transition. It turns out that the same phenomenon survives in a more robust form, if repulsive interactions between the Bosons are present. In the interacting Bose Einstein Condensate, the field operator $\psi(x)$ for the bosons actually acquires a macroscopic expectation value

  $$\langle\psi(x)\rangle = \sqrt{\rho_o}e^{i\phi(x)} \tag{6.75}$$

  In a non-interacting Bose condensate, the phase $\phi(x)$ lacks rigidity, and does not have a well-defined meaning. In an interacting condensate, the phase $\phi(x)$ is uniform, and gradients of the phase result in a *superflow* of particles- a flow of atoms which is completely free from viscosity.

Example: Using the results of the previous section, show that the ideal gas law is modified by the interference between identical particles, so that

$$P = nk_BT\mathcal{F}^{\pm}(\mu/k_BT) \tag{6.76}$$

where n is the number density of particles, $\mathcal{F}^{\pm}(z) = g^{\pm}(z)/h^{\pm}(z)$ and

$$\begin{aligned} g^{\pm}(z) &= \pm\int_0^\infty dx\sqrt{x}\ln[1\pm e^{-(x-z)}] \\ h^{\pm}(z) &= \int_0^\infty dx\sqrt{x}\frac{1}{e^{(x-z)}\pm 1} \end{aligned} \tag{6.77}$$

where the upper sign refers to fermions, the bottom to bosons. Sketch the dependence of pressure on temperature for a gas of identical bosons and a gas of identical fermions with the same density.

Solution: Let us begin by deriving an explicit expression for the Free energy of a free gas of fermions, or bosons. We start with

$$F = \mp(2S+1)k_BTV\int_{\mathbf{k}}\ln[1\pm e^{-\beta(\epsilon_{\mathbf{k}}-\mu)}] \tag{6.78}$$

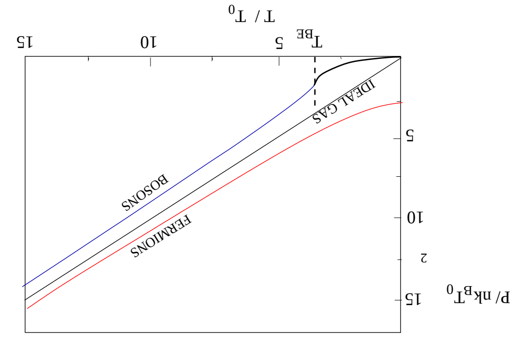


Figure 6.7: Pressure dependence in a Fermi or Bose gas, where temperature is measured in units of $k_BT_0 = \hbar^2/ma^2$ Showing P/nk_B

where S is the spin of the particle. Making the change of variables,

$$\begin{aligned} x &= \beta\epsilon_{\mathbf{k}} = \beta\frac{\hbar^2k^2}{2m}, \\ \frac{d^3k}{(2\pi)^3} &\rightarrow \frac{2}{\tilde{\lambda}_T^3\sqrt{\pi}}\sqrt{x}dx \end{aligned} \tag{6.79}$$

where $\tilde{\lambda}_T = \sqrt{2\pi\hbar^2/(mk_BT)}$ is the rescaled Thermal de Broglie wavelength, we obtain

$$F = \mp(2S+1)k_BT\frac{V}{\tilde{\lambda}_T^3}\frac{2}{\sqrt{\pi}}\int dx\sqrt{x}\ln[1\pm e^{-(x+\mu\beta)}] \tag{6.80}$$

Taking the derivative with respect to volume, and chemical potential, we obtain the following results for the Pressure and the particle density.

$$\begin{aligned} P &= -\frac{\partial F}{\partial V} = \pm(2S+1)\frac{k_BT}{\tilde{\lambda}_T^3}\frac{2}{\sqrt{\pi}}\int dx\sqrt{x}\ln[1\pm e^{-(x-\mu\beta)}] \\ n &= -\frac{\partial F}{V\partial\mu} = \frac{(2S+1)}{\tilde{\lambda}_T^3}\frac{2}{\sqrt{\pi}}\int dx\sqrt{x}\frac{1}{e^{(x-\mu\beta)}\pm 1} \end{aligned} \tag{6.81}$$

Dividing the pressure by the density, we obtain the quoted result for the ideal gas.

To plot these results, it is convenient to rewrite the temperature and pressure in the form

$$\begin{aligned} T &= T_o[h^{\pm}(\mu\beta)]^{-2/3} \\ \frac{P}{nk_BT_0} &= \frac{g^{\pm}(\mu\beta)}{[h^{\pm}(\mu\beta)]^{5/3}}, \end{aligned} \tag{6.82}$$

where $k_BT_o = \frac{\hbar^2}{ma^2}$, permitting both the pressure and the temperature to be plotted parametrically as a function of $\mu\beta$. Fig 6.7 shows the results of such a plot.

6.5 Exercises for chapter 6

1. (i)Use the Jordan Wigner transformation to show that the one dimensional anisotropic XY model

$$H = -\sum_j [J_1 S_x(i)S_x(i+1) + J_2 S_y(i)S_y(i+1)] \tag{6.83}$$

can be written as

$$H = -\sum_j [t(d^{\dagger}{}_{i+1}d_i + \text{H.c}) + \Delta(d^{\dagger}{}_{i+1}d^{\dagger}{}_i + \text{H.c})] \tag{6.84}$$

where $t = \frac{1}{4}(J_1 + J_2)$ and $\Delta = \frac{1}{4}(J_2 - J_1)$.

(ii)Calculate the excitation spectrum for this model and sketch your results. Comment specifically on the two cases $J_1 = J_2$ and $J_2 = 0$.

2. (a) Consider the non-interacting Hubbard model for next nearest neighbor hopping on a two dimensional lattice

$$H - \mu N = -t \sum_{j,\hat{a}=\hat{x},\hat{y},\sigma} [c^{\dagger}{}_{j+\hat{a}\sigma}c_{j\sigma} + \text{H.c}] - \mu \sum_{j\sigma} c^{\dagger}{}_{j\sigma}c_{j\sigma}$$

where $n_{j\sigma} = c^{\dagger}{}_{j\sigma}c_{j\sigma}$ represents the number of electrons of spin component $\sigma = \pm 1/2$ at site j. Show that the dispersion of the electrons in the absence of interactions is given by

$$\epsilon(\vec{k}) = -2t(\cos k_xa + \cos k_ya) - \mu$$

where a is the distance between sites, and $\vec{k} = (k_x, k_y)$ is the wavevector.

(b) Derive the relation between the number of electrons per site n_e and the area of the Fermi surface.

(c) Sketch the Fermi surface when

i. $n_e < 1$.

ii. "half filling" where $n_e = 1$

(d) The corresponding interacting Hubbard model, with an interaction term $Un_{\uparrow}n_{\downarrow}$ at each site describes a class of material called "Mott insulators", which includes the mother compounds for high temperature superconductors. What feature of the Fermi surface at half-filling makes the non-interacting ground-state unstable to spin density wave formation and the development of a gap around the Fermi surface ?

(e) Derive the dispersion for the case when, in the one-particle Hamiltonian there is an additional next-nearest neighbor hopping matrix element of strength across the diagonal, $-t'$. (Hint: use the Fourier transform of $t(R)$, given by $t(\vec{k}) = \sum_{\vec{R}} t(\vec{R})e^{-i\vec{k}\cdot\vec{R}}$). How does this affect the dispersion at half filling?

3. Consider an atom trap where the confining potential is given by a harmonic potential

$$V(x, y, z) = \frac{1}{2}m\omega^2(x^2 + y^2 + z^2)$$

so that the quantized kinetic energy of an atom in the trap is

$$\begin{aligned} E_{lmn} &= \hbar\omega(l + \frac{3}{2}) \\ l &= n_1 + n_2 + n_3 \end{aligned} \tag{6.85}$$

where $n_{1,2,3} \geq 0$ are non-negative integers.

(a) Show that in thermal equilibtrium, the total number of particles in the trap is given by

$$N = \frac{z}{1-z} + \sum_{l \neq 0} \frac{1}{z^{-1}e^{\beta\hbar\omega l} - 1}$$

where $z = e^{\beta\mu^*}$, $\mu^* = \mu - \frac{3}{2}\hbar\omega$ and the sum over l, denotes a sum over all values of $n_{1,2,3}$. What is the interpretation of the first term? Why must μ^* be negative? What happens to z when condensation develops?

(b) Show that below the Bose Einstein condensation temperature,

$$N = N_0(T) + \sum_{k=1}^{\infty} \left[\left(\frac{1}{1 - e^{-xk}} \right)^3 - 1 \right], \qquad (x = \beta\hbar\omega)$$

where $N_0(T)$ is the number of atoms condensed in the lowest energy state. (Hint, Taylor expand the second term in (a) and then invert the order of summation.)

(c) Show that when x is small,

$$N = N_o(T) + \frac{T^3}{(\hbar\omega)^3}\zeta(3) + \frac{T^2}{(\hbar\omega)^2}\zeta(2) + O(T)$$

where $\zeta(n) = \sum_{k=1}^{\infty} \frac{1}{k^n}$. Notice that if the first term is of order N, the second term is of order $N^{2/3} << N$, if N is large.

(d) Calculate an expression for the Bose Einstein condensation temperature T_{BE} of the trap, and show that to a good approximation,

$$\frac{N_o(T)}{N} = 1 - \left(\frac{T}{T_{BE}} \right)^3.$$

(e) Qualitatively: what do you expect to happen to the density profile across the trap, once the atoms start to condense?

Chapter 7

Greens Functions

Ultimately, we are interested in more than just free systems. We should like to understand what happens to our system as we dial up the interaction strength from zero, to its full value. We also want to know response of our complex systemto external perturbations, such as an electromagnetic field. We have to recognize that we can not, in general expect to diagonalize the problem of interest. We do not even need interactions to make the problem complex: a case in interest is a disordered metal, where we our interest in averaging over typically disordered configurations introduces effects reminiscent of interactions, and can even lead to new kinds of physics, such as electron localization. We need some general way of examinining the change of the system in response to these effects even though we can't diagonalize the Hamiltonian.

In general then, we will be considering problems where we introduce new terms to a non-interaction Hamiltonian, represented by V. The additional term might be due to

- External electromagnetic fields, which modify the Kinetic energy in the Hamiltonian as follows

$$-\frac{\hbar^2}{2m}\nabla^2 \rightarrow -\frac{\hbar^2}{2m}\left(\nabla - i\frac{e}{\hbar}\mathbf{A}\right)^2 \tag{7.1}$$

- Interactions between particles.

$$\hat{V} = \frac{1}{2}\int d\mathbf{1}d\mathbf{2}\psi^{\dagger}(\mathbf{1})\psi^{\dagger}(\mathbf{2})\psi(\mathbf{2})\psi(\mathbf{1}) \tag{7.2}$$

- A random potential

$$\hat{V} = \int d\mathbf{1}V(\mathbf{1})\rho(\mathbf{1}) \tag{7.3}$$

where $V(x)$ is a random function of position.

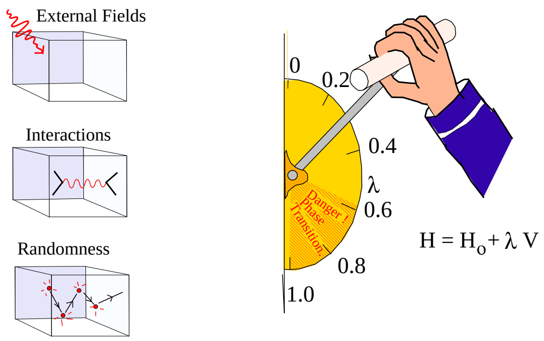


Figure 7.1: "Dialing up the interaction". Motivating the need to be able to treat perturbations to a non-interacting Hamiltonian by dialing up the strength of the perturbation.

One of the things we would like to do, is to examine what happens when we consider the change in the Hamiltonian to small enough to be considered a perturbation. Even if the term of interest is not small, we can still try to make it small by writing

$$H = H_o + \lambda\hat{V} \tag{7.4}$$

This is a useful excercise, for it enables us to consider the effect of adiabatically dialing up the strength of the additional term in the Hamiltonian from zero, to its full value, as illustrated in fig7.1. This is a dangerous procedure, but sometimes it really works. Life is interesting, because in macroscopic systems the perturbation of interest often leads to an instability. This can sometimes occur for arbitrarily small λ. Othertimes, when the instability occurs when the strength of the new term reaches some critical value λ_c. When this happens, the ground-state can change. If the change is a continuous one, then the point where the instability develops is a *Quantum Critical Point*, a point of great interest. Beyond this point, for $\lambda > \lambda_c$, if we are lucky, we can find some new starting $H'_o = H_o + \Delta H$, $\hat{V}' = \hat{V} - \Delta H$. If H'_o is a good description of the ground-state, then we can once again apply this adiabatic procedure, writing,

$$H = H'_o + \lambda'\hat{V}' \tag{7.5}$$

If a phase transition occurs, then H_o' will in all probability have display a spontaneous *broken symmetry*. The region of Hamiltonian space where $H \sim H_o'$ describes a new phase of the system, and H_o' is closely associated with the notion of a "fixed point" Hamiltonian.

All of this discussion motivates us developing a general perturbative approach to many body systems, and this rapidly leads us into the realm of Greens functions and Feynman diagrams. A Green's function describes the elementary correlations and responses of a system. Feynman diagrams are a way of graphically displaying the scattering processes that result from a perturbation.

7.1 Interaction representation

Up until the present, we have known two representations of quantum theory- the Schrödinger representation, where it is the wavefunction that evolves, and the Heisenberg, were the operators evolve and the states are stationary. We are interested in observable quantities more than wavefunctions, and so we aspire to the Heisenberg representation. In practice however, we always want to know what happens if we change the Hamiltonian a little. If we change H_o to H_o+V, but we stick to the Heisenberg representation for H_o, then we are now using the "interaction" representation.

Table. 5.1. Representations .

Representation	States	Operators
Schrödinger	Change rapidly $i\frac{\partial}{\partial t}\vert\psi_S(t)\rangle = H\vert\psi_S(t)\rangle$	O_s- operators constant
Heisenberg	Constant	Evolve $-i\frac{\partial O_H(t)}{\partial t} = [H, O_H(t)]$
Interaction $H = H_o + V$	States change slowly $i\frac{\partial}{\partial t}\vert\psi_I(t)\rangle = V_I(t)\vert\psi_I(t)\rangle$	Evolve according to H_o $-i\frac{\partial O_I(t)}{\partial t} = [H_o, O_I(t)]$

Let us now examine the interaction representation in greater detail. We begin by writing the Hamiltonian as two parts $H = H_o + V$. States and operators in this representation are defined as

$$\left.\begin{aligned} |\psi_I(t)\rangle &= e^{iH_o t}|\psi_S(t)\rangle, \\ O_I(t) &= e^{iH_o t}O_S e^{-iH_o t} \end{aligned}\right\}\text{Removes rapid state evolution due to } H_o \qquad (7.6)$$

The evolution of the wavefunction is thus

$$\left.\begin{aligned} |\psi_I(t)\rangle &= U(t)|\psi_I(0)\rangle, \\ U(t) &= e^{iH_o t}e^{-iHt} \end{aligned}\right] \qquad (7.7)$$

or more generally,

$$\begin{aligned} |\psi_I(t)\rangle &= S(t,t')|\psi_I(t')\rangle, \\ S(t) &= U(t)U^\dagger(t') \end{aligned} \qquad (7.8)$$

The time evolution of $U(t)$ can be derived as follows

$$\begin{aligned} i\frac{\partial U}{\partial t} &= i\left(\frac{\partial e^{iH_o t}}{\partial t}\right)e^{-iHt} + ie^{iH_o t}\left(\frac{\partial e^{-iHt}}{\partial t}\right) \\ &= e^{iH_o t}(-H_o + H)e^{-iHt} \\ &= [e^{iH_o t}Ve^{-iH_o t}]U(t) \\ &= V_I(t)U(t) \end{aligned} \qquad (7.9)$$

so that

$$i\frac{\partial S(t_2,t_1)}{\partial t_1} = V(t_2)S(t_2,t_1) \qquad (7.10)$$

where from now on, all operators are implicitly assumed to be in the interaction representation.

Now we should like to exponenentiate this time-evolution equation, but unfortunately, the operator $V(t)$ is not constant, and furthermore, $V(t)$ at one time, does not commute with $V(t')$ at another time. To overcome this difficulty, Schwinger invented a device called the "time-ordering operator".

> **Time ordering operator** Suppose $\{O_1(t_1), O_2(t_2)\dots O_N(t_N)\}$ is a set of operators at different times $\{t_1, t_2 \dots t_N\}$. If P is the permutation that orders the times, so that $t_{P_1} > t_{P_2}\dots t_{P_N}$, then if the operators are entirely bosonic, containing an even number of fermionic operators,the time ordering operator is defined as
>
> $$T\big[O_1(t_1)O_2(t_2)\dots O_N(t_N)\big] = O_{P_1}(t_{P_1})O_{P_2}(t_{P_2})\dots O_{P_N}(t_{P_N}) \qquad (7.11)$$
>
> For later use, we note that if the operator set contains fermionic operators, composed of an odd number of fermionic operators, then
>
> $$T\big[F_1(t_1)F_2(t_2)\dots F_N(t_N)\big] = (-1)^P F_{P_1}(t_{P_1})F_{P_2}(t_{P_2})\dots F_{P_N}(t_{P_N}) \qquad (7.12)$$
>
> where P is the number of pairwise permutations of fermions involved in the time ordering process.

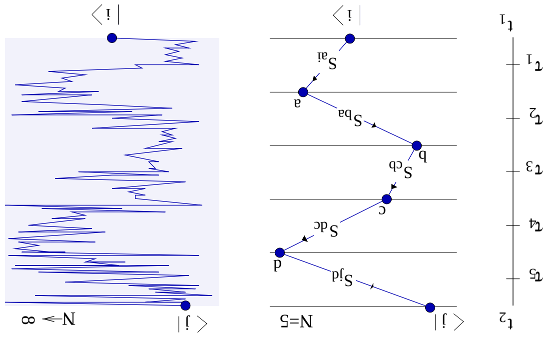


Figure 7.2: Each contribution to the time-ordered exponential corresponds to the amplitude to follow a particular path in state space. The S-matrix is given by the limit of the process where the number of time segments is sent to infinity.

Suppose we divide the time interval $[t_1, t_2]$, where $t_2 > t_1$ into N identical segments of period $\Delta t = (t_2 - t_1)/N$, where the time at the midpoint of the nth segment is $\tau_n = t_1 + (n - \frac{1}{2})\Delta t$. The S-matrix can be written as a product of S-matrices over each intermediate time segment, as follows:

$$S(t_2,t_1) = S(t_2,\tau_N - \tfrac{\Delta t}{2})S(\tau_{N-1} + \tfrac{\Delta t}{2},\tau_{N-1} - \tfrac{\Delta t}{2})\dots S(\tau_1 + \tfrac{\Delta t}{2}, t_1) \qquad (7.13)$$

Provided N is large, then over the short time interval Δt, we can approximate

$$S(\tau + \tfrac{\Delta t}{2}, \tau - \tfrac{\Delta t}{2}) = e^{-iV(\tau)\Delta t} + O(1/N^2) \qquad (7.14)$$

so that we can write

$$S(t_2,t_1) = e^{-iV(\tau_N)\Delta t}e^{-iV(\tau_{N-1})\Delta t}\dots e^{-iV(\tau_1)\Delta t} + O(1/N) \qquad (7.15)$$

Using the time-ordering operator, this can be written

$$S(t_2,t_1) = T[\prod_{j=1}^{N} e^{-iV(\tau_j)\Delta t}] + O(1/N) \qquad (7.16)$$

The beauty of the time-ordering operator, is that even though $A(t_1)$ and $A(t')$ don't commute, we can treat them as commuting operators so long as we always time-order them. This means that we can write

$$T[e^{A(t_1)}e^{A(t_2)}] = T[e^{A(t_1)+A(t_2)}] \qquad (7.17)$$

because in each time-ordered term in the Taylor expansion, we never have to commute operators, so the algebra is the same as for regular complex numbers. With this trick, we can write,

$$S(t_2,t_1) = Lim_{N\to\infty}T[e^{-i\sum_j V(\tau_j)\Delta t}] \qquad (7.18)$$

The limiting value of this time-ordered exponential is written as

$$\boxed{S(t_2,t_1) = T\left[\exp\left\{-i\int_{t_1}^{t_2}V(t)dt\right\}\right], \qquad \textbf{Time-ordered exponential} \qquad (7.19)}$$

This is the famous time-ordered exponential of the interaction representation.

Remarks

- The time-ordered exponential is intimately related to Feynman's notion of the path integral. The time-evolution operator $S(\tau_j + \Delta\tau/2, \tau_j - \Delta\tau/2) = S_{fr}(\tau_j)$ across each segment of time is a matrix that takes one from state r to state f. The total time evolution operator is just a matrix product over each intermediate time segment. Thus the amplitude to go from state i at time t_1 to state f at time t_2 is given by

  $$S_{fi}(t_2,t_1) = \sum_{\text{path}=\{p_1,\dots p_{N_1}\}} S_{f,p_{N-1}}(\tau_N)\dots S_{p_2 p_1}(\tau_2)S_{p_1 i}(\tau_1) \qquad (7.20)$$

  Each term in this sum is the amplitude to go along the path of states

  $$\text{path } i \ \to \ f: \ i \to p_1 \to p_2 \to \dots p_{N-1} \to f. \qquad (7.21)$$

  The limit where the number of segments goes to infinity is a path integral.

- One can formally expand the time-ordered exponential as a power series, writing,

  $$S(t_2,t_1) = \sum_{n=0,\infty}\frac{(-i)^n}{n!}\int_{t_1}^{t_2}d\tau_1\dots d\tau_n T[V(\tau_1)\dots V(\tau_n)] \qquad (7.22)$$

  The nth term in this expansion can be simply interpreted as the amplitude to go from the initial, to the final state, scattering n times off the perturbation V. This form of the S-matrix is very useful in making a perturbation expansion. By explicitly time-ordering the $n-th$ term, one obtains $n!$ identical terms, so that

$$S(t_2,t_1)=\sum_{n=0,\infty}(-i)^n\int_{t_1,\ \{\tau_n>\tau_{n-1}\ldots>\tau_1\}}^{t_2}d\tau_1\ldots d\tau_nV(\tau_n)\ldots V(\tau_1) \tag{7.23}$$

This form for the S-matrix is obtained by iterating the equation of motion,

$$S(t_2,t_1)=1-i\int_{t_1}^{t_2}d\tau V(\tau)S(\tau,t_1) \tag{7.24}$$

which provides an alternative derivation of the time-ordered exponential.

7.1.1 Driven Harmonic Oscillator

To illustrate the concept of the time-ordered exponential, we shall show how it is possible to evaluate the S-matrix for a driven harmonic oscillator, where $H=H_o+V(t)$,

$$\left.\begin{array}{rcl}H_o&=&\omega(b^\dagger b+\frac{1}{2})\\ V(t)&=&\bar z(t)b+b^\dagger z(t)\end{array}\right\} \tag{7.25}$$

Here the forcing terms are written in their most general form. $z(t)$ and $\bar z(t)$ are forces which "create" and "annihilate" quanta respectively. A conventional force in the Hamiltonian, $H=H_o-f(t)\hat x$ gives rise to a particular case, where $\bar z(t)=z(t)=(\hbar/2m\omega)^{\frac{1}{2}}f(t)$. We shall show that if the forcing terms are zero in the distant past and distant future and the system is initially in the ground-state, the amplitude to stay in this state is

$$\boxed{\langle 0|Te^{-i\int_{-\infty}^{\infty}dt[\bar z(t)b(t)+b^\dagger(t)z(t)]}|0\rangle=\exp\left[-i\int_{-\infty}^{\infty}dtdt'\bar z(t)G(t-t')z(t')\right]. \qquad (7.26)}$$

where $G(t-t')=-i\theta(t-t')e^{-i\omega(t-t')}$ is our first example of a one particle "Green's function". The importance of this result, is that we have a precise algebraic result for the response of the ground-state to an arbitrary force term. Once we know the response to an arbitrary force, we can, as we shall see, deduce the n-th ordered moments, or correlation functions of the Bose fields.

Remarks:

- The time-ordered exponential is an example of a "functional": a quantity which is a function of a function (in this case, $z(t)$ and $\bar z(t)$). With this result we can examine how the ground-state responds to an arbitrary external force. The quantity $G(t-t')$ which determines the response of the ground-state to the forces, $z(t)$ and $\bar z(t)$, is called the "one particle Green's function", defined by the relation

$$G(t-t')=-i\langle 0|Tb(t)b^\dagger(t')|0\rangle. \tag{7.27}$$

We may confirm this relation by expanding both sides of (7.26) to first order in $\bar z$ and z. The left hand side gives

$$1+(-i)^2\int dtdt'\bar z(t)\langle 0|Tb(t)b^\dagger(t')|0\rangle.z(t')+O(\bar z^2,z^2) \tag{7.28}$$

whereas the right-hand side gives

$$1-i\int dtdt'\bar z(t)G(t-t')z(t')+O(\bar z^2,z^2) \tag{7.29}$$

By comparing the coefficients, we are able to confirm the above relation.

- By expanding the time-ordered exponential as a power-series in z and $\bar z$, we find that the n-th order term is

$$\frac{(-i)^n}{n!}\int_{-\infty}^{\infty}\prod_{r=1,n}dt_rdt'_r\bar z(t_r)z(t'_r)\times\ \text{coeff} \tag{7.30}$$

where

$$\text{coeff}=G(1,\ldots n;1'\ldots n')=(-i)^n\langle 0|Tb(1)\ldots b(n)b^\dagger(n')\ldots b^\dagger(1')|0\rangle \tag{7.31}$$

is called the n-particle Greens function. Here we have used the conventient notation $r\equiv t_r$, $r'\equiv t'_r$. By expanding the right-hand-side, we find that the corresponding coefficient of z and $\bar z$ is given by the sum over all possible ways of connecting initial times $\{r'\}$ with final times $\{r\}$ by a single-particle Green's function,

$$G(1,\ldots n;1'\ldots n')=\sum_P\prod_r G(r-P'_r), \tag{7.32}$$

a result known as Wick's theorem. It is a remarkable property of non-interacting systems, that the n-particle Green's functions are determined entirely in terms of the one-particle Green functions. In (7.32) each destruction event at time $t_r\equiv r$ is paired up with a corresponding creation event at time $t'_{P_r}\equiv P'_r$. The connection between these two events is often called a "contraction", denoted as follows

$$(-i)^n\langle\phi|T\ldots b(1)\ldots b^\dagger(P'_r)\ldots|\phi\rangle\ \ =G(r-P'_r)\times(-i)^{n-1}\langle 0|T\ldots|0\rangle \tag{7.33}$$

Notice that since particles are conserved, we can only contract a creation operator with a destruction operator. According to Wick's theorem, the expansion of the n-particle Green function in (7.31) is carried out as a sum over all possible contractions, denoted as follows

$$G(1\ldots n')=\sum_P G(1-P'_1)G(2-P'_2)\ldots G(r-P'_r)\ldots$$

$$=\ \sum_P(-i)^n\langle\phi|Tb(1)b(2)\ldots b(r)\ldots b^\dagger(P'_r)\ldots b^\dagger(P'_1)\ldots b^\dagger(P'_2)\ldots|\phi\rangle \tag{7.34}$$

Physically, this result follows from the identical nature of the bosonic quanta or particles. When we take the n particles out at times $t_1\ldots t_n$, there is no way to know in which order we are taking them out. The net amplitude is the sum of all possible ways of taking out the particles- This is the meaning of the sum over permutations P.

- This result can be generalized to an arbitrary number of oscillators by replacing $(z,\ \bar z)\rightarrow(z_r,\bar z_r)$, whereupon

$$\begin{array}{rl}&\langle\ 0|T\exp\left[-i\int_{-\infty}^{\infty}dt[\bar z_r(t)b_r(t)+{b_r}^\dagger(t)z_r(t)]\right]|0\rangle\\ =&\exp\left[-i\int_{-\infty}^{\infty}dtdt'\bar z_r(t)G_{rs}(t-t')z_s(t')\right]\end{array} \tag{7.35}$$

where now, $G_{rs}(t-t')=-i\langle 0|Tb_r(t){b^\dagger}_s(t')|0\rangle=-i\delta_{rs}\theta(t-t')e^{-i\omega_r(t-t')}$, and summation over repeated indices is implied. This provides the general basis for Wick's theorem.

- The concept of a generating functional can also be generalized to Fermions, with the proviso that now we must use replace $(z,\bar z)$ by anticommuting numbers $(\eta,\bar\eta)$.

Proof: To demonstrate this result, we need to evaluate the time ordered exponential

$$\langle\quad 0\quad|T\exp\left[-i\int_{-t_1}^{t_2}dt[\bar z(t)b(t)+b^\dagger(t)z(t)]\right]|0\rangle \tag{7.36}$$

where $b(t)=be^{i\omega t}$ and $b^\dagger(t)=b^\dagger e^{i\omega t}$. To evaluate this integral, we divide up the interval $t\in(t_1,t_2)$ into N segments, $t\in(\tau_j-\Delta\tau/2,\tau_j+\Delta\tau_j)$ of width $\Delta\tau=(t_2-t_1)/N$ and write down the discretized time-ordered exponential as

$$S_N=e^{A_N-{A^\dagger}_N}\times\ldots e^{A_r-{A^\dagger}_r}\times\ldots e^{A_1-{A^\dagger}_1} \tag{7.37}$$

where we have used the short-hand notation,

$$\begin{array}{rcl}A_r&=&-i\bar z(\tau_r)b(\tau_r)\Delta\tau,\\ {A^\dagger}_r&=&ib^\dagger(\tau_r)z(\tau_r)\Delta\tau\end{array} \tag{7.38}$$

To evaluate the ground-state expectation of this exponential, we need to "normal" order the exponential, bringing the terms involving annihilation operators e^{A_r} to the right-hand side of the expression. To do this , we use the result

$$e^{\alpha+\beta}=e^\beta e^\alpha e^{[\alpha,\beta]/2} \tag{7.39}$$

and the related result ,

$$e^\alpha e^\beta=e^\beta e^\alpha e^{[\alpha,\beta]} \tag{7.40}$$

which hold if $[\alpha,\beta]$ commutes with α and β. We observe that in our case, the A_r commute with each other, as do the the ${A^\dagger}_r$. Fortunately, the commutator

$$[A_r,{A^\dagger}_s]=\Delta\tau^2\bar z(\tau_r)z(\tau_s)e^{-i\omega(\tau_r-\tau_s)} \tag{7.41}$$

is a c-number, so we can use the above theorem. We first normal order each term in the product, writing $e^{A_r-{A^\dagger}_r}=e^{-{A^\dagger}_r}e^{A_r}e^{-[A_r,{A^\dagger}_r]/2}$ so that

$$S_N=e^{-{A^\dagger}_N}e^{A_N}\ldots e^{-{A^\dagger}_1}e^{A_1}e^{-\sum_r[A_r,{A^\dagger}_r]/2} \tag{7.42}$$

Now we move the general term e^{A_r} to the right-hand side, picking up the residual commutators along the way to obtain

$$S_N=\overbrace{e^{-\sum_r{A^\dagger}_r}e^{\sum_rA_r}}^{:S_N:}\exp[-\sum_{r\geq s}[A_r,{A^\dagger}_s](1-\frac{1}{2}\delta_{rs})] \tag{7.43}$$

The vacuum expectation value of the first term is unity, so that

$$\begin{array}{rcl}S(t_2,t_1)&=&\lim_{\Delta\tau\rightarrow 0}\exp\left[-\sum_{s\leq r}\Delta\tau^2\bar z(\tau_r)z(\tau_s)e^{-i\omega(\tau_r-\tau_s)}(1-\frac{1}{2}\delta_{rs})\right]\\ &=&\exp\left[-\int_{t_1}^{t_2}d\tau d\tau'\bar z(\tau)\theta(\tau-\tau')e^{-i\omega(\tau-\tau')}z(\tau')\right]\end{array} \tag{7.44}$$

So placing $G(t-t')=-i\theta(\tau-\tau')e^{-i\omega(\tau-\tau')}$,

$$S(t_2,t_1)=\exp\left[-i\int_{t_1}^{t_2}d\tau d\tau'\bar z(\tau)G(t-t')z(\tau')\right] \tag{7.45}$$

Finally, taking the limits of the integral to infinity, we obtain the quoted result.

> **Example:** Show that the probability that a charged particle of charge q in a harmonic potential with mass m and characteristic frequency ω when exposed to an electric field E , remains in the ground-state after time T is given by
>
> $$p=\exp[-4g^2\sin^2(\omega T/2)] \tag{7.46}$$
>
> where ω is the frequency of the oscillator
>
> $$g^2=\frac{V_{spring}}{\hbar\omega} \tag{7.47}$$
>
> is the ratio between the classical energy $V_{spring}=q^2E^2/(2m\omega^2)$ stored in a classical "spring" stretched by a force qE to the quantum of energy $\hbar\omega$.

7.2 Greens Functions

Green's functions are the elementary response functions of a many body system. The one particle Green's function is defined as

$$G_{\lambda\lambda'}(t-t') = -i\langle\phi|T\psi_\lambda(t)\psi^\dagger{}_{\lambda'}(t')|\phi\rangle \tag{7.48}$$

where $|\phi\rangle$ is the <u>true</u> ground-state, $\psi_\lambda(t)$ is the field in the Heisenberg representation and

$$T\psi_\lambda(t)\psi^\dagger{}_{\lambda'}(t') = \left\{\begin{array}{ll} \psi_\lambda(t)\psi^\dagger{}_{\lambda'}(t') & (t > t') \\ \pm\psi^\dagger{}_{\lambda'}(t')\psi_\lambda(t) & (t < t') \end{array}\right. \qquad \pm\left\{\begin{array}{l}\text{Bosons}\\ \text{Fermions}\end{array}\right. \tag{7.49}$$

defines the time-ordering for fermions and bosons. Diagrammatically, this quantity is represented as follows

$$G_{\lambda\lambda'}(t-t') = \overset{\lambda,t}{}\xleftarrow{\qquad\qquad\qquad}\overset{\lambda',t'}{} \tag{7.50}$$

Quite often, we shall be dealing with translationally invariant systems, where λ denotes the momentum and spin of the particle $\lambda \equiv \mathbf{p}\sigma$. If spin is a good quantum number, (no magnetic field, no spin-orbit interactions), then

$$G_{\mathbf{k}\sigma,\mathbf{k}'\sigma'}(t-t') = \delta_{\sigma\sigma'}\delta_{\mathbf{k}\mathbf{k}'}G(\mathbf{k},t-t') \tag{7.51}$$

is diagonal, (where in the continuum limit, $\delta_{\mathbf{k}\mathbf{k}'} \to (2\pi)^D\delta^{(D)}(\mathbf{k}-\mathbf{k}')$). In this case, we denote

$$G(\mathbf{k},t-t') = -i\langle\phi|T\psi_{\mathbf{k}\sigma}(t)\psi^\dagger{}_{\mathbf{k}\sigma}(t')|\phi\rangle = \text{t}\xleftarrow{\qquad\mathbf{k}\qquad}\text{t'} \tag{7.52}$$

We can also define Green's function in real time,

$$G(\mathbf{x}-\mathbf{x}',t) = -i\langle\phi|T\psi_\sigma(\mathbf{x},t)\psi^\dagger{}_\sigma(\mathbf{x}',t')|\phi\rangle \tag{7.53}$$

which we denote diagramatically, by

$$G(\mathbf{x}-\mathbf{x}',t) = \text{(x,t)}\xleftarrow{\qquad\qquad\qquad}\text{(x',t')} \tag{7.54}$$

By writing $\psi_\sigma(\mathbf{x},t) = \int_\mathbf{k}\psi_{\mathbf{k}\sigma}e^{i(\mathbf{k}\cdot\mathbf{x})}$, we see that the real-space Green's function is just the Fourier transform of the momentum-space Green's function:

$$\begin{aligned} G(\mathbf{x}-\mathbf{x}',t) &= \int_{\mathbf{k},\mathbf{k}'} e^{i(\mathbf{k}\cdot\mathbf{x}-\mathbf{k}'\cdot\mathbf{x}')}\overbrace{-i\langle\phi|T\psi_{\mathbf{k}\sigma}(t)\psi^\dagger{}_{\mathbf{k}'\sigma}(0)|\phi\rangle}^{\delta_{\mathbf{k}\mathbf{k}'}G(\mathbf{k},t-t')} \\ &= \int\frac{d^3k}{(2\pi)^3}G(\mathbf{k},t)e^{i\mathbf{k}\cdot(\mathbf{x}-\mathbf{x}')} \end{aligned} \tag{7.55}$$

It is also often convenient to Fourier transform in time, so that

$$G(\mathbf{k},t) = \int_{-\infty}^{\infty}\frac{d\omega}{2\pi}G(\mathbf{k},\omega)e^{-i\omega t} \tag{7.56}$$

The quantity

$$\begin{aligned} G(\mathbf{k},\omega) &= \int_{-\infty}^{\infty}dtG(\mathbf{k},t)e^{i\omega t} \\ &= \xleftarrow{\qquad\mathbf{k,\omega}\qquad} \end{aligned} \tag{7.57}$$

is known as the propagator. We can then relate the Green's function in real space to its propagator, as follows

$$-i\langle\phi|T\psi_\sigma(\mathbf{x},t)\psi_\sigma(\mathbf{x}',t')|\phi\rangle = \int\frac{d^3kd\omega}{(2\pi)^4}G(\mathbf{k},\omega)e^{i[(\mathbf{k}\cdot(\mathbf{x}-\mathbf{x}')-\omega(t-t')]} \tag{7.58}$$

7.2.1 Green's function for free Fermions

As a first example, let us calculate the Green's function of a dengenerate Fermi liquid of non-interacting Fermions in its ground-state. We shall take the heat-bath into account, using a Heisenberg representation where the heat-bath contribution to the energy is subtracted away, so that

$$H = \hat{H}_o - \mu N = \sum_\sigma \epsilon_\mathbf{k}c^\dagger{}_{\mathbf{k}\sigma}c_{\mathbf{k}\sigma}. \tag{7.59}$$

is the Hamiltonian used in the Heisenberg representation and $\epsilon_\mathbf{k} = \frac{p^2}{2m} - \mu$. The ground-state for a fluid of fermions is given by

$$|\phi\rangle = \prod_{\sigma|\mathbf{k}|<k_f} c^\dagger{}_{\mathbf{k}\sigma}|0\rangle \tag{7.60}$$

In the Heisenberg representation, $c^\dagger{}_{\mathbf{k}\sigma}(t) = e^{i\epsilon_\mathbf{k}t}c^\dagger{}_{\mathbf{k}\sigma}$, $c_{\mathbf{k}\sigma}(t) = e^{-i\epsilon_\mathbf{k}t}c_{\mathbf{k}\sigma}$. For forward time propagation, it is only possible to add a fermion above the Fermi energy, and

$$\begin{aligned} \langle\phi|c_{\mathbf{k}\sigma}(t)c^\dagger{}_{\mathbf{k}'\sigma'}(t')|\phi\rangle &= \delta_{\sigma\sigma'}\delta_{\mathbf{k}\mathbf{k}'}e^{-i\epsilon_\mathbf{k}(t-t')}\langle\phi|c_{\mathbf{k}\sigma}c^\dagger{}_{\mathbf{k}\sigma}|\phi\rangle \\ &= \delta_{\sigma\sigma'}\delta_{\mathbf{k}\mathbf{k}'}(1-n_\mathbf{k})e^{-i\epsilon_\mathbf{k}(t-t')} \end{aligned} \tag{7.61}$$

where $n_\mathbf{k} = \theta(|k_F| - |\mathbf{k}|)$. For backward time propagators, it is only possible to destroy a fermion, creating a hole, below the Fermi energy

$$\langle\phi|c^\dagger{}_{\mathbf{k}'\sigma'}(t')c_{\mathbf{k}\sigma}(t)|\phi\rangle = \delta_{\sigma\sigma'}\delta_{\mathbf{k}\mathbf{k}'}n_\mathbf{k}e^{-i\epsilon_\mathbf{k}(t-t')} \tag{7.62}$$

so that

$$G(\mathbf{k},t) = -i[(1-n_\mathbf{k})\theta(t) - n_\mathbf{k}\theta(-t)]e^{-i\epsilon_\mathbf{k}t}$$

$$= \left\{\begin{array}{lll} -i\theta_{|\mathbf{k}|-|\mathbf{k}_F|}e^{-i\epsilon_\mathbf{k}t} & (t>0) & \text{“electrons”} \\ i\theta_{|\mathbf{k}_F|-|\mathbf{k}_F|}e^{-i\epsilon_\mathbf{k}t} & (t<0) & \text{holes = “electrons moving backwards in time”} \end{array}\right. \tag{7.63}$$

This unification of hole and electron excitations in a single function is one of the great utilities of the time-ordered Green's function. [1]

Next, let us calculate the Fourier transform of the Green's function. This is given by

$$\begin{aligned} G(\mathbf{k},\omega) &= -i\int_{-\infty}^{\infty}dte^{i(\omega-\epsilon_\mathbf{k})t}\overbrace{e^{-|t|\delta}}^{\text{cnvgnce factor}}\left[\theta_{k-k_F}\theta(t) - \theta_{k_F-k}\theta(-t)\right] \\ &= -i\left[\frac{\theta_{k-k_F}}{\delta - i(\omega-\epsilon_\mathbf{k})} - \frac{\theta_{k_F-k}}{\delta + i(\omega-\epsilon_\mathbf{k})}\right] = \frac{1}{\omega - \epsilon_\mathbf{k} + i\delta_\mathbf{k}} \end{aligned} \tag{7.64}$$

where $\delta_\mathbf{k} = \text{sign}(\text{k} - \text{k}_\text{F})$. The free fermion propagator is then

$$\boxed{G(\mathbf{k},\omega) = \frac{1}{\omega - \epsilon_\mathbf{k} + i\delta_\mathbf{k}} = \xleftarrow{\qquad\mathbf{k,\omega}\qquad}} \tag{7.65}$$

The Green's function contains both static, and dynamic information about the motion of particles in the many-body system. For example, we can use it to calculate the density of particles in a Fermi gas

$$\begin{aligned} \langle\hat{\rho}(x)\rangle &= \sum_\sigma\langle\psi^\dagger{}_\sigma\psi_\sigma\rangle = -\sum_\sigma\langle\phi|T\psi_\sigma(x,0^-)\psi^\dagger{}_\sigma(x,0)|\phi\rangle \\ &= -i(2S+1)G(\mathbf{x},0^-)|_{\mathbf{x}=0} \end{aligned} \tag{7.66}$$

where S is the spin of the fermion. We can also use it to calculate the Kinetic energy density, which is given as follows

$$\begin{aligned} \langle\hat{T}(x)\rangle &= -\frac{\hbar^2}{2m}\sum_\sigma\langle\psi^\dagger{}_\sigma\nabla_x^2\psi_\sigma(x)\rangle = \frac{\hbar^2\nabla_x^2}{2m}\sum_\sigma\langle\phi|T\psi_\sigma(x,0^-)\psi^\dagger{}_\sigma(\vec{x}',0)|\phi\rangle\Big|_{\mathbf{x}-\mathbf{x}'=0} \\ &= i(2S+1)\frac{\hbar^2\nabla^2}{2m}G(\mathbf{x},0^-)\Big|_{\mathbf{x}=0} \end{aligned} \tag{7.67}$$

---

[1] According to aprocyphyll story, the relativistic counterpart of this notion, that positrons are the electrons travelling backwards in time, was invented by Richard Feynman as a graduate student of John Wheeler. Wheeler was very strict, allowing Feynman precisely half an hour of discussion, and using a chess clock as a timer. When the time was up, Wheeler stopped the clock and announced that the session was over. At the second meeting, when Feynman and Wheeler were discussing the physics of positrons, Feynman arrived with his own clock, and at the end of the half hour, Feynman stopped his own clock, as if to say that his advisors time was up. At the third meeting, having come up with the idea that a positron was an electron travelling backwards in time, Feynman arrived at the meeting with a clock started at 30 minutes and ran backwards to zero!

Example: By relating the particle density and kinetic energy density to one-particle Green's function to the particle density, calculate the particle and kinetic energy density of particles in a degenerate Fermi liquid.

<u>*Solution:*</u> We begin by writing $\langle\hat{\rho}(x)\rangle = -i(2S+1)G(\vec{0},0^-)$. Writing this out explicitly we obtain

$$\langle\rho(x)\rangle = (2S+1)\int\frac{d^3k}{(2\pi)^3}\left[\int\frac{d\omega}{2\pi i}e^{i\omega\delta}\frac{1}{\omega - \epsilon_\mathbf{k} + i\delta_\mathbf{k}}\right] \tag{7.68}$$

where the convergence factor appears because we are evaluating the Green's function at a small negative time $-\delta$. We have explicitly separated out the frequency and momentum integrals. The poles of the propagator are at $\omega = \epsilon_\mathbf{k} - i\delta$ if $k > k_F$, but at $\omega = \epsilon_\mathbf{k} + i\delta$ if $k < k_F$, as illustrated in Fig. 7.3. The convergence factor means that we can calculate the complex integral using Cauchy's theorem by completing the contour in the upper half complex plane, where the integrand dies away exponentially. The pole in the integral will only pick up those poles associated with states below the Fermi energy, so that

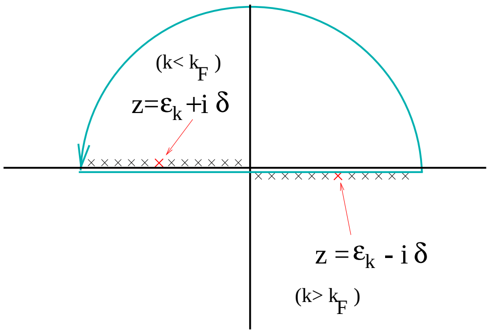


Figure 7.3: Showing how the path of integration in (7.69) picks up the pole contributions from the occupied states beneath the Fermi surface.

$$\int\frac{d\omega}{2\pi i}e^{i\omega\delta}\frac{1}{\omega - \epsilon_\mathbf{k} + i\delta_\mathbf{k}} = \theta_{k_F - |\mathbf{k}|} \tag{7.69}$$

and hence

$$\rho = (2S+1)\int_{k<k_F}\frac{d^3k}{(2\pi)^3} = (2S+1)\frac{V_F}{(2\pi)^3} \qquad (7.70)$$

In a similar way, the kinetic energy density is written

$$\begin{aligned}\langle T(x)\rangle &= (2S+1)\int\frac{d^3k}{(2\pi)^3}\frac{\hbar^2k^2}{2m}\left[\int\frac{d\omega}{2\pi i}e^{i\omega\delta}\frac{1}{\omega-\epsilon_{\mathbf{k}}+i\delta_{\mathbf{k}}}\right]\\ &= (2S+1)\int_{k<k_F}\frac{d^3k}{(2\pi)^3}\frac{\hbar^2k^2}{2m} = \frac{3}{5}\epsilon_F\rho \qquad (7.71)\end{aligned}$$

7.2.2 Green's function for free Bosons

As a second example, let us examine the Green's function of a gas of non-interacting bosons, described by

$$H = \sum_{\mathbf{q}}\omega_{\mathbf{q}}[b^\dagger{}_{\mathbf{q}}b_{\mathbf{q}} + \frac{1}{2}] \qquad (7.72)$$

where physical field operator is related to a sum of creation and annihilation operators:

$$\begin{aligned}\phi(x) &= \int_q \phi_{\mathbf{q}}e^{i\mathbf{q}\cdot\mathbf{x}}\\ \phi_{\mathbf{q}} &= \frac{\hbar}{2m\omega_{\mathbf{q}}}[b_{\mathbf{q}} + b^\dagger{}_{-\mathbf{q}}] \qquad (7.73)\end{aligned}$$

Since there are no bosons present in the ground-state, boson destruction operators annihilate the ground-state $|\phi\rangle$. The only terms contributing to the Green function are then

$$\begin{aligned}-i\langle\phi|Tb_{\mathbf{q}}(t)b^\dagger{}_{\mathbf{q}}(0)|\phi\rangle &= -i\theta(t)e^{-i\omega_{\mathbf{q}}t},\\ -i\langle\phi|Tb^\dagger{}_{-\mathbf{q}}(t)b_{-\mathbf{q}}(0)|\phi\rangle &= -i\theta(-t)e^{i\omega_{\mathbf{q}}t}, \qquad (7.74)\end{aligned}$$

so that

$$D(\mathbf{q},t) = -i\langle\phi|\phi(\mathbf{q},t)\phi(-\mathbf{q},t)|\phi\rangle = -i\frac{\hbar}{2m\omega_{\mathbf{q}}}[\theta(t)e^{-i\omega_{\mathbf{q}}t} + \theta(-t)e^{i\omega_{\mathbf{q}}t}] \qquad (7.75)$$

If we Fourier transform this quantity, we obtain the boson propgator,

$$\begin{aligned}D(\mathbf{q},\nu) &= \int_{-\infty}^{\infty}dte^{-\delta|t|+i\nu t}D(\mathbf{q},t)\\ &= -i\frac{\hbar}{2m\omega_{\mathbf{q}}}\left[\frac{1}{\delta-i(\nu-\omega_{\mathbf{q}})} + \frac{1}{\delta+i(\nu-\omega_{\mathbf{q}})}\right] \qquad (7.76)\end{aligned}$$

or

$$\boxed{D(\mathbf{q},\nu) = \frac{\hbar}{2m\omega_{\mathbf{q}}}\left[\frac{2\omega_{\mathbf{q}}}{\nu^2-(\omega_{\mathbf{q}}-i\delta)^2}\right], \qquad \text{Bose propagator} \qquad (7.77)}$$

Remarks:

- Note that the bose propagator has two poles at $\nu = \pm(\omega - i\delta)$. You can think of the bose propagator as a sum of two terms, one involving a boson emission, the other involving boson absorption.

$$D(\mathbf{q},\nu) = \frac{\hbar}{2m\omega_{\mathbf{q}}}\left[\overbrace{\frac{1}{\nu-(\omega_{\mathbf{q}}-i\delta)}}^{\text{emission}} + \overbrace{\frac{1}{-\nu-(\omega_{\mathbf{q}}-i\delta)}}^{\text{absorption}}\right] \qquad (7.78)$$

- We shall shortly see that amplitude to absorb and emit bosons by propagating fermions is directly related to the Boson propagator. For example, when there is an interaction of the form

$$H_{int} = g\int d^3x\phi(\mathbf{x})\rho(\mathbf{x}) \qquad (7.79)$$

The exchange of virtual bosons between particles gives rise to *retarded* interactions,

$$V(\mathbf{q},t-t') = \frac{g^2}{\hbar}D(\mathbf{q},t-t'), \qquad (7.80)$$

whereby a passing fermion produces a the potential change in the environment which lasts lasts a characteristic time $\Delta\tau \sim 1/\omega_o$ where ω_o is the characteristic value of $\omega_{\mathbf{q}}$. From the Fourier transform of this expression, you can see that at long times, this interaction becomes negative, i.e. attractive.

7.3 Adiabatic concept

The adiabatic concept is one of the most valuable concepts in many body theory. What does it mean to understand a many body problem when we can never, except in the most special cases, expect to solve the problem exactly? The adiabatic concept provides an answer to this question.

Suppose we are interested in a many body problem with Hamiltonian H, with ground-state $|\Psi_g\rangle$ which we can not solve exactly. Instead we can often solve a simplified version of the many body Hamiltonian H_o where the ground-state $|\tilde\Psi_g\rangle$ has the same *symmetry* as $|\Psi_g\rangle$. Suppose we start in the ground-state $|\tilde\Psi_g\rangle$, and now slowly evolve the Hamiltonian

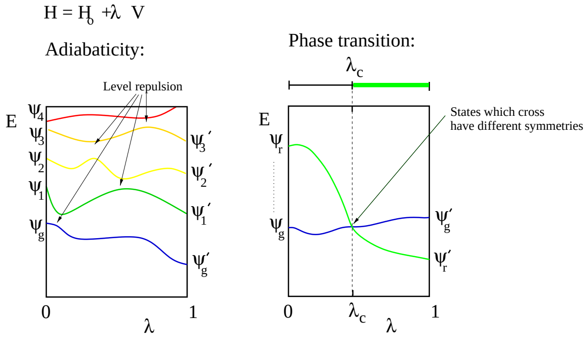


Figure 7.4: Illustrating the evolution of the Hilbert space as the Hamiltonian is adiabatically evolved. In the first case, the ground-state can be adiabatically evolved all the way to $\lambda = 1$. In the second case, a phase transition occurs at $\lambda = \lambda_c$, where a previously excited state, with a different symmetry to the ground-state crosses below the ground-state.

from H_o to H, i.e, if $\hat V = H - H_o$, we imagine that the state time-evolves according to the Hamiltonian

$$\begin{aligned}H(t) &= H_o + \lambda(t)V\\ \lambda(t) &= e^{-|t|\delta} \qquad (7.81)\end{aligned}$$

where δ is arbitrarily small.

As we adiabatically evolve the system, the ground-state, and excited states will evolve, as shown in Fig. 7.4. In such an evolution process, the energy levels will typically show "energy level repulsion". If any two levels get too close together, matrix elements between the two states will cause them to repel one-another. However, it is possible for states of different symmetry to cross, because selection rules prevent them from mixing. Sometimes, such an adiabatic evolution will lead to "level crossing", whereby at $\lambda = \lambda_c$ when some excited state ψ_r with different symmetry to the ground-state, crosses to a lower energy than the ground-state. Such a situation leads to "spontaneous symmetry breaking". A simple example is when a Ferromagnetic ground-state becomes stabilized by interactions.

In general however, if there is no symmetry changing phase transition as the interaction V is turned on, the procedure of adiabatic evolution, can be used to turn on "interactions", and to evolve the ground-state from $\tilde\Psi_g$ to Ψ_g.

These ideas play a central role in the development of perturbation theory and Feynman diagrams. They are however also of immense qualitative importance, for the physics of adiabatically related ground-states is equivalent. Adiabatic evolution defines an equivalence class of ground-states with the same qualitative physics. The adiabatic principle was first employed with great success in the fifties. Gell Mann and Lowe used it to prove their famous relation linking non-interacting, and interacting Green's functions. Around the same time, Landau used the adiabatic idea in a brilliantly qualitative fashion, to formulate his theory of interacting Fermi liquids. We will now look at both applications of the adiabatic principle.

7.3.1 Gell-Man Lowe Theorem

Suppose we turn on an interaction $V(t)$ in the distant past. Let the interaction and Heisenberg representations coincide at $t = -\infty$. The Gell Man Lowe formula states that

$$\boxed{\begin{aligned}\langle 0|TA(t_1)B(t_2)\dots R(t_r)|0\rangle_H &= \langle +\infty|TS[\infty,-\infty]A(t_1)B(t_2)\dots R(t_r)|-\infty\rangle_I\\ S[\infty,-\infty] &= T\exp\Big[-i\int_{-\infty}^{\infty}V(t')dt'\Big] \qquad (7.82)\end{aligned}}$$

where the subscript H and I indicate that the operators, and states are to be evaluated in the Heisenberg and interaction representations, respectively, and $\hat V(t) = e^{-\epsilon|t|}V$, where ϵ is infinitesimal, is the part of the Hamiltonian that is slowly turned on, then later allowed to revert back to zero. The states $|0\rangle_H \equiv |-\infty\rangle_I$ correspond to the Heisenberg ground-state at time $t = -\infty$. The state $|+\infty\rangle$ corresponds to the ground-state, in the interaction representation in the distant future. If adiabaticity holds, then the process of slowly turning on, and then turning off the interaction, will return the system to to its original state. If this is the case, then $|+\infty\rangle = e^{2i\delta}|-\infty\rangle$, so that

$$\langle +\infty| = \frac{\langle -\infty|}{\langle -\infty|+\infty\rangle} \qquad (7.83)$$

and the Gell-Mann Lowe formula becomes

$$\boxed{\langle 0|TA(t_1)B(t_2)\dots R(t_r)|0\rangle_H = \frac{\langle -\infty|TS[\infty,-\infty]A(t_1)B(t_2)\dots R(t_r)|-\infty\rangle_I}{\langle -\infty|S[\infty,-\infty]|-\infty\rangle} \qquad (7.84)}$$

Remarks:

- The second Gell-Mann Lowe relation is the starting point for the Feynman diagram expansion of Green's functions. When we expand the time-ordered exponential as a power-series in V, each term in the expansion corresponds to a particular Feynman diagram.

- When we expand the vacuum expectation value of the S-matrix, we will see that this leads to "Linked Cluster" diagrams.

Proof: To prove this result, let $S(t,-\infty)$ be the time-evolution operator for the interaction representation. Since the interaction, and Heisenberg states coincide at $t=-\infty$, and $|\psi_H\rangle$ does not evolve with time,

$$|\psi_I(t)\rangle = U(t)|\psi_H\rangle \tag{7.85}$$

Since $U(t)A_H(t)|\psi_H\rangle = A_I(t)|\psi_I(t)\rangle = A_I(t)U(t)|\psi_H\rangle$, the relation between operators in the two representations must be

$$A_H(t) = U^\dagger(t)A_IU(t) \tag{7.86}$$

Suppose $t_1 > t_2 > t_3 \dots t_r$, then using this relation we may write

$$\langle 0|A(t_1)\dots R(t_r)|0\rangle_H = \langle -\infty|U^\dagger(t_1)A_I(t_1)\overbrace{U(t_1)U^\dagger(t_2)}^{S(t_1,t_2)}\dots\overbrace{U(t_{r-1})U^\dagger(t_r)}^{S(t_{r-1},t_r)}R_I(t_r)U(t_r)|-\infty\rangle$$

where we have identified $|0\rangle_H \equiv |-\infty\rangle$. Now $S(t_1,t_2) = U(t_1)U^\dagger(t_2)$ is the operator that time evolves the states of the interaction representation, so we may rewrite the above result as

$$\langle 0|A(t_1)\dots R(t_r)|0\rangle_H = \langle -\infty|\ \overbrace{U^\dagger(t_1)}^{S^\dagger(t_1,-\infty)}\ A_I(t_1)S(t_1,t_2)\dots S(t_{r-1},t_r)R_I(t_r)\ \overbrace{U(t_r)}^{S(t_r,-\infty)}\ |-\infty\rangle$$

where we have replaced $U(t)\to S(t,\infty)$. Now $S(\infty,t_1)S(t_1,-\infty)|-\infty\rangle = |\infty\rangle$ and since S is a unitary matrix, $S^\dagger(\infty,t_1)S(\infty,t_1)=1$, so multiplying both sides by $S^\dagger(\infty,t_1)$, $S(t_1,-\infty)|-\infty\rangle = S^\dagger(\infty,t_1)|\infty\rangle$ and by taking its complex conjugate,

$$\langle -\infty|S^\dagger(t_1,-\infty) = \langle\infty|S(\infty,t_1) \tag{7.87}$$

Inserting this into the above expression gives,

$$\langle 0|A(t_1)\dots R(t_r)|0\rangle_H = \langle +\infty|S(\infty,t_1)A_I(t_1)S(t_1,t_2)\dots S(t_{r-1},t_r)R_I(t_r)S(t_r,-\infty)|-\infty\rangle$$

Finally, since we assumed $t_1 > t_2 > \dots t_r$, we can write,

$$\langle 0|T[A(t_1)\dots R(t_r)]|0\rangle_H = \langle +\infty|T[S(\infty,-\infty)A_I(t_1)B(t_2)\dots R_I(t_r)]|-\infty\rangle \tag{7.88}$$

Although we proved this expression for a particular time-ordering, it is clear that if we permute the operators the time-ordering will always act to time-order both sides, and thus this expression holds for an arbitary time-ordering of operators.

7.3.2 Generating Function for Free fermions

The generating function derived for the harmonic oscillator can be generalized to free fermions by the use of "anticommuting" or Grassman numbers η and η. The simplest model is

$$\left.\begin{array}{rcl} H &=& \epsilon c^\dagger c \\ V(t) &=& \bar\eta(t)c(t) + c^\dagger(t)\eta(t) \end{array}\right\} \tag{7.89}$$

The corresponding Generating functional is given by

$$\boxed{\begin{array}{rcl} S[\bar\eta,\eta] = \langle\phi|T\exp -i\int dt\left[\bar\eta(t)c(t)+c^\dagger(t)\eta(t)\right]|\phi\rangle &=& \exp\left[-i\int d1d2\bar\eta(1)G(1-2)\eta(2)\right] \\ G(1-2) &=& -i\langle\phi|Tc(1)c^\dagger(2)|\phi\rangle \qquad (7.90) \end{array}}$$

where $|\phi\rangle$ is the ground-state for the non-interacting Hamiltonian. To prove this result, we use the same method as used for the harmonic oscillator. As before we split up the S matrix into N discrete time-slices, writing

$$S_N = e^{A_N - A^\dagger{}_N}\times\dots e^{A_r - A^\dagger{}_r}\times\dots e^{A_1-A^\dagger{}_1} \tag{7.91}$$

where

$$\begin{array}{rcl} A_r &=& \bar\eta(t_r)(-ice^{-i\epsilon t_r})\Delta t, \\ A^\dagger{}_r &=& \eta(t_r)(ic^\dagger e^{i\epsilon t_r})\Delta t. \end{array} \tag{7.92}$$

The next step requires a little care, for when $\epsilon < 0$, $|\phi\rangle = c^\dagger|0\rangle$ is the vacuum for holes $h = c^\dagger$, rather than particles, so that in this case we need to "anti-normal order" the S matrix. Carrying out the ordering process, we obtain

$$S_N = \begin{cases} e^{-\sum_r A^\dagger{}_r}e^{\sum_r A_r}\exp\left[-\sum_{r\geq s}[A_r,A^\dagger{}_s](1-\frac{1}{2}\delta_{rs})\right] & (\epsilon>0) \\ e^{\sum_r A_r}e^{-\sum_r A^\dagger{}_r}\exp\left[\sum_{r\leq s}[A_r,A^\dagger{}_s](1-\frac{1}{2}\delta_{rs})\right] & (\epsilon<0) \end{cases} \tag{7.93}$$

When we take the expectation value $\langle\phi|S_N|\phi\rangle$, the first term in these expressions gives unity. Calculating the commutators, in the exponent, we obtain

$$\begin{array}{rcl} [A_r,A^\dagger{}_s] &=& \Delta t^2[\bar\eta(t_r)c, c^\dagger\eta(t_s)]e^{-i\epsilon(t_r-t_s)} \\ &=& \Delta t^2\bar\eta(t_r)\{c,c^\dagger\}\eta(t_s)e^{-i\epsilon(t_r-t_s)} \\ &=& \Delta t^2\bar\eta(t_r)\eta(t_s)]e^{-i\epsilon(t_r-t_s)}. \end{array} \tag{7.94}$$

(Notice how the anticommuting property of the Grassman variables $\bar\eta(t_r)\eta(t_s) = -\eta(t_s)\bar\eta(t_r)$ means that we can convert a commutator of $[A_r, A_s]$ into an anticommutator $\{c, c^\dagger\}$.) Next,

that taking the limit $N\to\infty$, we obtain

$$S[\bar\eta,\eta] = \begin{cases} \exp\left[-\int_{-\infty}^{\infty}dtdt'\bar\eta(t)\theta(t-t')\eta(t')e^{-i\epsilon(t-t')}\right] & (\epsilon>0) \\ \exp\left[\int_{-\infty}^{\infty}d\tau d\tau'\bar\eta(\tau)\theta(t'-t)\eta(\tau')e^{-i\epsilon(t-t')}\right] & (\epsilon<0) \end{cases} \tag{7.95}$$

By introducing the Green function,

$$G(t) = -i\left[(1-f(\epsilon))\theta(t) - f(\epsilon))\theta(-t)\right]e^{-i\epsilon t}$$

we can compactly combine these two results into the final form

$$S(t_2,t_1) = \exp\left[-i\int_{-\infty}^{\infty}dtdt'\bar\eta(t)G(t-t')\eta(t')\right]. \tag{7.96}$$

A more heuristic derivation however, is to recognized that derivatives of the generating functional bring down fermi operators inside the time-ordered exponential,

$$\begin{array}{rcl} i\dfrac{\delta}{\delta\eta(t)}\langle\phi|T\hat S\dots|\phi\rangle &=& \langle\phi|T\hat Sc^\dagger(t)\dots|\phi\rangle \\ i\dfrac{\delta}{\delta\bar\eta(t)}\langle\phi|T\hat S\dots|\phi\rangle &=& \langle\phi|T\hat Sc(t)\dots|\phi\rangle \end{array} \tag{7.97}$$

where $\hat S = T\exp\left[-i\int dt'\left(\bar\eta(t')c(t') + c^\dagger(t')\eta(t')\right)\right]$ so that inside the expectation value,

$$\begin{array}{rcl} i\dfrac{\delta}{\delta\eta(t)} &\equiv& c^\dagger(t) \\ i\dfrac{\delta}{\delta\bar\eta(t)} &\equiv& c(t), \end{array} \tag{7.98}$$

and

$$i\frac{\delta\ln S}{\delta\eta(1)} = \frac{\langle\phi|Tc^\dagger(1)\hat S|\phi\rangle}{\langle\phi|\hat S|\phi\rangle} \equiv \langle c^\dagger(1)\rangle, \tag{7.99}$$

where $\hat S = T\exp\left[-i\int V(t')dt'\right]$. Here, we have used the Gell-Mann Lowe theorem to identify the quotient above as the expectation value for $c^\dagger(1)$ in the presence of the source terms. Differentiating one more time,

$$\begin{array}{rcl} (i)^2\dfrac{\delta^2\ln S[\bar\eta,\eta]}{\delta\bar\eta(2)\delta\eta(1)} &=& \dfrac{\langle\phi|Tc^\dagger(2)c^\dagger(1)\hat S|\phi\rangle}{\langle\phi|\hat S|\phi\rangle} - \dfrac{\langle\phi|Tc(2)\hat S|\phi\rangle}{\langle\phi|\hat S|\phi\rangle}\dfrac{\langle\phi|Tc^\dagger(1)\hat S|\phi\rangle}{\langle\phi|\hat S|\phi\rangle} \\ &=& \langle Tc(2)c^\dagger(1)\rangle - \langle c(2)\rangle\langle c^\dagger(1)\rangle \\ &=& \langle T\delta c(2)\delta c^\dagger(1)\rangle. \end{array} \tag{7.100}$$

This quantity describes the variance in the fluctuations $\delta c^{(\dagger)}(2) \equiv c^{(\dagger)}(2) - \langle c^{(\dagger)}(2)\rangle$ of the fermion field about their average value. When the source terms η and $\bar\eta$ are introduced, they will change the average values of the fields $\langle c(1)\rangle$ and $\langle c^\dagger(1)\rangle$ but the absence of interactions between the modes mean they won't change the amplitude of fluctuations about the mean, so that

$$(i)^2\frac{\delta^2\ln S[\bar\eta,\eta]}{\delta\bar\eta(2)\delta\eta(1)} = \langle Tc(1)c^\dagger(2)\rangle\Big|_{\eta,\ \bar\eta=0} = iG(1-2),$$

and we can then deduce that

$$\ln S[\bar\eta,\eta] = -i\int d1d2\bar\eta(2)G(2-1)\eta(1). \tag{7.101}$$

There is no constant term, because $S=1$ when the source terms are removed, and we arrive back at (refwick00).

The generalization of the generating functional to a gas of Fermions with many one-particle states is just a question of including an appropriate sum over one-particle states, i.e

$$\left.\begin{array}{rcl} H &=& \sum_\lambda \epsilon_\lambda c^\dagger{}_\lambda c_\lambda \\ V(t) &=& \sum_\lambda \bar\eta_\lambda(t)c_\lambda(t) + c_\lambda{}^\dagger(t)\eta_\lambda(t) \end{array}\right\} \tag{7.102}$$

The corresponding Generating functional is given by

$$\boxed{\begin{array}{rcl} S[\bar\eta,\eta] = \langle\phi|T\exp\left[-i\int dtV(t)\right]|\phi\rangle &=& \exp\left[-i\sum_\lambda\int d1d2\bar\eta_\lambda(1)G_\lambda(1-2)\eta_\lambda(2)\right] \\ G_\lambda(1-2) &=& -i\langle\phi|Tc_\lambda(1)c^\dagger{}_\lambda(2)|\phi\rangle \qquad (7.103) \end{array}}$$

Example: Show using the generating function, that in the presence of a source term,

$$\langle c_\lambda(t')\rangle = \int dt'G_\lambda(t-t')\eta(t').$$

7.3.3 The Spectral Representation

In the non-interacting Fermi liquid, we saw that the propagator contained a single pole, at $\omega = \epsilon_{\mathbf{k}}$. What happens to the propagator when we turn on the interactions? Remarkably it retains its same general analytic structure, excepting that now, the single pole divides into a plethora of poles, each one corresponding to an excitation energy for adding, or removing a particle from the ground-state. The general result, is that

$$G(\mathbf{k},\omega) = \sum_\lambda\frac{|M_\lambda|^2}{\omega-\epsilon_\lambda+i\delta_\lambda} \tag{7.104}$$

where $\delta_\lambda = \delta \mathrm{sign}(\epsilon_\lambda)$ and the total pole strength

$$\sum_\lambda |M_\lambda|^2 = 1 \tag{7.105}$$

is unchanged. If the ground-state is an N particle state, then the state $|\lambda\rangle$ is either an $N+1$, or $N-1$ particle state. The corresponding excitation energies are

$$\epsilon_\lambda = \begin{cases} E_\lambda - E_g & (|\lambda\rangle \in |N+1\rangle) \\ E_g - E_\lambda & (|\lambda\rangle \in |N-1\rangle) \end{cases} \tag{7.106}$$

and the corresponding matrix elements are

$$M_\lambda = \begin{cases} \langle\lambda|c^{\dagger}{}_{\mathbf{k}\sigma}|\phi\rangle, & (|\lambda\rangle \in |N+1\rangle), \\ \\ \langle\lambda|c_{\mathbf{k}\sigma}|\phi\rangle, & (|\lambda\rangle \in |N-1\rangle). \end{cases} \tag{7.107}$$

In practice, the poles in the interacting Green function blur into a continuum of excitation energies, with an infinitesimal separation. To deal with this situation, we define a quantity known as the spectral function, given by the imaginary part of the Green's function,

$$A(\mathbf{k},\omega) = \frac{1}{\pi}\mathrm{Im}G(\mathbf{k},\omega - i\delta), \qquad \textbf{Spectral Function} \tag{7.108}$$

Using the Cauchy's principle part equation, $1/(x-i\delta) = P(1/x) + i\pi\delta(x)$, where P denotes the principal part, we can use the spectral representation (7.104) to write

$$A(\mathbf{k},\omega) = \sum |M_\lambda|^2 \delta(\omega - \epsilon_\lambda) \tag{7.109}$$

where now, the normalization of the pole-strengths means that

$$\int_{-\infty}^{\infty} A(\mathbf{k},\omega)d\omega = \sum_\lambda |M_\lambda|^2 = 1 \tag{7.110}$$

Since the excitation energies are always positive, ϵ_λ is positive for electron states and negative for electron states, so

$$A(\mathbf{k},\omega) = \theta(\omega)\rho_e(\mathbf{k},\omega) + \theta(-\omega)\rho_h(\mathbf{k},-\omega) \tag{7.111}$$

where $\rho_e(\omega)$ and $\rho_h(\omega)$ are the spectral functions for adding or holes of energy ω to the system respectively. To a good approximation, in high energy spectroscopy, $\rho_{e,h}(\mathbf{k},\omega)$ is directly proportional to the cross-section for adding, or removing an electron of energy $|\omega|$ to the material. Photoemission and inverse photoemission experiments can, in this way, be used to directly measure the spectral function of electronic systems.

To derive this spectral decomposition, we imagine that we know the complete Hilbert space of energy eigenstates $\{|\lambda\rangle\}$. By injecting the completeness relation $\sum |\lambda\rangle\langle\lambda| = 1$

between the creation and annihilation operators in the Green's function, we can expand it as follows

$$G(\mathbf{k},t) \quad = \quad -i\sum_\lambda \Big[\langle\phi|c_{\mathbf{k}\sigma}(t)\overbrace{|\lambda\rangle\langle\lambda|}^{=1}c^{\dagger}{}_{\mathbf{k}\sigma}(0)|\phi\rangle\theta(t) + i\langle\phi|c^{\dagger}{}_{\mathbf{k}\sigma}(0)\overbrace{|\lambda\rangle\langle\lambda|}^{=1}c_{\mathbf{k}\sigma}(t)|\phi\rangle\theta(-t)\Big]$$

By using energy eigenstates, we are able to write

$$\begin{aligned} \langle\phi|c_{\mathbf{k}\sigma}(t)|\lambda\rangle &= \langle\phi|e^{iHt}c_{\mathbf{k}\sigma}e^{-iHt}|\lambda\rangle = \langle\phi|c_{\mathbf{k}\sigma}|\lambda\rangle e^{i(E_g-E_\lambda)t} \\ \langle\lambda|c_{\mathbf{k}\sigma}(t)|\phi\rangle &= \langle\lambda\phi|e^{iHt}c_{\mathbf{k}\sigma}e^{-iHt}|\phi\rangle = \langle\lambda|c_{\mathbf{k}\sigma}|\phi\rangle e^{i(E_\lambda-E_g)t} \end{aligned} \tag{7.112}$$

Notice that the first term involves adding a particle of momentum $\mathbf{k}$, spin σ, so that the state $|\lambda\rangle = |N+1; \mathbf{k}\sigma\rangle$ is an energy eigenstate with $N+1$ particles, momentum $\mathbf{k}$ and spin σ. Similarly, in the second matrix element, a particle of momentum $\mathbf{k}$, spin σ has been *subtracted*, so that $|\lambda\rangle = |N-1; -\mathbf{k} \ -\sigma\rangle$. We can thus write the Greens function in the form:

$$G(\mathbf{k},t) \quad = \quad -i\sum_\lambda \Big[|\langle\lambda|c^{\dagger}{}_{\mathbf{k}\sigma}|\phi\rangle|^2 e^{-i(E_\lambda-E_g)t}\theta(t) - |\langle\lambda|c_{\mathbf{k}\sigma}|\phi\rangle|^2 e^{-i(E_g-E_\lambda)t}\theta(-t)\Big],$$

where we have simplified the expression by writing $\langle\phi|c_{\mathbf{k}\sigma}|\lambda\rangle = \langle\lambda|c^{\dagger}{}_{\mathbf{k}\sigma}|\phi\rangle^*$ and $\langle\lambda|c_{\mathbf{k}\sigma}|\phi\rangle = \langle\phi|c^{\dagger}{}_{\mathbf{k}\sigma}|\lambda\rangle^*$. This has precisely the same structure as a non-interacting Greens function, except that $\epsilon_{\mathbf{k}} \rightarrow E_\lambda - E_g$ in the first term, and $\epsilon_{\mathbf{k}} \rightarrow E_g - E_\lambda$ in the second term. We can use this observation to quickly carry out the Fourier transform, whereapon

$$G(\mathbf{k},\omega) \quad = \quad \sum_\lambda \left[\frac{|\langle\lambda|c^{\dagger}{}_{\mathbf{k}\sigma}|\phi\rangle|^2}{\omega - (E_\lambda - E_g)) + i\delta} + \frac{|\langle\lambda|c_{\mathbf{k}\sigma}|\phi\rangle|^2}{\omega - (E_g - E_\lambda) - i\delta}\right]$$

which is the formal expansion of the result quoted above.

To show that the total pole-strength is unchanged by interactions, we expand the sum over pole strengths, and then use completeness again, as follows

$$\begin{aligned} \sum_\lambda |M_\lambda|^2 &= \sum_\lambda |\langle\lambda|c^{\dagger}{}_{\mathbf{k}\sigma}|\phi\rangle|^2 + |\langle\lambda|c_{\mathbf{k}\sigma}|\phi\rangle|^2 \\ &= \sum_\lambda \langle\phi|c_{\mathbf{k}\sigma}\overbrace{|\lambda\rangle\langle\lambda|}^{=1}c^{\dagger}{}_{\mathbf{k}\sigma}|\phi\rangle + \langle\phi|c^{\dagger}{}_{\mathbf{k}\sigma}\overbrace{|\lambda\rangle\langle\lambda|}^{=1}c_{\mathbf{k}\sigma}|\phi\rangle \\ &= \langle\phi|\overbrace{\{c_{\mathbf{k}\sigma}, c^{\dagger}{}_{\mathbf{k}\sigma}\}}^{=1}|\phi\rangle = 1 \end{aligned} \tag{7.113}$$

7.4 Many particle Green's functions

The n-particle Green's function determines the amplitude for n-particles to go from one starting configuration to another:

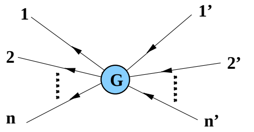
$$\overbrace{\{1', 2' \dots n'\}}^{\text{initial particle positions}} \quad \xrightarrow{G} \quad \overbrace{\{1', 2' \dots n'\}}^{\text{final particle positions}} \tag{7.114}$$

where $1' \equiv (\mathbf{x}', t')$, *etc.* and $1 \equiv (\mathbf{x}, t)$, *etc.*. The n-particle Green's function is defined as

$$\boxed{G(1,2,\dots n; 1', 2', \dots n') = (-i)^n \langle\phi|T\psi(1)\psi(2)\dots\psi(n)\psi^\dagger(n')\dots\psi^\dagger(1')|\phi\rangle}$$

and represented diagramatically as

$G(1,2,\dots n; 1', 2', \dots n') =$



(7.115)

In systems without interactions, the n-body Green's function can always be decomposed in terms of the one-body Green's function, a result known as "Wick's theorem". This is because particles propagate without scattering off one-another. Suppose a particle which ends up at $\mathbf{r}$ comes from location P'_r, where P_r is the r-th element of a permutation P of $(1, 2, \dots n)$. The amplitude for this process is

$$G(\mathbf{r} - P'_{\mathbf{r}}) \tag{7.116}$$

and the overall amplitude for all n-particles to go from locations P'_r to positions r is then

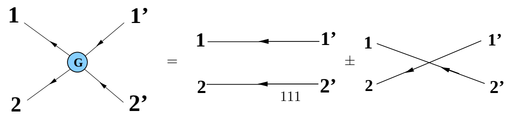
$$\zeta^p G(1 - P'_1)G(2 - P'_2)\dots G(n - P'_n) \tag{7.117}$$

where $\zeta = \pm$ for bosons (+) and fermions (-) and p is the number of pairwise permutations required to make the permutation P. This prefactor arises because for fermions, every time we exchange two of them, we pick up a minus sign in the amplitude. Wick's theorem states the physically reasonable result that the n-body Green's function of a non-interacting system is given by the sum of all such amplitudes:

$$G(\mathbf{1},\mathbf{2},\dots\mathbf{n};\mathbf{1}',\mathbf{2}',\dots\mathbf{n}') = \sum \zeta^P \prod_{r=1,n} G(\mathbf{r} - P'_r) \tag{7.118}$$

For example, the two-body Green's function is given by

$$G(\mathbf{1},\mathbf{21}',\mathbf{2}') \quad = \quad G(\mathbf{1},\mathbf{1}')G(\mathbf{2},\mathbf{2}') \pm G(\mathbf{1},\mathbf{2}')G(\mathbf{2},\mathbf{1}')$$



The process of identifying pairs of initial, and final states in the n-particle Green's function is often referred to as a "contraction". When we contraction two field operators inside a Green's function, we associate an amplitude with the contraction as follows

$$\langle 0|T[\dots\psi(\mathbf{1})\dots\psi^\dagger(\mathbf{2})\dots]|0\rangle \quad \longrightarrow \quad \langle 0|T[\psi(\mathbf{1})\psi^\dagger(\mathbf{2})]|0\rangle = iG(\mathbf{1}-\mathbf{2})$$

$$\langle 0|T[\dots\psi^\dagger(\mathbf{2})\dots\psi(\mathbf{1})\dots]|0\rangle \quad \longrightarrow \quad \langle 0|T[\psi^\dagger(\mathbf{2})\psi(\mathbf{1})]|0\rangle = \pm iG(\mathbf{1}-\mathbf{2})$$

Each product of Green's functions in the Wick-expansion of the propagator is a particular "contraction" of the n-body Green's function, thus

$$\begin{aligned} &\langle 0|T[\psi(\mathbf{1})\psi(\mathbf{2})\dots\psi(\mathbf{n})\dots\psi^\dagger(\mathbf{P'_2})\dots\psi^\dagger(\mathbf{P'_1})\dots\psi^\dagger(\mathbf{P'_n})]|0\rangle \\ &= \ \zeta^P G(\mathbf{1} - P'_1)G(\mathbf{2} - P'_2)\dots G(\mathbf{n} - P'_n) \end{aligned} \tag{7.119}$$

where now P is just the number of times the contraction lines cross-one another. Wick's theorem then states that the n-body Green's function is given by the sum over all possible contractions

$$\langle\phi| \quad T \quad \psi(1)\psi(2)\dots\psi^\dagger(n')|\phi\rangle =$$

$$\sum_{\text{All contractions}} \langle 0|T[\psi(\mathbf{1})\psi(\mathbf{2})\dots\psi(\mathbf{n})\dots\psi^\dagger(\mathbf{P'_2})\dots\psi^\dagger(\mathbf{P'_1})\dots\psi^\dagger(\mathbf{P'_n})]|0\rangle$$

> **Example:** Show how the expansion of the generating functional in the absence of interactions can be used to derive Wick's theorem.

7.5 Landau's Fermi Liquid Theory

One of Landau's most creative inventions, is the idea of Fermi liquid theory. In the early fifties, the availability of isotopic pure $He-3$ as a biproduct of the Manhattan project, made it possible for the first time, to experimentally study an almost ideal Fermi liquid. $He-3$ atoms contain an odd number of nucleii, neutralized by two orbital electrons in a singlet state. It behaves as a composite neutral fermion with spin 1/2.

Prior to Landau's theory, the only available theory of a Fermi fluid was Sommerfelds model for a non-interacting Fermi liquid. A key property of the non-interacting Fermi-gas, is the presence of a large, finite density of single-particle excitations at the Fermi energy, given by

$$N(0) = 2\frac{(4\pi)p^2}{(2\pi\hbar)^3}\frac{dp}{dE}\bigg|_{p=p_F} = \frac{mp_F}{\pi^2\hbar^3} \qquad (7.120)$$

In such a fluid, application of a magnetic field splits the "up" and "down" Fermi seas, changing the energy by an amount $\mp g\mu_B B$, where $g\mu_B$ is the magnetic moment of the Fermion. The number of "up" and "down fermions is thereby shifted by an amount $\delta N_\uparrow = -\delta N_\downarrow = \frac{1}{2}N(0)\mu_B B$ thereby changing the magnetization by an amount $M = \chi B$ where,

$$\chi = g\mu_B(N_\uparrow - N_\downarrow)/B = \mu_f^2 N(0) \qquad (7.121)$$

is the "Pauli paramagnetic susceptibility" . In a degenerate Fermi liquid, the energy is given by

$$E(T) - \mu N = \sum_{\mathbf{k}\sigma=\pm\mathbf{1/2}} \epsilon_{\mathbf{k}}\frac{1}{e^{\beta\epsilon_{\mathbf{k}}}+1} \qquad (7.122)$$

The variation of this quantity at low temperatures (where to order T^2, the chemical potential is constant) depends only on the density of states at the Fermi energy, so the low temperature specific heat

$$\begin{aligned} C_V = \frac{dE}{dT} &= N(0)\int_{-\infty}^{\infty} d\epsilon\epsilon\frac{d}{dT}\left(\frac{1}{e^{\beta\epsilon}+1}\right) \\ &= N(0)k_B^2 T\overbrace{\int_{-\infty}^{\infty} dx\frac{x^2}{(e^x+1)(e^{-x}+1)}}^{\pi^2/3} = \overbrace{\frac{\pi^2}{3}}^{=\gamma}N(0)k_B^2 T \qquad (7.123) \end{aligned}$$

is linear in the temperature. Since both the specific heat, and the magnetic susceptibility are proportional to the density of states, their ratio is set purely by the size of the magnetic moment:

$$\frac{\chi}{\gamma} = g^2\frac{3\mu_B^2}{\pi^2 k_B^2} \qquad (7.124)$$

Remarkably, the early experiments by Fairbank, Ard and Walters at Duke University confirmed the paramagnetic character and the linearity of the specific heat in Helium-3, but more careful analysi revealed that to fit the experiments required required an effective He-3 mass and an enhanced magnetic moment given by

$$\begin{aligned} m^* &= (3.1)m_{(\mathrm{He}^3)}, \\ (g^*)^2 &\approx 3(g^2)_{(\mathrm{He}^3)}, \qquad (7.125) \end{aligned}$$

Landau's approach to this problem was elegantly simple. He imagined starting with a hypothetical gas of Helium atoms with no forces of repulsion between them: this is case he could understand using Sommerfeld's model. Landau imagined gradually turning back on the interactions between the atoms until they reached their full value. What would happen, if one could do this extremely slowly, or "adiabatically"? Nothing! Landau argued that since the fermions near the Fermi surface had nowhere to scatter to, as interactions were smoothly turned on, the quantum states of the metal would evolve smoothly, without any of the energies of the quantum states crossing one-another to become equal. With this reasoning, Landau concluded that each quantum state of the fully-interacting liquid Helium-3, would be in *precise one-to-one correspondence with the states of the idealized "non-interacting" Fermi-liquid.*[6]

Each one particle of the original non-interacting Fermi liquid has a momentum $\vec{\mathrm{p}}$ and a spin $\sigma = \pm 1/2$. The number of fermions which occupy it $n_{\mathrm{p}\sigma}$, is either one, or zero. The complete quantum state of the non-interacting system is labeled by these occupancies. We write

$$\Psi = |n_{\mathrm{p}_1\sigma_1},\ n_{\mathrm{p}_2\sigma_2},\ldots\rangle \qquad (7.126)$$

In the ground-state, Ψ_o all states with momentum p less than the Fermi momentum are occupied, all states above the Fermi surface are empty

$$\mathrm{Ground-state}\ \Psi_\mathrm{o} \quad : \quad n_{\mathrm{p}\sigma} = \begin{cases} 1 & (\mathrm{p}\ <\ \mathrm{p_F}) \\ 0 & (\mathrm{otherwise}\ \mathrm{p} > \mathrm{p_F}) \end{cases} \qquad (7.127)$$

Landau argued, that if one turned on the interactions slowly, then this state would evolve smoothly into the ground-state of the interacting Fermi liquid. The energy of this state is unknown, but we can call it E_0. Suppose we now add one fermion to the original state with momentum $\mathrm{p_o} > \mathrm{p_F}$. Once again we can slowly turn on the interactions. This does not change the momentum of the state, and providing nothing catastrophic takes place, our original state will now evolve smoothly into the a final state that we can label as follows:

$$\mathrm{Quasi-particle:}\ \Psi_{\mathrm{p_o}} \qquad n_\mathrm{p} = \begin{cases} 1 & (\mathrm{p} < \mathrm{p_F}\ \mathrm{and}\ \mathrm{p} = \mathrm{p_o}) \\ 0 & (\mathrm{otherwise}) \end{cases} \qquad (7.128)$$

This state has total momentum $\mathrm{p_o}$ and an energy $E(\mathrm{p_o}) > E_o$ larger than the ground-state. It is called a "quasiparticle-state" because it behaves in every respect like a single particle. This concept is a triumph of Landau's theory, for it enables us to continue using the idea of an independent particle, even in the presence of strong interactions; it also provides a framework for understanding the robustness of the Fermi surface whilst accounting for the effects of interactions. The "excitation energy" required to create a single quasiparticle, is

$$\epsilon_{\mathrm{p_o}} = E(p_o) - E_o \qquad (7.129)$$

The quasiparticle concept would be of limited value if it was limited to individual excitations. At a finite temperature, a dilute gas of these particles is excited around the Fermi surface

and these particles interact. At first sight, this is a hopeless situation: how can the particle concept survive once one has a finite density of excitations?

Landau's appreciation of a very subtle point enabled him to go much further: he realized that near the Fermi surface, electron-electron scattering is severely limited by the phase space constraints of the exclusion principle. In particular, the amount of momentum that two particles can exchange in a collision goes to zero for particles that are on the Fermi surface:

$$(\mathrm{p}_1,\mathrm{p}_2) \to (\mathrm{p}_1 - \mathrm{q},\mathrm{p}_2 + \mathrm{q}) \qquad (\mathrm{q} = 0 \qquad \mathrm{On\ Fermi\ surface.}) \qquad (7.130)$$

In the low density Fermi gas formed around the Fermi surface, particles *only* scatter in the *forward direction*, and in the asymptotic low-energy limit, the number of particles at a given momentum is unchanged by scattering, becoming a constant of the motion.

These physical considerations led Landau to conclude that the energy of a gas of quasiparticles could be expressed as a functional of the average number of quasiparticles, n_p at momentum p. Since the density of quasiparticles is low, it is sufficient to expand the energy in the small deviations in particle number $\delta n_{\mathrm{p}\sigma} = n_{\mathrm{p}\sigma} - n_{\mathrm{p}\sigma}^{(o)}$ from equilibrium. This leads to the Landau energy functional for the Fermi surface,

$$E(\{n_{\mathrm{p}\sigma}\}) = E_0 + \sum_{\mathrm{p}\sigma}\epsilon_\mathrm{p}\delta n_{\mathrm{p}\sigma} + \frac{1}{2}\sum_{\mathrm{p},\mathrm{p}',\sigma,\sigma'} f_{\mathrm{p}\sigma,\mathrm{p}'\sigma'}\delta n_{\mathrm{p}\sigma}\delta n_{\mathrm{p}'\sigma'} + \ldots \qquad (7.131)$$

where

$$\begin{aligned} \epsilon_\mathrm{p} &= \frac{\delta E}{\delta n_{\mathrm{p}\sigma}} \\ f_{\mathrm{p}\sigma,\mathrm{p}'\sigma'} &= \frac{\delta^2 E}{\delta n_{\mathrm{p}\sigma}\delta n_{\mathrm{p}'\sigma'}} \qquad (7.132) \end{aligned}$$

are the first and second-derivatives of the functional, evaluated in the ground-state ($\delta n_\mathrm{p} = 0$). This functional proves of immense facility in understanding the properties of interacting Fermi gases, for it turns out that many physical quantities can be directly related to the first two terms in this expansion, and higher order terms are generally not needed. The first term in the expansion, ϵ_p is just the single quasi-particle energy mentioned above. It is easily seen that the change in total energy when $n_\mathrm{p} \to n_\mathrm{p} + \delta n_\mathrm{p}$ is

$$\frac{\delta E}{\delta n_{\mathrm{p}\sigma}} = \epsilon_\mathrm{p} + \sum_{\mathrm{p}'\sigma'} f_{\mathrm{p}\sigma,\mathrm{p}',\sigma'}\delta n_{\mathrm{p}'\sigma'}. \qquad (7.133)$$

The second-term is naturally interpreted as the change in the quasiparticle energy energy due to a the low density of quasiparticles $\delta n_{\mathrm{p}'\sigma'}$ at momentum p'. In Helium-3, which is an isotropic Fermi liquid, the interaction is invariant under both spin rotations, which means that

$$f_{\mathrm{p}\sigma,\mathrm{p}',\sigma'} = f^s_{\mathrm{p},\mathrm{p}'} + f^a_{\mathrm{p},\mathrm{p}'}\sigma\sigma'. \qquad (7.134)$$

Furthermore, since the interaction is invariant under spatial rotations, on the Fermi surface these terms only depend on the relative angle between p and p′, which permits them to be expanded in terms of Legendre polynomials. By convention one writes

$$N(0)f^{s,a}_{\mathrm{p},\mathrm{p}'} = F^{s,a}_{\mathrm{p},\mathrm{p}'} = \sum_{l=0}^{\infty} F_l^{s,a}P_l(\cos\theta_{\vec{\mathrm{p}},\vec{\mathrm{p}}'}) \qquad (7.135)$$

where

$$N(0) = \frac{m^* p_F}{\pi^2\hbar^3} \qquad (7.136)$$

is the density of one-particle quasiparticle states at the Fermi energy. The parameters F_l^s and F_l^a are called the Landau parameters.

To determine the equilibrium distribution of quasiparticles, we need the Free energy $F = E - TS$. However, here Landau's application of adiabaticity comes to the rescue. When we turn on the interactions, we do not change the entropy, which must still have the same form as in the non-interacting system, i.e.

$$S = -k_B\sum_{\mathbf{p},\sigma}[n_{\mathbf{p}\sigma}\ln n_{\mathbf{p}\sigma} + (1 - n_{\mathbf{p}\sigma})\ln(1 - n_{\mathbf{p}\sigma})] \qquad (7.137)$$

The complete free energy is then the sum of (7.133) and (7.137). Taking the variation with respect to small changes in $n_{\mathbf{p}\sigma}$, we obtain

$$\delta F = \sum_{\mathbf{p}\sigma}\delta n_{\mathbf{p}\sigma}\left[\epsilon_\mathbf{p} + k_B T\ln\left(\frac{n_{\mathbf{p}\sigma}}{1 - n_{\mathbf{p}\sigma}}\right)\right] + \emptyset(\delta n_{\mathbf{p}\sigma}{}^2) \qquad (7.138)$$

The condition that the Free energy be stationary w.r.t. small variations in $n_{\mathbf{p}\sigma}$ means that the first term in this expression must vanish, i.e.

$$n_{\mathbf{p}\sigma} = \frac{1}{e^{\beta\epsilon_\mathbf{p}} + 1} \qquad (7.139)$$

obeys the Fermi distribution function.

Using this formulation of the interacting Fermi gas, Landau was able to deduce three major consequences. The first consequence of the Landau quasiparticle interactions, is the renormalization of the quasi-particle mass. As the fermion moves through the medium, it produces a "wake" of other quasiparticle excitations which moves along with it (Fig. 7.5). This changes its inertia, modifying its energy, as follows

$$\begin{aligned} m &\longrightarrow m^* \\ \epsilon(\mathrm{p}) &= \frac{\mathrm{p}^2}{2m^*} - \epsilon_F. \qquad (7.140) \end{aligned}$$

Landau was able to relate the renormalized mass m^* to the interactions. He did this by considering two situations (Fig. 7.6).

1. A stationary Fermi surface observed from a reference frame moving at velocity **u**.
2. A Fermi surface in which the distribution functions have been modified to produce a Fermi surface that is centered around the momentum $-m\mathbf{u}$.

Using the "Galilean" equivalence of the two situations, Landau argued that the momentum carried by the quasiparticle could be written

$$\vec{p} = m\vec{v}(1 + \frac{1}{3}F_1^s) \tag{7.141}$$

where the additional term is derived from the back-flow of particles displaced by the quasiparticle. Since the velocity at which the particle moves is given by $\vec{v} = \vec{p}/m^*$, it follows that $\vec{p} = \frac{m}{m^*}(1 + \frac{1}{3}F_1^s)\vec{p}$ or

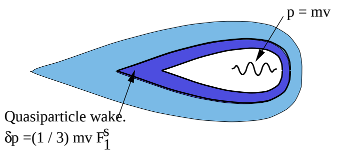


Figure 7.5: Illustrating the wake of particle-hole excitations that moves with a quasiparticle.

$$\frac{m^*}{m} = 1 + \frac{1}{3}F_1^s \tag{7.142}$$

Detailed Discussion To see how Gallilean invariance works, recall that if (E, P) are the energy and momentum of the Lab frame, then in a frame moving with velocity **u**, to leading order in **u**, the energy and momenta are

$$(E', \mathbf{P}') = (E - \mathbf{P}\cdot\mathbf{u}, \mathbf{P} - M\mathbf{u}) \tag{7.143}$$

Let us apply this to a Landau Fermi liquid. Suppose we have a distribution of quasiparticles, then in the Lab frame, the energy and momentum are

$$\begin{aligned} E &= E[n_{\mathbf{p}\sigma}], \\ \mathbf{P} &= \sum_{\mathbf{p},\sigma} \mathbf{p} n_{\mathbf{p}\sigma}. \end{aligned} \tag{7.144}$$

Now suppose we move to a moving frame. We know that in the moving frame, the distribution of quasiparticles is now shifted, so that it is now centered around a momentum $-m\mathbf{u}$, i.e.

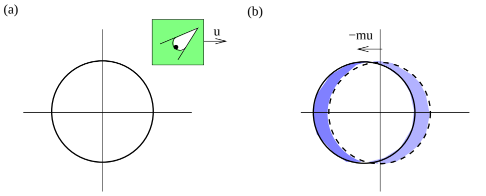


Figure 7.6: Gallilean equivalent quasiparticle distributions: (a) Fermi sea observed from frame moving to right at velocity **u**, (b) Fermi sea with distribution functions modified so as to translate the Fermi sea a momentum $-m\mathbf{u}$ to the left.

$$n'_{\mathbf{p}\sigma} = n_{\mathbf{p}+m\mathbf{u}\sigma} = n_{\mathbf{p}\sigma} + m\mathbf{u}\cdot\nabla_{\mathbf{p}}\mathbf{n}_{\mathbf{p}\sigma}. \tag{7.145}$$

We can now compute the energy in the moving frame by two different methods:

1. Using a Gallilean boost to compute $\Delta E = -\mathbf{P}\cdot\mathbf{u}$.
2. By microscopically simulating a Gallilean boost, adjusting the distribution functions with $\delta n_{\mathbf{p}\sigma} = m\mathbf{u}\cdot\nabla_{\mathbf{p}}\mathbf{n}_{\mathbf{p}\sigma}$, and then computing $\Delta E = \sum_{\mathbf{p}\sigma}\frac{\delta E}{\delta n_{\mathbf{p}\sigma}}\delta n_{\mathbf{p}\sigma}$.

Here's our strategy. Following Landau, we compare these two expressions, to obtain two separate expressions for the total momentum **P** of the Fermi fluid. When we differentiate these expressions with respect to the particle occupancy $n_{\mathbf{p}\sigma}$, we will be able to relate the momentum of each quasiparticle to its group velocity. The coefficient of $\mathbf{v_p}$ in the expression for the momentum will then be the effective mass $\mathbf{p} = \mathbf{m^*v}$.

Let us first compute the energy in the moving frame. This is

$$E' = E[n'_{\mathbf{p}\sigma}] = E[n_{\mathbf{p}\sigma}] + \sum_{\mathbf{p}\sigma}\frac{\delta E}{\delta n_{\mathbf{p}\sigma}} m\mathbf{u}\cdot\nabla_{\mathbf{p}}\mathbf{n}_{\mathbf{p}\sigma} \tag{7.146}$$

The second term can be integrated by parts to yield

$$E[n'_{\mathbf{p}\sigma}] = E[n_{\mathbf{p}\sigma}] - \mathbf{u}\cdot\sum_{\mathbf{p}\sigma} m\nabla_{\mathbf{p}}\left(\frac{\delta\mathbf{E}}{\delta\mathbf{n}_{\mathbf{p}\sigma}}\right)\mathbf{n}_{\mathbf{p}\sigma} \tag{7.147}$$

It is convenient at this point to identify an effective group velocity of each quasiparticle by

$$\mathbf{v}_{\mathbf{p}\sigma} = \nabla_{\mathbf{p}}\left(\frac{\delta E}{\delta n_{\mathbf{p}\sigma}}\right), \tag{7.148}$$

so that

$$E[n'_{\mathbf{p}\sigma}] = E[n_{\mathbf{p}\sigma}] - \mathbf{u}\cdot\sum_{\mathbf{p}\sigma} m\mathbf{v}_{\mathbf{p}\sigma}n_{\mathbf{p}\sigma} \tag{7.149}$$

By comparing (7.147) with (7.143) we thus see that in the original Lab frame there are two ways of writing the momentum

$$\mathbf{P} = \sum_{\mathbf{p}\sigma}\mathbf{p}n_{\mathbf{p}\sigma} = m\sum_{\mathbf{p}\sigma}\mathbf{v}_{\mathbf{p}\sigma}n_{\mathbf{p}\sigma} \tag{7.150}$$

To obtain the quasiparticle momentum, we must differentiate these expressions with respect to the particle occupancy $\delta n_{\mathbf{p}\sigma}$. The left hand-side of this expression gives us

$$\frac{\delta P}{\delta n_{\mathbf{p}\sigma}} = \mathbf{p}.$$

When we come to consider the right-hand side of this expression, we must be careful to realize that because of interactions, $\mathbf{v}_{\mathbf{p}\sigma}$ itself depends on the distribution of particles.

If we examine the variation of the right-hand-side of (7.150) with respect to the quasiparticle occupancies, we obtain

$$\delta\mathbf{P} = m\sum_{\mathbf{p}\sigma}\mathbf{v}_{\mathbf{p}\sigma}\delta n_{\mathbf{p}\sigma} + (\delta\mathbf{v}_{\mathbf{p}\sigma})n_{\mathbf{p}\sigma} \tag{7.151}$$

Using (7.133), we see that

$$\delta(v_{\mathbf{p}\sigma}) = \sum_{\mathbf{p}'\sigma'}\nabla_{\mathbf{p}}\left(\frac{\delta^2 E}{\delta n_{\mathbf{p}\sigma}\delta n_{\mathbf{p}'\sigma'}}\right)\delta n_{\mathbf{p}'\sigma'} = \sum_{\mathbf{p}\sigma'}\nabla_{\mathbf{p}}f_{\mathbf{p}\sigma,\mathbf{p}'\sigma'}\delta n_{\mathbf{p}'\sigma'} \tag{7.152}$$

so that

$$\begin{aligned} \delta\mathbf{P} &= m\sum_{\mathbf{p}\sigma}\delta n_{\mathbf{p}\sigma}\Big(\mathbf{v}_{\mathbf{p}\sigma} + (\nabla_{\mathbf{p}'}f_{\mathbf{p}\sigma,\mathbf{p}'\sigma'})n_{\mathbf{p}'\sigma'}\Big) \\ &= \sum_{\mathbf{p}\sigma}\delta n_{\mathbf{p}\sigma}\Big(m\mathbf{v}_{\mathbf{p}\sigma}\overbrace{-mf_{\mathbf{p}\sigma,\mathbf{p}'\sigma'}\nabla_{\mathbf{p}'}n_{\mathbf{p}'\sigma'}}^{\mathbf{p}_{\rm wake}}\Big) \end{aligned} \tag{7.153}$$

where we have integrated the second-term by parts. Physically, the second term is the momentum associated with the "wake" of particle- hole pairs that accompanies the quasiparticle.

To calculate the "wake" momentum we use the ground-state distribution, $n_{\mathbf{p}\sigma} = n_{\mathbf{p}\sigma}{}^{(0)}$, so that $\nabla_{\mathbf{p}}n_{\mathbf{p}\sigma}{}^{(0)} = -\nabla_{\mathbf{p}}\epsilon_{\mathbf{p}}(\partial n_{\mathbf{p}}/\partial\epsilon_{\mathbf{p}}) = -\mathbf{v}_{\mathbf{p}}\delta(\epsilon_p)$. Carrying out the integral for **p** on the Fermi surface, we obtain

$$\mathbf{p}_{\rm wake} = -m\sum_{\mathbf{p}\sigma'}f_{\mathbf{p}\sigma,\mathbf{p}'\sigma'}\nabla_{\mathbf{p}'}n^{(0)}_{\mathbf{p}'\sigma'} \quad = \quad 2m\int_{\mathbf{p}'}f^s_{\mathbf{p}\mathbf{p}'}\mathbf{v}_{\mathbf{p}'}\delta(\epsilon_{\mathbf{p}'}) \tag{7.154}$$

Replacing

$$2\int_{\mathbf{p}'}\delta(\epsilon_{\mathbf{p}'}) = N(0)\int\frac{d\Omega_{\hat{\mathbf{p}}'}}{4\pi} \tag{7.155}$$

where $d\Omega_{\hat{\mathbf{p}}'}$ is the element of solid angle, and resolving $\mathbf{v}_{\mathbf{p}'}$ along $\mathbf{v}_{\mathbf{p}}$ we obtain

$$\mathbf{p}_{\rm wake} \quad = \quad m\mathbf{v}\int\frac{d\Omega_{\hat{\mathbf{p}}'}}{4\pi}\overbrace{N(0)f^s(\cos\theta)}^{F^s(\cos\theta)}\cos\theta \tag{7.156}$$

where $\cos\theta = \hat{\mathbf{p}}\cdot\hat{\mathbf{p}}'$. Using the Legendre decomposition of the interaction (7.135), this is then

$$p_{wake} = m\mathbf{v}\overline{F^s(\cos\theta)\cos\theta} = \frac{1}{3}m\mathbf{v}F_1^s, \tag{7.157}$$

so that

$$\vec{\mathrm{p}} = m\vec{v}(1 + \frac{1}{3}F_1^s), \tag{7.158}$$

as in the main text.

"Mass renormalization" has the effect of compressing the the spacing between the fermion energy levels, which increases the number of quasi-particles that are excited at a given temperature by a factor m^*/m: this enhances the linear specific heat to the renormalized value

$$C_V^* = \frac{m^*}{m}C_V \tag{7.159}$$

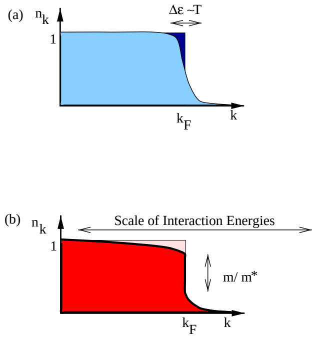


Figure 7.7: (a) A temperature T that is smaller than the Fermi energy, slightly "blurs" the Fermi surface; (b) even though the interaction energy is greater than the temperature, often greater than the Fermi energy, in a Fermi liquid, the exclusion principle stabilizes the jump in occupancy at the Fermi surface.

where C_V is the Sommerfeld value for the specific heat capacity. Experimentally, the specific heat of Helium-3 *is* greater than that expected based on the Sommerfeld model and from the observed enhancement, we know that the quasiparticle mass in Helium three is $m^* \approx 3m$.

Lastly, when a Fermi gas is spin-polarized by a magnetic field, interactions polarize the cloud surrounding each quasiparticle. This leads to an additional renormalization of the susceptibility relative to the specific heat capacity,

$$\chi^* = \frac{m^*}{m(1-F_0^a)}\chi \tag{7.160}$$

This enabled Landau to account for the observation that the Pauli susceptibility of He-3 is enhanced four times more than the linear specific heat capacity.

Helium-3 is a much simpler Fermi liquid than real metals, nevertheless many aspects of the Fermi-liquid picture generalize to the electron fluid. Amazingly, even when the Coulomb interactions are comparable or bigger than the electron kinetic energies, the effects of the Pauli Exclusion principle are seen to be strong enough to sustain the Fermi liquid in simple metals. In the early sixties, Luttinger and Ward provided a detailed mathematical foundation for Landau's picture, and showed that provided one can adiabatically turn on the interactions, the "precipice", or jump in occupation survives, but reduced by the factor m/m^* (Fig. 7.7(b)).

7.6 Exercises for chapter 7

1. A particle with $S = 1/2$ is placed in a large magnetic field $\vec{B} = (B_1\cos(\omega t), B_1\sin(\omega t), B_o)$, where $B_o >> B_1$.

   (a) Treating the oscillating part of the Hamiltonian as the interaction, write down the Schrödinger equation in the interaction representation.

   (b) Find $U(t) = \mathrm{T}\exp\left[-iH_{int}(t')dt'\right]$ by whatever method proves most convenient.

   (c) If the particle starts out at time $t = 0$ in the state $S_z = -\frac{1}{2}$, what is the probability it is in this state at time t ?

2. (Optional derivation of bosonic generating functional.) Consider the forced Harmonic oscillator

$$H(t) = \omega b^\dagger b + \bar{z}(t)b + b^\dagger z(t) \tag{7.161}$$

where $z(t)$ and $\bar{z}(t)$ are arbitrary, independent functions of time. Consider the S-matrix

$$S[z,\bar{z}] = \langle 0|\mathrm{T}\hat{S}(\infty,-\infty)|0\rangle = \langle 0|\mathrm{T}\exp\left(-i\int_{-\infty}^{\infty}dt[\bar{z}(t)b(t) + \bar{b}(t)^\dagger z(t)]\right)|0\rangle, \tag{7.162}$$

where $\hat{b}(t)$ denotes $\hat{b}$ in the interaction representation. Consider changing the function $\bar{z}(t)$ by an infinitesimal amount

$$\bar{z}(t) \to \bar{z}(t) + \Delta\bar{z}(t_o)\delta(t-t_o), \tag{7.163}$$

The quantity

$$\lim_{\Delta\bar{z}(t_o)\to 0}\frac{\Delta S[z,\bar{z}]}{\Delta\bar{z}(t_o)} = \frac{\delta S[z,\bar{z}]}{\delta\bar{z}(t_o)}$$

is called the "functional derivative" of S with respect to $\bar{z}$. Using the Gell-Man Lowe formula $\langle\psi(t)|b|\psi(t)\rangle = \frac{\langle 0|T\hat{S}(\infty,-\infty)b(t)|0\rangle}{\langle 0|T\hat{S}(\infty,-\infty)|0\rangle}$ prove the following identity

$$i\delta\ln S[z,\bar{z}]/\delta\bar{z}(t) \equiv \tilde{b}(t) = \langle\hat{b}(t)\rangle = \langle\psi(t)|\hat{b}|\psi(t)\rangle. \tag{7.164}$$

(ii) Use the equation of motion to show that

$$\frac{\partial}{\partial t}\tilde{b}(t) = i\langle[H(t),\hat{b}(t)]\rangle = -i[\epsilon\tilde{b}(t) + z(t)].$$

(iii) Solve the above differential equation to show that

$$\tilde{b}(t) = \int_{-\infty}^{\infty}G(t-t')z(t') \tag{7.165}$$

where $G(t-t') = -i\langle 0|T[b(t)b^\dagger(t')]|0\rangle$ is the free Green's function for the harmonic oscillator.

(iv) Use (iii) and (i) together to obtain the fundamental result

$$S[z,\bar{z}] = \exp\left[-i\int_{-\infty}^{\infty}dtdt'\bar{z}(t)G(t-t')z(t')\right] \tag{7.166}$$

3. (Harder problem for extra credit).

   Consider a harmonic oscillator with charge e, so that an applied field changes the Hamiltonian $H \to H_o - eE(t)\hat{x}$, where x is the displacement and $E(t)$ the field. Let the system initially be in its ground-state, and suppose a constant electric field E is applied for a time T.

   (i) Rewrite the Hamiltonian in the form of a forced Harmonic oscillator

$$H(t) = \omega b^\dagger b + \bar{z}(t)b + b^\dagger z(t) \tag{7.167}$$

and show that

$$z(t) = \bar{z}(t) = \begin{cases} \omega\alpha & (T > t > 0) \\ 0 & (\text{otherwise}) \end{cases}, \tag{7.168}$$

deriving an explicit expression for α in terms of the field E, mass m, and frequency ω of the oscillator.

(ii) Use the explicit form of $S(\bar{z}, z)$

$$S[z,\bar{z}] = \exp\left[-i\int_{-\infty}^{\infty}dtdt'\bar{z}(t)G(t-t')z(t')\right] \tag{7.169}$$

where $G(t-t') = -i\langle 0|T[b(t)b^\dagger(t')]|0\rangle$ is the free bosonic Green-function, to calculate the probability $p(T)$ that the system is still in the ground-state after time T. Please express your result in terms of α, ω and T. Sketch the form of $p(T)$ and comment on your result.

Chapter 8

Feynman Diagrams: T=0

The preceeding chapter discussed adiabaticity, and we learned how Green's functions functions of an interacting system, can be written in terms Green's functions of the non-interacting system, weighted by the S-matrix, e.g.

$$\langle\phi|T\psi(1)\psi^\dagger(2)|\phi\rangle \;=\; \frac{\langle\phi_o|T\hat{S}\psi(1)\psi^\dagger(2)|\phi_o\rangle}{\langle\phi_o|\hat{S}|\phi_o\rangle}$$

$$\hat{S} \;=\; T\exp\left[-i\int_{-\infty}^{\infty}V(t')dt'\right] \qquad (8.1)$$

where $|\phi_o\rangle$ is the ground-state of H_o. In this chapter we shall learn how to expand to expand these quantities, order by order in the strength of the interaction. The Feynman diagram approach provides a succinct visual rendition of this expansion which is physically intuitive, but also allows us to manipulate and resum the various terms in this vast expansion.

From the Feynman rules, we learn how to evaluate

- The ground-state $S-$ matrix

$$S = \langle\phi_o|\hat{S}|\phi_o\rangle = \sum\{\text{Unlinked Feynman Diagrams}\}\,. \qquad (8.2)$$

- The logarithm of the $S-$ matrix, which is directly related to the shift in the ground-state energy due to interactions.

$$E - E_o = \lim_{\tau\to\infty}\frac{\partial}{\partial\tau}\ln\langle\phi_o|S[\tau/2,-\tau/2]|\phi_o\rangle = i\sum\{\text{Linked Feynman Diagrams}\} \quad (8.3)$$

  where each Linked Feynman diagrams describes a different virtual excitation induced by the perturbation.

- Green's functions.

$$G(1-2) = \sum\{\text{Two-legged Feynman Diagrams}\} \qquad (8.4)$$

- Response functions. These are a different type of Green's function, of the form

$$\mathcal{R}(1-2) = -i\langle\phi|[A(1),B(2)]|\phi\rangle\theta(t_1-t_2) \qquad (8.5)$$

8.1 Heuristic Derivation

Feynman initially derived his diagramatic expansion as a mnemonic device for calculating scattering amplitudes. His approach was heuristic: each diagram has a physical meaning in terms of a specific scattering process. Feynman derived a set of rules rules that explained *how* to convert the diagrams into concrete scattering amplitudes. These rules were fine tuned and tested in the simple cases where they could be checked by other means; later, he applied his method to cases where the direct algebraic approach was impossibly cumbersome. It was only later that Dyson showed how his diagramatic expansion could be developed systematically.

Formally, a perturbation theory for the fully interacting S-matrix is is obtained by expanding the S-matrix as a power-series, then using Wick's theorem to write the resulting correlation functions as a sum of contractions.

$$\langle\phi_o|\hat{S}|\phi_o\rangle = \sum_{n=0}^{\infty}\frac{(-i)^n}{n!}\int_{-\infty}^{\infty}dt_1\ldots dt_n \sum_{\text{Contractions}}\langle\phi_o|T\,V(t_1)V(t_2)\ldots V(t_n)\;|\phi_o\rangle \qquad (8.6)$$

The Feynman rules tell us how to expand these contractions as a sum of diagrams, where each diagram provides a precise, graphical representation of a scattering amplitude that contributes to the complete S-matrix.

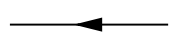
Let us see examine how we might develop, heuristically, a Feynman diagram exapnsion for simple potential scattering, for which

$$V(1) \equiv \int d^3x_1 U(\vec{x}_1)\psi^\dagger(\vec{x}_1,t_1)\psi(\vec{x}_1,t_1). \qquad (8.7)$$

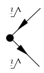
where we've suppressed spin indices into the background. When we start to make contractions we will break up each product $V(1)V(2)\ldots V(r)$ into pairs of creation and annihilation operators, replacing each pair as follows

$$\psi(2)\ldots\psi^\dagger(1) \;\longrightarrow (\sqrt{i})^2\times G(2-1). \qquad (8.8)$$

where we have divided up the the prefactor of i two factors of $\sqrt{i}$, which we will transfer onto the scattering amplitudes where the particles are created and annihilated. This contraction is denoted by

$$G(2-1) = 2$$  $$1 \qquad (8.9)$$

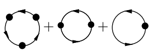
representing the propagation of a particle from "1" to "2". Pure potential scattering gives us one incoming, and one outgoing propagator, so we denote a single potential scattering event by the diagram



$$-iU(x) \qquad = (\sqrt{i})^2\times -iU(x) \equiv U(x) \qquad (8.10)$$

Here, the "$-i$" has been combined with the two factors of $\sqrt{i}$ taken from the incoming, and outgoing propagators to produce a purel *real* scattering amplitude $(\sqrt{i})^2\times -iU(x) = U(x)$.

The Feynman rules for pure potential scattering tell us that the S-matrix for potential scattering is the exponential of a sum of connected "vacuum" diagrams

$$S = \exp\,[$$  $$+\ldots]\,. \qquad (8.11)$$

The "vacuum diagrams" appearing in the exponential do not have any incoming or outgoing propagators- they represent the amplitudes for the various possible processes by which electron-hole pairs can bubble out of the vacuum. Let us examine the first, and second order contractions for potential scattering. To first order

$$-i\langle\phi_0|V(t_1)\;|\phi_0\rangle \;=\; -i\sum_\sigma\int d^3xU(x)\langle\phi_0|T\,\psi^\dagger_\sigma(x,t_1^+)\psi_\sigma(x,t_1^-)\;|\phi_0\rangle \qquad (8.12)$$

This contraction describes a single scattering event at $(\vec{x},t_1)$. Note that the creation operator occurs to the *left* of the annihilation operator, and to preserve this ordering inside the time-ordered exponential, we say that the particle propagates "backwards in time" from $t = t_1^+$ to $t = t_1^-$. When we replace this term by a propagator the backward time propagation introduces a factor of $\zeta = -1$ for fermions, so that

$$\langle\phi_0|T\,\psi^\dagger_\sigma(x,t_1^+)\psi_\sigma(x,t_1^-)\;|\phi_0\rangle = i\zeta G(\vec{x}-\vec{x},t_1^- - t_1^+) = i\zeta G(\vec{0},0^-) \qquad (8.13)$$

We carry along the factor $U(\vec{x})$ as the amplitude for this scattering event. The result of this contraction procedure is then

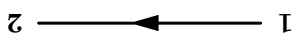
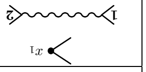
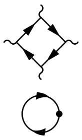
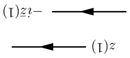
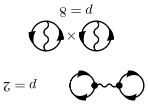
$$-i\int_{-\infty}^{\infty}dt_1\langle\phi_0|V(t_1)\;|\phi_0\rangle \;=\; -i(2S+1)\int dt_1\times\int d^3xU(x)\times i\zeta G(\vec{0},0^-)$$

$$=$$  $$, \qquad (8.14)$$

where we have translated the scattering amplitude into a a single diagram. You can think of it as the spontaneous creation, and re-annhilation of a single particle. Here we may

tentatively infer a number of important "Feynman rules" - listed in Table 8.1: that we must associate each scattering event with an amplitude $U(x)$, connected by propagators that describe the amplitude for electron motion between scattering events. The overall amplitude involves an integration over the space time co-ordinates of the scattering events, and apparantly, when a particle loop appears, we need to introduce the factor $\zeta(2S+1)$ (where $\zeta = -1$ for fermions) into the scattering amplitude to account for the presence of an odd-number of backwards-time propagators and the $2S+1$ spin components of the particle field. These rules are summarized in the table below:

Table. 8.1 Real Space Feynman Rules .

 **1** **2**	$G(\mathbf{2}-\mathbf{1})$
 x_1 **1** **2**	$U(x_1)$ $iV(\mathbf{1}-\mathbf{2})$
$\prod_i\int d^3x_i dt_i$	Integrate over all intermediate times and positions.
	$-(2S+1)G(\vec{0},0^-)$ $[-(2S+1)]^F$, $F =$ no. Fermion loops.
 $z(1)$ $-i\bar{z}(1)$	$z(1)$ $-i\bar{z}(1)$
 $p=2$ $p=8$	$\frac{1}{p}$ $p =$ order of symmetry group.

Physically, the vacuum diagram we have drawn here can be associated with the small first-order shift in the energy ΔE_1 of the particle due to the potential scattering. This inturn produces a phase shift in the scattering S-matrix,

$$S \sim \exp\left[-i\Delta E_1\int dt\right] \sim 1 - i\Delta E_1\int dt, \tag{8.15}$$

where the exponential has been audaciously expanded to linear order in the strength of the scattering potential. If we compare this result with our leading Feynman diagram expansion of the S-matrix,

$\langle\phi_o|\hat{S}|\phi_o\rangle = 1 +$  ,

we see that we can interprete the overall factor of $\int dt_1$ in (8.14) as the time period over which the scattering potential acts on the particle. If we factor this term out of the expression we may identify

$$\Delta E_1 = \overbrace{i\zeta(2S+1)G(\vec{0},0^-)}^{\rho}\int d^3xU(x) \tag{8.16}$$

Here, following our work in the previous chapter, we have identified $i\zeta(2S+1)G(\vec{0},0^-) = \sum_\sigma\langle\psi^\dagger{}_\sigma(x)\psi_\sigma(x)\rangle = \rho$ as the density of particles. giving $\Delta E_1 = \rho\int d^3xU(x)$. The correspondence of our result with first order perturbation theory is a check that the tentative Feynman rules are correct.

Let us go on to look at the second order contractions

$$\langle\phi_0|TV(t_1)V(t_2)\ |\phi_0\rangle = \langle\phi_0|T\overset{\sqcap}{V}(t_1)\overset{\sqcap}{V}(t_2)\ |\phi_0\rangle + \langle\phi_0|T\ \overbrace{V(t_1)V(t_2)}\ |\phi_0\rangle \tag{8.17}$$

which now generate two diagrams

$\frac{1}{2!}(-i)^2\int_{-\infty}^{\infty}dt_1dt_2\langle\phi_0|T\overset{\sqcap}{V}(t_1)\overset{\sqcap}{V}(t_2)\ |\phi_0\rangle = \frac{1}{2}[$  $]^2 = [$   $]$

$\frac{1}{2!}(-i)^2\int_{-\infty}^{\infty}dt_1dt_2\langle\phi_0|T\ \overbrace{V(t_1)V(t_2)}\ |\phi_0\rangle =$  , (8.18)

The first term is simply a product of two first order terms- the beginning of an exponential combination of such terms. Notice how the square of one diagram is the original diagram, repeated twice. The factor of 1/2 that occurs in the expression on the left hand-side is absorbed into this double diagram as a so-called "symmetry factor". We shall return to this issue shortly, but briefly, this diagram has a permutation symmetry described by a group of dimension $d = 2$, according to the Feynman rules, this generates a prefactor $1/d = 1/2$. The second term derives from the second-order shift in the particle energies due to scattering, and which, like the first order shift, produces a phase shift in the S-matrix. This diagram has a cyclic group symmetry of dimension $d = 2$, and once again, there is

a symmetry factor of $1/d = 1/2$. This connected, second-order diagram gives rise to the scattering amplitude

 $= \frac{1}{2}\zeta(2S+1)\int d1d2U(1)U(2)G(1-2)G(2-1)$ (8.19)

where $1 \equiv (\vec{x_1}, t_1)$, so that

$$\begin{aligned}\int d1 &\equiv \int dt_1d^3x_1\\ G(2-1) &\equiv G(\vec{x}_2-\vec{x_1},t_2-t_1).\end{aligned} \tag{8.20}$$

Once again, the particle loop gives a factor $\zeta(2S+1)$, and the amplitude involves an integral over all possible space-time co-ordinates of the two scattering events. You may interpret this diagram in various ways- as the creation of a particle-hole pair at $(\vec{x}_1, t_1)$ and their subsequent reannilation at $(\vec{x}_2, t_2)$ (or vice versa). Alternatively, we can adopt an idea that Feynman developed as a graduate student with John Wheeler- the idea than that an anti-particle (or hole), is a particle propagating backwards in time. From this perspective, this second-order diagram represents a *single* particle that propagates around a loop in space time. Equation (8.19) can be simplified by first making the change of variables $t = t_1 - t_2$, $T = (t_1+t_2)/2$, so that $\int dt_1dt_2 = \int dT \times \int dt$. Next, if we Fourier transform the scattering potential and Green functions, we obtain

 $= \int dT \times \frac{1}{2}\zeta(2S+1)\int dtd^3qd^3k|U(\vec{q_1})|^2G(\vec{k}+\vec{q},t)G(\vec{k},-t)$ (8.21)

Once again, an overall time-integral factors out of the overall expression, and we can identify the remaining term as the *second-order* shift in the energy

$$\Delta E_2 = \frac{i}{2}\zeta(2S+1)\int dt\frac{d^3k}{(2\pi)^3}\frac{d^3q}{(2\pi)^3}|U(\vec{q_1})|^2G(\vec{k}+\vec{q},t)G(\vec{k},-t). \tag{8.22}$$

To check that this result is correct, let us consider the case of fermions, where

$$G(\mathbf{k},t) = -i[(1-n_{\mathbf{k}})\theta(t) - n_{\mathbf{k}}\theta(-t)]e^{-i\epsilon_{\mathbf{k}}t} \tag{8.23}$$

which enables us to do the integral

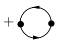
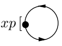
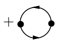
$$i\int dte^{-\delta|t|}G(\vec{k}+\vec{q},t)G(\vec{k},-t) = \frac{(1-n_{\mathbf{k+q}})n_{\mathbf{k}}}{\epsilon_{\mathbf{k+q}}-\epsilon_{\mathbf{k}}} + (\mathbf{k}\leftrightarrow\mathbf{k+q}) \tag{8.24}$$

We recognize the first process as the virtual creation of an electron of momentum $\vec{k}+\vec{q}$, leaving behind a hole in the state with momentum $\vec{k}$. The second-term is simply a duplicate of the first, with the momenta interchanged, and the sum of the two terms cancels the factor of 1/2 infront of the integral. The final result

$$\Delta E_2 = -(2S+1)\int\frac{d^3k}{(2\pi)^3}\frac{d^3q}{(2\pi)^3}|U(\vec{q})|^2\frac{(1-n_{\mathbf{k+q}})n_{\mathbf{k}}}{\epsilon_{\mathbf{k+q}}-\epsilon_{\mathbf{k}}}$$

is recognized as the second-order correction to the energy derived from these virtual processes. Of course, we could have derived these results directly, but the important point, is that we have established a tentative link between the diagramatic expansion of the contractions, and the perturbation expansion for the ground-state energy. Moreover, we begin to see that our diagrams have a direct interpretation in terms of the virtual excitation processes that are generated by the scattering events.

To second-order, our results do indeed correspond to the leading order terms in the exponential

$S = 1 + [$  $+$  $\ldots] + \frac{1}{2!}[$  $+\ldots]^2 + \ldots = exp\,[$  $+$  $+\ldots]\,.$

Before we go on to complete this connection more formally in the next section, we need to briefly discuss "source terms", which couple directly to the creation and annihilation operators. The source terms let us examine how the S-matrix responds to incoming currents of particles. Source terms add directly to the scattering potential, so that

$$V(1) \longrightarrow V(1) + \bar{z}(1)\psi(1) + \psi^\dagger(1)z(1).$$

The source terms terms involve a single creation or annihilation operator, thus produce either the beginning

 $z(1) \equiv \int d1\ldots\times z(1)$

(8.25)

or the end

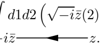
$-i\bar{z}$  $\equiv -i\int d2\bar{z}(2)\times\ldots$

(8.26)

of a Feynman diagram. In practice, each $\bar{z}$ and z arrive in pairs, and the factor $-i$ which multiplies $\bar{z}$ combines the two factors of $-i$ from a pair $(\bar{z}, z)$ with the factor of i derived from the propagator line they share. We need these terms, so that we can generate diagrams which involve incoming and outgoing electrons. The simplest contraction with these terms generates the bare propagator

$$\frac{(-i)^2}{2!}\int d2d1\langle 0|\left[V(2)+\bar{z}(2)\psi(2)+\psi^\dagger(2)z(2)\right]\left[V(1)+\bar{z}(1)\psi(1)+\psi^\dagger(1)z(1)\right]|0\rangle$$

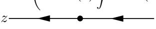
$$= \int d1d2\left(\sqrt{-i}\bar{z}(2)G(2-1)\sqrt{-i}z(1)\right)$$

$= -i\bar{z}$  $z.$ (8.27)

If we now include the contraction with the first scattering term we produce the first scattering correction to the propagator

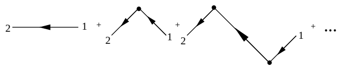
$$\frac{(-i)^3}{3!}\int d2dXd1\langle 0|\left\{[\ldots+\bar{z}(2)\psi(2)+\ldots]\left[U(X)\psi^\dagger(X)\psi(X)+\ldots\right]\left[\ldots+\psi^\dagger(1)z(1)\right]+\text{perms}\right\}|0\rangle$$

$$= \int d1d2\left(\sqrt{-i}\bar{z}(2)\int dXG(2-X)V(X)G(X-1)\sqrt{-i}z(1)\right)$$

$= -iz$  $z.$ (8.28)

where we have only shown one of *six* equivalent contractions on the first line. This diagram is simply interpreted as a particle, created at 1, scattering at position X before propagating onwards to position 2. Notice how we must integrate over the the space-time co-ordinate of the intermediate scattering event at X, to obtain the total first order scattering amplitude. Higher order corrections will merely generate multiple insertions into the propagator and we will have to integrate over the space-time co-ordinate of each of these scattering events. Diagramatically, the sum over all such diagrams generates the "renormalized propagator", denoted by

$G^*(2-1) = 2$  1

$=$  (8.29)

Indeed, to second-order in the scattering potential, we can see that all the allowed contractions are consistent with the following exponential form for the generating functional

$S = exp\,[$  $+$  $+\ldots - i\bar{z}$  $z]\,.$ (8.30)

To prove this result formally requires a little more work, that we now go into in more detail. The important point for you to grasp right now, is that the sum over all contractions in the S-matrix can be represented by a sum of diagrams which concisely represent the contributions to the scattering amplitude as a sum over all possible virtual excitation processes about the vacuum.

8.2 Developing the Feynman Diagram Expansion

A neat way to organize this expansion is obtained using the source term approach we encountered in the last chapter. There we found we could completely evaluate the the response of a non-interacting the system to a source term which injected and removed particles. We start with the source term S-matrix

$$\hat{S}[\bar{z},z] = T\exp\left[-i\int d1[\psi^\dagger(1)z(1)+\bar{z}(1)\psi(1)]\right]. \tag{8.31}$$

Here, for convenience, we shall hide details of the spin away with the space-time co-ordinate, so that $1 \equiv (\mathbf{x}_1, t_1, \sigma_1)$, $\psi(1) \equiv \psi_\sigma(\mathbf{x}, t)$. You can think of the quantities $z(1)$ and $\bar{z}(1)$ as "control-knobs" which we dial up, or down, the rate at which we are adding, or subtracting particles to the system. For fermions, these numbers must be anticommuting Grassman numbers: numbers which anticommute with each and all Fermion field operators. The vacuum expectation value of this S-matrix is then

$$S[\bar{z},z] = \langle\phi|\hat{S}[\bar{z},z]|\phi\rangle = \exp\left[-i\int d1d2\bar{z}(1)G(1-2)z(2)\right] \tag{8.32}$$

where here, $G(1-2) \equiv \delta_{\sigma\sigma_2}G(\mathbf{x}_1-\mathbf{x}_2, t_1-t_2)$ is diagonal in spin. In preparation for our diagramatic approach, we shall denote

$$\int d1d2\bar{z}(1)G(1-2)z(2) = \bar{z} \;\longleftarrow\; z \tag{8.33}$$

where an integral over the space-time variables $(\mathbf{x}_1, t_1)$ and $(\mathbf{x}_2, t_2)$ and a sum over spin variables σ_1, σ_2 is implied by the diagram. The S-matrix equation can then be written

$$S[\bar{z},z] = \exp\Big[-i\bar{z} \;\longleftarrow\; z\Big] \tag{8.34}$$

This is called a "generating functional". By differentiating this quantity with respect to the source terms, we can compute the expectation value of any product of operators. Each time we differentiate the S-matrix with respect to $\bar{z}(1)$, we pull down a field operator inside the time-ordered product

$$\begin{aligned} i\frac{\delta}{\delta\bar{z}(1)} &\rightarrow \psi(1) \\ i\frac{\delta}{\delta\bar{z}(1)}\langle\phi|T\hat{S}\{\ldots\}|\phi\rangle &= \langle\phi|T\hat{S}\{\psi(1)\ldots\}|\phi\rangle \end{aligned} \tag{8.35}$$

For example, the field operator has an expectation value

$$\begin{aligned} \langle\psi(1)\rangle &= \frac{\langle\phi|\hat{S}[\bar{z},z]\psi(1)|\phi\rangle}{\langle\phi|\hat{S}[\bar{z},z]|\phi\rangle} = i\frac{\delta}{\delta\bar{z}(1)}\ln S[\bar{z},z] \\ &= \int G(1-2)z(2)d2 \\ &\equiv [1 \longleftarrow z] \end{aligned} \tag{8.36}$$

Notice how the differential operator $i\frac{\delta}{\delta\bar{z}(1)}$ "grabs hold" of the end of a propagator and connects it up to space-time co-ordinate 1. Likewise, each time we differentiate the S-matrix with respect to $z(1)$, we pull down a field creation operator inside the time-ordered product [1]

$$i\frac{\delta}{\delta z(1)} \rightarrow \psi^\dagger(1), \tag{8.37}$$

---

[1] When z is a Grassman variable, then we have to be careful about the ordering of numbers. The differential operator $\frac{\delta}{\delta z}$ is defined via the Euler expansion $F = F_o + \bar{z}\frac{\partial F}{\partial\bar{z}} + \frac{\partial F}{\partial z}z$, so that $\frac{\partial F}{\partial z}$ is the coefficient lying to the *left* of z. This means that the differential operator $\frac{\delta}{\delta z}$ acts on an expression from the *right*, so that for example, the differential of a product fg is $\frac{\delta}{\delta z}(fg) = f\frac{\delta g}{\delta z} - \frac{\delta f}{\delta z}g$ and the chain rule is $\frac{\delta}{\delta z}F[g] = F'[g]\frac{\delta g}{\delta z}$. This definition avoids the need to carry a factor of ζ in equation (8.37).

so that the creation operator has the value

$$\begin{aligned} \langle\psi^\dagger(2)\rangle &= \frac{\langle\phi|\hat{S}[\bar{z},z]\psi^\dagger(2)|\phi\rangle}{\langle\phi|\hat{S}[\bar{z},z]|\phi\rangle} = i\frac{\delta}{\delta z(2)}\ln S[\bar{z},z] \\ &= \int d1\bar{z}(1)G(1-2) \\ &\equiv [\bar{z} \longleftarrow 2] \end{aligned} \tag{8.38}$$

(Remember that for fermions, the differential operator $\frac{\delta}{\delta z(2)}$ acts from the right). If we differentiate either (8.36) w.r.t. $z(2)$, or (8.38) w.r.t. $\bar{z}(1)$ we obtain

$$i\frac{\delta}{\delta z(2)}\langle\psi(1)\rangle\Big|_{z=\bar{z}=0} = i\frac{\delta}{\delta\bar{z}(1)}\langle\psi(2)\rangle\Big|_{z=\bar{z}=0} = \langle\phi|T\psi(1)\psi^\dagger(2)|\phi\rangle = iG(1-2) \tag{8.39}$$

as expected.

In general, we can calculate arbitrary functions of the field operators by acting on the S-matrix with the appropriate function of derivative operators.

$$\langle\phi|T\hat{S}[\bar{z},z]F[\psi^\dagger,\psi]|\phi\rangle = F\left[i\frac{\delta}{\delta z}, i\frac{\delta}{\delta\bar{z}}\right]\exp\Big[-i\bar{z} \;\longleftarrow\; z\Big]. \tag{8.40}$$

If we now set $F[\psi^\dagger,\psi] = Te^{-i\int V[\psi^\dagger,\psi]dt}$, then

$$S_I[\bar{z},z] = \langle\phi|Te^{-i\int_{-\infty}^{\infty}dt\left(V(\psi^\dagger,\psi)+\text{source terms}\right)}|\phi\rangle \tag{8.41}$$

can be written completely algebraically, in the form

$$S_I[\bar{z},z] = e^{-i\int_{-\infty}^{\infty}V(i\frac{\delta}{\delta z},i\frac{\delta}{\delta\bar{z}})dt}\exp\Big[-i\bar{z} \;\longleftarrow\; z\Big] \tag{8.42}$$

The action of the exponentiated differential operator on the source terms generates all of the contractions. It is convenient to recast this expression in a form that groups all the factors of "i". To do this, we write $\alpha = z, \bar{\alpha} = -i\bar{z}$, this enables us to rewrite the expression as $S_I[\bar{z},z] = \mathcal{S}_I[\bar{\alpha},\alpha]|_{\alpha=z,\bar{\alpha}=-i\bar{z}}$, where

$$\mathcal{S}_I[\bar{\alpha},\alpha] = e^{(i)^{n-1}\int_{-\infty}^{\infty}V(\frac{\delta}{\delta\alpha},\frac{\delta}{\delta\bar{\alpha}})dt}\exp\Big[\bar{\alpha} \;\longleftarrow\; \alpha\Big]$$

where we have written

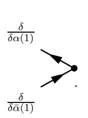
$$V(i\frac{\delta}{\delta z}, i\frac{\delta}{\delta\bar{z}}) = i^nV(\frac{\delta}{\delta\alpha},\frac{\delta}{\delta\bar{\alpha}}) \tag{8.43}$$

for an interaction involving n creation and n annihilation operators (n-particle interaction). This equation provides the basis for all Feynman diagram expansions.

To develop the Feynman expansion, we need to recast our expression in a more graphical form. To see how this works, let us first consider a one-particle scattering potential ($n = 1$). In this case, we write

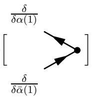
$$i^{n-1}V(\frac{\delta}{\delta\alpha},\frac{\delta}{\delta\bar{\alpha}}) = \int d^3xU(x)\frac{\delta}{\delta\alpha(x)}\frac{\delta}{\delta\bar{\alpha}(x)} \tag{8.44}$$

which we denote as



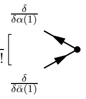
(8.45)

Notice that the basic scattering amplitude for scattering at point x is simply $U(x)$ (or $U(x)/\hbar$ if we reinstate Planck's constant). Schematically then, our Feynman diagram expansion can be written as



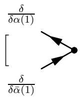
$$\boxed{\mathcal{S}_I[\bar{\alpha},\alpha] = \exp\Big[\qquad\Big]\exp\Big[\bar{\alpha} \;\longleftarrow\; \alpha\Big]}$$

The differential operators acting on the bare S-matrix, glue the scattering vertices to the ends of the propagators, and thereby generate a sum of all possible Feynman diagrams. Formally, we must expand the exponentials on both sides, e.g.

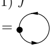


$$\mathcal{S}_I[\bar{\alpha},\alpha] = \sum_{n,m}\frac{1}{n!m!}\Big[\qquad\Big]^n\Big[\bar{\alpha} \longleftarrow \alpha\Big]^m \tag{8.46}$$

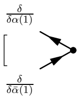
The action of the differential operator on the left hand-side is to glue the m propagators together with the n vertices, to make a series of Feynman diagrams. Now, at first sight, this sounds pretty frightening- we will have a profusion of diagrams. Let us just look at a few: do not at this stage worry about the details, just try to get a feeling for the general structure. The simplest $n = 1$, $m = 1$ term takes the form

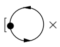


$$\begin{aligned} \Big[\qquad\Big]\Big[\bar{\alpha} \longleftarrow \alpha\Big] &= \zeta\int d1V(1)\frac{\delta^2}{\delta\bar{\alpha}(1^-)\delta\alpha(1)}\int dXdY\bar{\alpha}(X)G(X-Y)\alpha(Y) \\ &= \zeta\int d1V(1)G(1^- - 1) = \end{aligned} \tag{8.47}$$



This is the simplest example of a "linked-cluster" diagram, and it results from a single contraction of the scattering potential. The sign $\zeta = -1$ occurs for fermions, because the fermi operators need to be interchanged to write the expression as a time-ordered propagator. One can say that the expectation value involves the fermion propagating backwards in time from time t to an infinitesimally earlier time $t^- = t - \epsilon$. The term $n = 1$, $m = 2$ gives rise to two sets of diagrams, as follows:



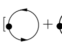


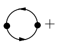
$$\Big[\qquad\Big]\Big[\bar{\alpha} \longleftarrow \alpha\Big]^2 = \bar{\alpha} \longleftarrow\!\bullet\!\longleftarrow \alpha + [\qquad \times\; \bar{\alpha} \longleftarrow \alpha] \tag{8.48}$$

The first term corresponds to the first scattering correction to the propagator, written out algebraically,

$$\bar{\alpha} \longleftarrow\!\bullet\!\longleftarrow \alpha = \int d1d2\bar{\alpha}(1)\int dXG(1-X)V(X)G(X-2)\alpha(2)$$

whereas the second term is an unlinked product of the bare propagator, and the first linked cluster diagram. The Feyman rules enable us to write each possible term in the expansion of the S-matrix as a sum of unlinked diagrams. Fortunately, we are able to systematically combine all of these diagrams together, with the end result that





$$\begin{aligned} S_I(\bar{\alpha},\alpha) &= \exp\Big[\sum\text{linked diagrams}\Big] \\ &= exp\,[\qquad + \qquad + \ldots\bar{\alpha} \Longleftarrow \alpha]\,. \end{aligned} \tag{8.49}$$

When written in this exponential form, the unlinked diagrams entirely disappear- a result of the so-called "link-cluster" theorem we are shortly to encounter. The Feynman rules tell us how to convert these diagrams into mathematical expressions. These rules are summarized in table 8.1.

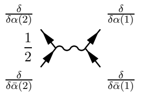
Let us now look at how the same procedure works for a two-particle interaction. Working heuristically, we expect a two-body interaction to involve two incoming and two outgoing propagators. We shall denote a two-body scattering amplitude by the following diagram

$$= (\sqrt{i})^4 \times -iV(1-2) \equiv iV(1-2). \tag{8.50}$$

Notice how, in contrast to the one-body scattering amplitude, we pick up four factors of $\sqrt{i}$ from the external legs, so that the net scattering ampligude involves an awkward factor of "i". If we now proceed using the generating function approach, we set $n = 2$ and then write

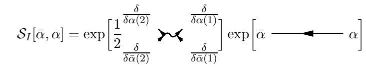
$$i^{n-1}V(\frac{\delta}{\delta\alpha},\frac{\delta}{\delta\bar{\alpha}}) = i\frac{1}{2}\int d^3xd^3x'V(x-x')\frac{\delta}{\delta\alpha(x)}\frac{\delta}{\delta\alpha(x')}\frac{\delta}{\delta\bar{\alpha}(x')}\frac{\delta}{\delta\bar{\alpha}(x)} \tag{8.51}$$

Notice how the amplitude for scattering two particles is now $iV(x-x')$ (or $iV(x-x')/\hbar$ if we reinstate Planck's constant). We can now formally denote the scattering vertex as



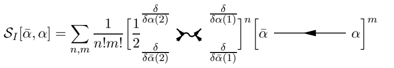
(8.52)

This gives rise to the following expression for the generating functional



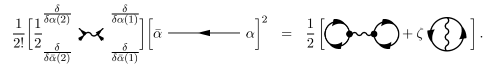
for the S-matrix of interacting particles.

As in the one-particle scattering case, the differential operators acting on the bare S-matrix, glue the scattering vertices to the ends of the propagators, and thereby generate a sum of all possible Feynman diagrams. Once again, we are supposed to formally expand the exponentials on both sides, e.g.



(8.53)

Let us again look at some of the leading diagrams that appear in this process. For instance



We shall see later that these are the Hartree and Fock contributions to the Ground-state energy. The prefactor of $\frac{1}{2}$ arises here because there are two distinct ways of contracting the vertices with the propagators. At each of the vertices in these diagrams, we must integrate over the space-time co-ordinates and sum over the spins. Since spin is conserved along each propagator, so this means that each loop has a factor of $(2S+1)$ associated with the spin sum. Once again, for fermions, we have to be careful about the minus signs. For each particle loop, there is always an odd number of fermion propagators propagating backwards in time, and this gives rise to a factor

$$\zeta(2S+1) = -(2S+1) \tag{8.54}$$

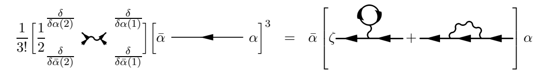
per fermion loop. This is the origin of the factor ζ in the second linked cluster diagram above. The algebraic rendition of these Feynman diagrams is then

$$\frac{1}{2}\int d1d2V(1-2)\Big[(2S+1)^2G(0,0^-)^2 + \zeta(2S+1)G(1-2)G(2-1)\Big] \tag{8.55}$$

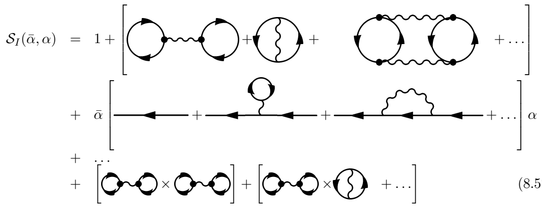
Notice finally, that the first Hartree diagram contains a propagator which "bites its own tail". This comes from a contraction of the density operator,

$$-i\sum_\sigma\langle\ldots\psi_\sigma{}^\dagger(\mathbf{x},t)\psi_\sigma(\mathbf{x},t)\ldots\rangle = \zeta(2S+1)G(\mathbf{x},0^-) \tag{8.56}$$

and since the creation operator lies to the left of the destruction operator, we pick up a minus sign for fermions. As a second example, consider



corresponding to the Hartree and Fock corrections to the propagator. Notice how a similar minus sign is associated with the single fermion loop in the Hartree self-energy. By convention the numerical prefactors are implicitly absorbed into the Feynman diagrams, by introducing two more rules: one which states that each fermion loop gives a factor of ζ, the other which relates the numerical pre-factor to the symmetry of the Feynman diagram. When we add all of these terms, the S-matrix becomes



(8.57)

The diagrams on the first line are "linked-cluster" diagrams: they describe the creation of virtual particle-hole pairs in the vacuum. The second-line of diagrams are the one-leg diagrams, which describe the one-particle propagators. There are also higher order diagrams (not shown) with $2n$ legs, coupled to the source terms, corresponding to the n-particle Green's functions. The diagrams on the third line are "unlinked" diagrams. We shall shortly see that we can remove these diagrams by taking the logarithm of the S-matrix.

8.2.1 Symmetry factors

Remarkably, in making the contractions of the S-matrix, the prefactors in terms like eq. (8.53) are almost completely absorbed by the combinatorics. Let us examine the number of ways of making the contractions between the two terms in (8.53). Our procedure for constructing a diagram is illustrated in Fig. 8.1

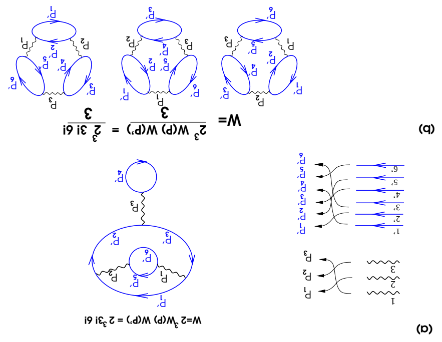


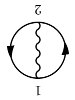
Figure 8.1: (a) Showing how six propagators and three interaction lines can be arranged on a Feynman diagram of low symmetry ($p=1$). (b) In a Feynman diagram of high symmetry, each possible assignment of propagators and interaction lines to the diagram belongs to a $p-$tuplet of topologically equivalent assignments, where p is the order of the symmetry group of permutations under which the topology of the diagram is unchanged. In the example shown above, $p=3$ is the order of the symmetry group. In this case, we need to divide the number of assignments W by a factor of p.

1. We label each propagator on the Feynman diagram 1 through m and label each vertex on the Feynman diagram (1) through (n).
2. The process of making a contraction corresponds to identifying each vertex and each propagator in (8.53) with each vertex and propagator in the Feynman diagram underconstruction. Thus the P'_r th propagator is placed at position r on the Feynman diagram, and the P_k-th interaction line is placed at position k on the Feynman diagram, where P is a permutation of $(1,\ldots n)$ and P' a permutation of $(1,\ldots,m)$.
3. Since each interaction line can be arranged 2 ways at each location, there are $2^nW(P) = 2^nn!$ ways of putting down the the interaction vertices and $W(P') = m!$ ways of putting down the propagators on the Feynman diagram, giving a total of $W = 2^nn!m!$ ways.
4. The most subtle point is notice that if the topology of the Feynman graph is invariant

under certain permutations of the vertices, then the above procedure overcounts the number of independent contractions by a "symmetry factor" p, where p is the dimension of the set of permutations under which the topology of the diagram is unchanged. The point is, that each of the $2^nn!m!$ choices made in (2) actually belongs to a $p-$tuplet of different choices which have actually paired up the propagators and vertices in exactly the same configuration. To adjust for this overcounting, we need to divide the number of choices by the symmetry factor p, so that the number of ways of making the same Feynman graph is

$$W = \frac{2^nn!m!}{p} \tag{8.58}$$

As an example, consider the simplest diagram,

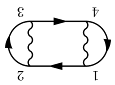


(8.59)

This diagram is topologically invariant under the group of permutations

$$\mathcal{G} \;=\; \{(12),(21)\} \tag{8.60}$$

so $p=2$. In a second example

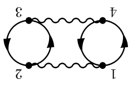


(8.61)

the invariance group is

$$\mathcal{G} \;=\; \{(1234),(3412)\} \tag{8.62}$$

so once again, $p=2$. By contrast, for the diagram



(8.63)

the invariance group is

$$\mathcal{G} \;=\; \{(1234),(3412),(2143),(4312)\} \tag{8.64}$$

so that $p=4$.

8.2.2 Linked Cluster Theorem

One of the major simplifications in developing a Feynman diagram expansion arise because of the Linked Cluster Theorem. Ultimately, we are more interested in calculating the logarithm of the S-matrix, $\ln S(\bar z, z)$. This quantity determines both the energy shift due to interactions, but also, it provides the n-particle (connected) Green's functions. In the Feynman diagram expansion of the S-matrix, we saw that there are two types of diagram: linked-cluster diagrams, and unlinked diagrams, which are actually products of linked-cluster diagrams. The linked cluster theorem states that the logarithm of the S-matrix involves just the sum of the linked cluster diagrams:

$$\ln S_I[\bar z, z] = \sum \{\text{Linked Cluster Diagrams}\} \tag{8.65}$$

To show this result, we shall employ a trick called the "replica trick", which takes advantage of the relation

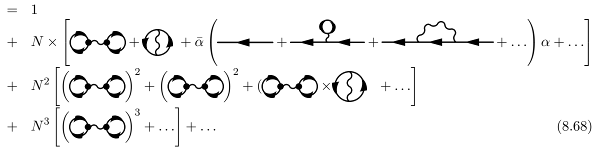
$$\ln S = \lim_{n\to 0}\left[\frac{S^n - 1}{n}\right] \tag{8.66}$$

In other words, if we expand S^n as a power-series in n, then the linear coefficient in the expansion will give us the logarithm of S. It proves much easier to evaluate S^n diagramatically. To do this, we introduce n identical, but independent replicas of the original system, each "replica" labelled by $\lambda = (1, n)$. The Hamiltonian of the replicated system is just $H = \sum_{\lambda=1,n}$ and since the operators of each replica live in a completely independent Hilbert space, they commute. This permits us to write

$$(S_I[\bar z, z])^N = \langle\phi|Te^{-i\int_{-\infty}^{\infty} dt \sum_\lambda (V(\psi_\lambda{}^\dagger, \psi_\lambda) + \text{source terms})}|\phi\rangle \tag{8.67}$$

When we expand this, we will generate exactly the same Feynman diagrams as in S, excepting that now, for each linked Feynman diagram, we will have to multiply the amplitude by N. The diagram expansion for interacting fermions will look like

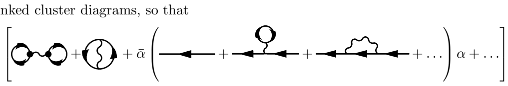
$\mathcal{S}_I(\bar\alpha, \alpha) = 1$



(8.68)

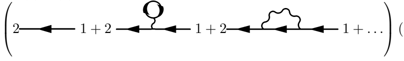
from which we see that the coefficient of N in the replica expansion of S^N is equal to the sum of the linked cluster diagrams, so that

$\ln\mathcal{S}_I(\bar\alpha, \alpha) =$



By differentiating the log of the S-matrix with respect to the source terms, extract the one-particle Green's functions as the sum of all two-leg diagrams

$$G(1-2) = \frac{\delta^2 \ln\mathcal{S}_I(\bar\alpha, \alpha)}{\delta\bar\alpha(1)\delta\alpha(2)} = \sum\{\text{Two leg diagrams}\}$$



(8.69)

This is a quite non-trivial result. Were we to have attempted a head-on Feynman diagram expansion of the Green's function using the Gell Mann Lowe theorem,

$$G(1-2) = -i\frac{\langle\phi|TS\psi(1)\psi^\dagger(2)|\phi\rangle}{\langle\phi|S|\phi\rangle} \tag{8.70}$$

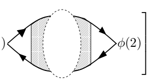
we would have to consider the quotient of two sets of Feynman diagrams, coming from the contractions of the denominator and numerator. Remarkably, the unlinked diagrams of the S matrix in the numerator cancel the unlinked diagrams appearing in the Wick expansion of the denominator, leaving us with this elegant expansion in terms of two-leg diagrams.

The higher order derivatives w.r.t. α and $\bar\alpha$ correspond to the connected n-body Green's functions

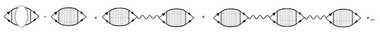
Example: By introducing a chemical potential source term into the original Hamiltonian,

$$H = \int d^3x\delta\phi(x,t)\hat\rho(x) \tag{8.71}$$

show that the change in the logarithm of the S-matrix is

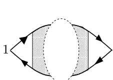
$\ln S[\phi] = \ln S[0] + \frac{1}{2}\Big[\phi(1)$  $\phi(2)\Big]$ (8.72)

where



(8.73)

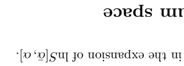
denotes the sum of all diagrams that connect two "density" vertices. Use this result to show that the time-ordered density correlation function is given by

$-i\langle\phi|T\delta\rho(1)\delta\rho(2)|\phi\rangle = i\frac{\delta^2}{\delta\phi(1)\delta\phi(2)}\ln S[\phi] = i$ 1  2 (8.74)

Example: Expand the S-matrix to quadratic order in α and $\bar\alpha$, and use this to show that the two-particle Green's function is given by

$$\frac{1}{S[\bar\alpha,\alpha]}\frac{\delta^4 S}{\delta\bar\alpha(1)\delta\bar\alpha(2)\delta\alpha(3)\delta\alpha(4)} = -\langle\phi|T[\psi(1)\psi(2)\psi^\dagger(3)\psi^\dagger(4)]|\phi\rangle$$

$=$

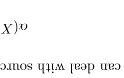


(8.75)

Show that the last term, which is the connected two-particle Green's function, is the quartic term coefficient in the expansion of $\ln S[\bar\alpha, \alpha]$.

8.3 Feynman rules in momentum space

Though it is easiest to motivate the Feynman rules in real space, practical computations are much more readily effected in momentum space. We can easily transform to momentum space by expanding each interaction line and Green's function in terms of their Fourier components:



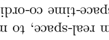
$$= G(X_1 - X_2) = \int \frac{d^dp}{(2\pi)^d} G(p) e^{ip(X_1 - X_2)}$$

$$= V(X_1 - X_2) = \int \frac{d^dq}{(2\pi)^d} V(q) e^{iq(X_1 - X_2)} \tag{8.76}$$

where we have used a short-hand notation $p = (\mathbf{p}, \omega)$, $q = (\mathbf{q}, \nu)$, $X = (\mathbf{x}, t)$, and $pX = \mathbf{p}\cdot\mathbf{x} - \omega t$. We can deal with source terms in similar way, writing

$$\alpha(X) = \int \frac{d^dp}{(2\pi)^d} e^{ipX}\alpha(p). \tag{8.77}$$

Having made these transformations, we see that the space-time co-ordinates associated with each vertex, now only appear in the phase factors. At each vertex, we can now carry out the integral over all space-time co-ordinates, which then imposes the conservation of frequency and momentum at each vertex.



$$= \int d^dXe^{i(p_1 - p_2 - q)X} = (2\pi)^d\delta^{(d)}(p_1 - p_2 - q) \tag{8.78}$$

Since momentum and energy are conserved at each vertex, this means that there is one independent energy and momentum per loop in the Feynman diagram. Thus the transformation from real-space, to momentum space Feynman rules is effected by replacing the sum over all space-time co-ordinates by the integral over all loop momenta and frequency. (Table 8.2). The convergence factor

$$e^{i\omega O^+} \tag{8.79}$$

is included in the loop integral. This term is only really needed when the loop contains a single propagator, propagating back to the point from which it eminated. In this case, the convergence factor builds in the information that the corresponding contraction of field operators is normal ordered.

Actually, since all propagators and interaction variables depend only on the difference of position, the integral over all n space-time co-ordinates can be split up into an integral over the center-or-mass co-ordinate

$$X_{cm} = \frac{X_1 + X_2 + \dots X_n}{n} \tag{8.80}$$

and the relative co-ordinates

$$\tilde X_r = X_r - X_1, \qquad (r > 1), \tag{8.81}$$

as follows

$$\prod_{r=1,n} d^dX_r = d^dX_{cm}\prod_{r=2,n} d^d\tilde X_r \tag{8.82}$$

The integral over the $\tilde X_r$ imposes momentum and frequency conservation, whilst the integral over X_{cm} can be factored out of the diagram, to give an overall factor of

$$\int d^dX_{cm} = (2\pi)^d\delta^{(d)}(0) \equiv VT \tag{8.83}$$

where V is the volume of the system, and T the time over which the interaction is turned on. This means that the proper expression for the logarithm of the S-matrix is

$$\ln S = VT\sum \text{ linked cluster diagrams in momentum space}\}. \tag{8.84}$$

In other words, the phase-factor associated with the S-matrix grows extensively with the volume and the time over which the interactions act.

8.3.1 Relationship between energy, and the S-matrix

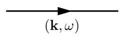
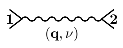
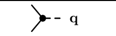
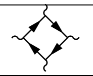
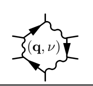
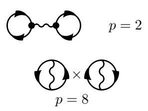
One of the most useful relationships of perturbation theory, is the link between the S-matrix and the ground-state energy. Here the basic idea is very simple. When we turn on the interaction, the ground-state energy changes which causes the phase of the S-matrix to evolve. If we turn on the interaction for a time T, then we expect that for sufficiently long times, the phase of the S-matrix will be given by $-i\Delta ET$:

$$S[T] = \langle -\infty|\hat U(T/2)U^\dagger(-T/2)|\infty\rangle \propto e^{-i\Delta ET} \tag{8.85}$$

where $\Delta E = E_g = E_o$ is the shift in the ground-state energy as a result of interactions. This means that at long times,

$$\ln S[T] = -i\Delta ET + \text{constant} \tag{8.86}$$

Table. 8.2 Momentum Space Feynman Rules .

	$G_o(\mathbf{k},\omega)$	Fermion propagator
	$iV(q)$ $ig_q^2D_o(q)$	Interaction Exchange Boson.
	$U(\mathbf{q})$	Scattering potential
	$[-(2S+1)]^F$,	F= no. Fermion loops
	$\int\frac{d^dqd\nu}{(2\pi)^{d+1}}e^{i\omega 0^+}$	Integrate over internal loop momenta and frequency.
	$\frac{1}{p}$	p = order of symmetry group.

But from the linked cluster theorem, we know that

$$\mathrm{S} = VT\sum\{\text{linked clusters in momentum space}\} \tag{8.87}$$

which then means that the change in the ground-state energy due to interactions is given by

$$\boxed{\Delta E = iV\sum\{\text{linked clusters in momentum space}\} \qquad (8.88)}$$

To show this result, let us turn on the interaction for a period of time T, writing the ground-state S-matrix as

$$S[T] = \langle -\infty|\hat{U}(T/2)U^\dagger(-T/2)|\infty\rangle \tag{8.89}$$

If we insert a complete set of energy eigenstates $\underline{1} = \sum_\lambda |\lambda\rangle\langle\lambda|$ into this expression for the S-matrix, we obtain

$$S[T] = \sum_\lambda \langle -\infty|\hat{U}(T/2)|\lambda\rangle\langle\lambda|U^\dagger(-T/2)|\infty\rangle \tag{8.90}$$

In the limit $T \to \infty$, the only state with an overlap with the time-evolved state $U^\dagger(-T/2)|\phi_o\rangle$ will be the true ground-state $|\psi_g\rangle$ of the interacting system, so we can write

$$S(T) \to \mathcal{U}(T/2)\mathcal{U}^\dagger(-T/2)\langle\phi|^\dagger(-T/2)|\infty\rangle \tag{8.91}$$

where $\mathcal{U}(\tau) = \langle -\infty|\hat{U}(\tau/2)|\phi\rangle$. Now differentiating the first term in this product, we obtain

$$\begin{aligned}\frac{\partial}{\partial\tau}\mathcal{U}(\tau) &= \frac{\partial}{\partial T}\langle\psi_o|e^{iH_o\tau/2}e^{-iH\tau/2}|\psi_g\rangle\\ &= \frac{i}{2}\langle\psi_o|\{H_oU(\tau/2) - U(\tau/2)H\}|\psi_g\rangle\\ &= -\frac{i\Delta E}{2}\mathcal{U}(\tau)\end{aligned} \tag{8.92}$$

Similarly, $\frac{\partial}{\partial\tau}\mathcal{U}^\dagger(-\tau) = -\frac{i\Delta E}{2}\mathcal{U}^\dagger(-\tau)$, so that

$$\frac{\partial S(T)}{\partial T} = -i\Delta E S(T) \tag{8.93}$$

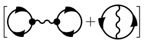
which proves the original claim.

8.4 Examples

8.4.1 Hartree Fock Energy

As a first example of the application of Feynman diagrams, we use the linked cluster theorem to expand the ground-state energy of an interacting electron gas to first order. To leading order in the interaction strength, the shift in the ground-state energy is given by

$$E_g = E_o + iV\left[\qquad\right] \tag{8.94}$$



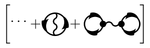
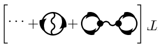
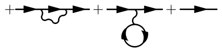
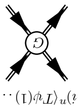
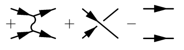
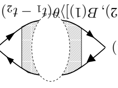
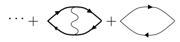
corresponding to the Hartree, and Fock contributions to the ground-state energy. Writing out this expression explicitly, noting that the symmetry factor associated with each diagram is $p = 2$, we obtain

$$\Delta E_{HF} = \frac{iV}{2}\int\frac{d^3kd^3k'}{(2\pi)^6}\frac{d\omega d\omega}{(2\pi)^2}\left[(-[2S+1])(iV_{\mathbf{k}-\mathbf{k}'}) + (-[2S+1])^2(iV_{\mathbf{q}=\mathbf{0}}\right]G(k)G(k')$$

In the last chapter, we obtained the result

$$\int\frac{d\omega}{2\pi}G(\mathbf{k},\omega) = if_{\mathbf{k}} = i\theta(\mathbf{k}_F - |\mathbf{k}|) \tag{8.95}$$

Table. 8.3 Relationship With Physical Quantities.

ΔE	$iV\sum\{\text{linked clusters}\}$	
ln$S$	$VT\sum\{\text{linked clusters}\}$	
 $-i\langle T\psi(2)\psi^\dagger(1)\rangle$	$\sum\{\text{Two leg diagrams}\}$	
$(-i)^n\langle T\psi(1)\ldots\psi^\dagger(2n)\rangle$  $n=2$	$\sum\{\text{2n- leg diagrams}\}$	
Response Functions $(-i)^2\langle\psi\vert T[A(2)B(1)]\vert\psi\rangle = \chi^T_{AB}$  $i\langle[A(2),B(1)]\rangle\theta(t_1-t_2) = \chi_{AB}$	$\chi_{AB} = -i\chi^T_{AB}(\omega - i\delta)$	

so that the shift in the ground-state energy is given by

$$\Delta E_{HF} = \frac{V}{2}\int\frac{d^3kd^3k'}{(2\pi)^6}\left[(2S+1)^2(V_{\mathbf{q}=\mathbf{0}}) - (2S+1)(V_{\mathbf{k}-\mathbf{k}'})\right]f_{\mathbf{k}}f_{\mathbf{k}'} \tag{8.96}$$

In the first term, we can identify $\rho = (2S+1)\sum f_{\mathbf{k}}$ as the density, so this term corresponds to the classical interaction energy of the fermi gas. Note that for the Coulomb interaction, without screening, the Hartree interaction becomes infinite! The second term is the exchange energy. This term is present because the spatial wavefunction of parallel spin electrons is antisymmetric, which keeps them apart, producing a kind of "correlation hole" between parallel spin electrons.

To illuminate this correlation hole between the parallel electrons, it is useful to consider the equal time density correlation function,

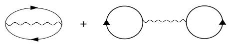
$$C_{\sigma\sigma'}(\vec{x}-\vec{x'}) = \langle\phi_0|:\rho_\sigma(x)\rho_{\sigma'}(x'):|\phi_0\rangle$$

In real space, the Hartree Fock energy is given by

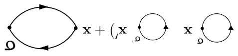
$$\begin{aligned}\langle\phi_0|\hat{V}|\phi_0\rangle &= \frac{1}{2}\sum_{\sigma,\sigma'}\int d^3xd^3yV(\vec{x}-\vec{y})\langle\phi_0|:\hat{\rho}_\sigma(\vec{x})\rho(\sigma')(\vec{y})|\phi_0\rangle\\ &= \frac{1}{2}\sum_{\sigma,\sigma'}\int d^3xd^3yV(\vec{x}-\vec{y})C_{\sigma\sigma'}(\vec{x}-\vec{y})\end{aligned} \tag{8.97}$$

Now if we look at the real-space Feynman diagrams for this energy,

$$\Delta E = i\left[\qquad + \qquad\right]$$

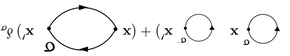


$$= -\frac{1}{2}\sum_{\sigma\sigma'}\int_{\mathbf{x},\mathbf{x}'}V(\mathbf{x}-\mathbf{x}')\left[\left(\quad\mathbf{x}\quad\mathbf{x}'\right) + \mathbf{x}\quad\mathbf{x}'\right] \tag{8.98}$$



since each interaction line contributes a $iV(\mathbf{x}-\mathbf{x}')$ to the total energy, we deduce that the Feynman diagram for the equal time density correlation functions are

$$C_{\sigma\sigma'}(\mathbf{x}-\mathbf{y}) = -\left[\left(\quad\mathbf{x}\quad\mathbf{x}'\right) + \left(\mathbf{x}\quad\mathbf{x}'\right)\delta_{\sigma\sigma'}\right] \tag{8.99}$$



Written out explicitly,

$$\begin{aligned}C_{\sigma\sigma'}(\vec{x}-\vec{y}) &= -\left[-\delta_{\sigma\sigma'}G(\vec{x}-\vec{y},0^-)G(\vec{y}-\vec{x},0^-) + (\overbrace{-G(\vec{0},O^-)}^{i\rho_0})^2)\right]\\ &= \rho_0^2 + \delta_{\sigma\sigma'}G(\vec{x}-\vec{y},0^-)G(\vec{y}-\vec{x},0^-)\end{aligned} \tag{8.100}$$

where we have identified $G(\vec{0},0^-) = i\rho_0$ with the density of electrons per spin. From this we see that $C_{\uparrow\downarrow}(\vec{x}-\vec{y}) = \rho_0^2$ is independent of separation- there are no correlations between the up and down-spin density in the non-interacting electron ground state. However, the correlation function between parallel spin electrons contains an additional term. We can calculate this term from the equal time electron propagator, which in real space is given by

$$\begin{aligned}G(\vec{x},0^-) &= \int_{\mathbf{k}}G(\mathbf{k},0^-)e^{i\vec{k}\cdot\vec{x}}\\ &= i\int_{k<k_F}\frac{k^2dk}{2\pi^2}\overbrace{\int\frac{d\cos\theta}{2}e^{ikr\cos\theta}}^{\frac{\sin kr}{kr}}\\ &= \frac{k_F}{2\pi^2}\left[\frac{\sin(k_Fr) - k_Fr\cos k_Fr}{r^2}\right]\\ &= \rho_0F(k_Fx)\end{aligned} \tag{8.101}$$

where $\rho_0 = \frac{k_F^3}{6\pi^2}$ and

$$F(x) = \frac{3\pi}{2x} j_1(x) = 3\frac{\sin x - x\cos(x)}{x^2} \tag{8.102}$$

so that

$$C_{\uparrow\uparrow}(\vec{x}-\vec{y}) = \rho_0^2\left[1 - F(k_F|\vec{x}-\vec{y}|)\right]$$

This function is shown in Fig. 8.2. At $\vec{x}-\vec{y}=0$, this function goes to zero, corresponding to the fact that the probability to find two "up" electrons in the same place actually vanishes. It is this hole in the correlation function that gives the interacting electron fluid a predisposition towards the development of ferromagnetism and triplet paired superfluids.

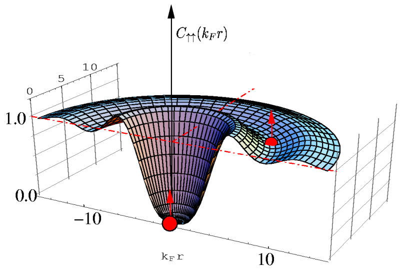


Figure 8.2: "Correlation hole". The equal time correlation function $C_{\uparrow\uparrow}(k_F r)$ for the non-interacting Fermi gas. Notice how this function vanishes at the origin, corresponding to a vanishing probability to find two "up" electrons at the same location in space.

8.4.2 Response functions

One of the most valuable applications of Feynman diagrams, is to evaluate response functions. Suppose we couple the interacting system up to an external source field,

$$H(t) = H_o + H_s(t) \tag{8.103}$$

where

$$H_s(t) = -A(t)f(t) \tag{8.104}$$

involves the coupling of an external force to a variable of the system. Examples would include

$$\begin{aligned} H_s(t) &= -\mu_B \int d^3x \mathbf{S}(x)\cdot\mathbf{B}(x,t), && \text{External magnetic field} \\ H_s(t) &= -\int d^3x \rho(\mathbf{x})\Phi(x,t) && \text{External potential} \end{aligned} \tag{8.105}$$

In each case, the system will respond by a change in the variable $A(t)$. To calculate this change, the interaction representation of $H(t)$, so that

$$A_H(t) = U^\dagger(t)A_I(t)U(t) \tag{8.106}$$

where, from chapter 7,

$$U(t) = T\exp\left[-i\int_{-\infty}^{t} H_s(t')dt'\right] \tag{8.107}$$

We shall now drop the subscript I, because $A_I(t) = A(t)$ also corresponds to the Heisenberg representation of H_o. Expanding (8.106) to linear order in H_s, we obtain

$$A_H(t) = A(t) - i\int_{-\infty}^{t}[A(t), H_s(t')]dt' + O(H_s^2) \tag{8.108}$$

Finally, taking expectation values, we obtain

$$\langle A_H(t)\rangle = \langle\phi|A(t)|\phi\rangle - i\int_{-\infty}^{t}\langle\phi|[A(t), H_s(t')]|\phi\rangle dt' \tag{8.109}$$

But if A is zero in the absence of the applied force, i.e. $\langle\phi|A(t)|\phi\rangle = 0$, then the linear response of the system is given by

$$\langle A_H(t)\rangle = \int_{-\infty}^{\infty} dt' \mathcal{G}(t-t')f(t')dt' \tag{8.110}$$

where

$$\boxed{\mathcal{R}(t-t') = i\langle\phi|[A(t), A(t')]|\phi\rangle\theta(t-t')} \tag{8.111}$$

and $A(t)$ is in the Heisenberg representation of the unperturbed system.

Now in diagramatic perturbation theory, we are able to evaluate time-ordered correlation functions, such as

$$G(1-2) = i\langle\phi|TA(1)A(2)|\phi\rangle \tag{8.112}$$

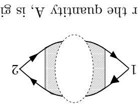
Fortunately, there is a very deep link between the dissipative response function, and the fluctuations associaed with a correlation function, called the "fluctuation-dissipation" theorem. The Fourier transforms of $\mathcal{R}$ and G are both governed by precisely the same many-body excitations, with precisely the same spectral functions, with one small difference: in the complex structure of $\mathcal{R}(\omega)$, all the poles lie just below the real axis, guaranteeing a retarded response. By contrast, in $G(\omega)$, the positive and negative energy poles give rise to retarded, and advanced responses, respectively. The spectral decomposition of these functions are then,

$$\boxed{\begin{aligned} \mathcal{R}(\omega) &= \sum_\lambda \frac{|M_\lambda|^2}{\omega_\lambda - \omega - i\delta} \\ G(\omega) &= \sum_\lambda \frac{|M_\lambda|^2}{\omega_\lambda - \omega - i\delta\mathrm{sgn}(\omega_\lambda)} \end{aligned}} \tag{8.113}$$

so that the response function can be simply related to the time-ordered response at a small imaginary frequency:

$$\mathcal{R}(\omega) = G(\omega + i\delta) \tag{8.114}$$

We can obtain the Feynman rules for the time-ordered correlation function, by introducing a source term H_s and calculating the S-matrix $S[f]$. In this case,

$$-i\frac{\delta^2}{\delta f(1)\delta f(2)}\ln S[f] = i\langle\phi|T[A(1)A(2)]|\phi\rangle = -i$$  (8.115)

Diagramatically, the time-ordered correlation function for the quantity A, is given by

$$G(\omega) = -i\sum\{\text{diagrams formed by connecting two "A" vertices together.}\} \tag{8.116}$$

as summarized in Table 8.3.

Example: Derive the Lindhard function for the zero-frequency susceptibility of the non-interacting electron gas.

8.4.3 Electron in a scattering potential

As an illustration of the utility of the Feynman diagram approach, we now consider an electron scattering off an attractive central scattering potential. Here, by resumming the Feynman diagrams, it is easy to show how in dimensions $d \leq 2$, an arbitrarily weak attractive potential gives rise to bound-states.

The Hamiltonian is given by

$$H = \sum_{\mathbf{k}} \epsilon_{\mathbf{k}} c^\dagger{}_{\mathbf{k}} c_{\mathbf{k}} + H_{sc} \tag{8.117}$$

where $\epsilon_{\mathbf{k}} = k^2/2m - \mu$ and the scattering potential is given by

$$H_{sc} = \int d^3x \psi^\dagger(x)\psi(x)U(x) \tag{8.118}$$

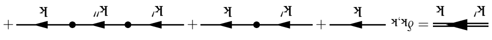
If we Fourier transform the scattering potential, writing

$$U(x) = \int_{\mathbf{q}} U(\mathbf{q})e^{i\mathbf{q}\cdot\mathbf{x}} \tag{8.119}$$

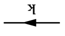
then the scattering potential becomes

$$H_{sc} = \int_{\mathbf{k},\mathbf{k}'} \underbrace{U_{\mathbf{k}-\mathbf{k}'}}_{\text{amplitude to transfer momentum } \mathbf{k}-\mathbf{k}'} c^\dagger{}_{\mathbf{k}} c_{\mathbf{k}'} \tag{8.120}$$

The Feynman diagrams for the one-electron Green's function are then

 (8.121)

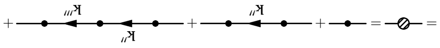
where

 $= G^o(\mathbf{k},\omega) = \dfrac{1}{\omega - \epsilon_{\mathbf{k}} - i\delta_{\mathbf{k}}}$ (8.122)

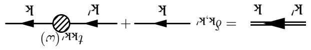
denotes the propagator in the absence of potential scattering and

 $= U_{\mathbf{k}-\mathbf{k}'}$ (8.123)

is the basic scattering vertex. The first diagram represents the amplitude to be transmitted without scattering; subsequent diagrams represent multiple scattering processes involving one, two three and more scattering events. We shall lump all scattering processes into a single amplitude, called the t-matrix, represented by

$t_{\mathbf{k},\mathbf{k}'}(\omega) =$  (8.124)

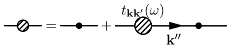
With this short-hand notation, the diagrams for the electron propagator become

 (8.125)

Written out as an equation, this is

$$G(\mathbf{k},\mathbf{k}',\omega) = \delta_{\mathbf{k},\mathbf{k}'}G^o(\mathbf{k},\omega) + G^o(\mathbf{k},\omega)t_{\mathbf{k},\mathbf{k}'}(\omega)G^o(\mathbf{k}',\omega) \tag{8.126}$$

If we look at the second, third and higher scattering terms in the t-matrix, we see that they are a combination of the t-matrix plus the bare scattering amplitude. This enables us to re-write the t-matrix as the following self-consistent set of Feynman diagrams



(8.127)

Written out explicitly, this is

$$t_{\mathbf{kk}'}(\omega) = U_{\mathbf{k}-\mathbf{k}'} + \sum_{\mathbf{k}''} U_{\mathbf{k}-\mathbf{k}''} G_o(\mathbf{k}'', \omega) t_{\mathbf{k}''\mathbf{k}'}(\omega) \tag{8.128}$$

Equations (8.126) and (8.128) fully describe the scattering off the impurity.

As a simplified example of the application of these equations, let us look at the case of s-wave scattering off a point-like scattering center:

$$U(\mathbf{x}) = U\delta^{(d)}(\mathbf{x}) \tag{8.129}$$

In this case, $U(\mathbf{q}) = U$ is independent of momentum transfer. By observation, this means that the t-matrix will also be independent of momentum, i.e. $t_{\mathbf{k},\mathbf{k}'}(\omega) - t(\omega)$. The equation for the t-matrix then becomes

$$t(\omega) = U + U \sum_{\mathbf{k}''} G^o(\mathbf{k}'', \omega) t(\omega) \tag{8.130}$$

or

$$t(\omega) = \frac{U}{1 - UF(\omega)} \tag{8.131}$$

where

$$\begin{aligned} F(\omega) &= \int \frac{d^d p}{(2\pi)^d} \frac{1}{\omega - \epsilon_{\mathbf{k}} + i\delta_{\mathbf{k}}} \\ &= \int_0^\Lambda d\epsilon N(\epsilon) \frac{1}{\omega - \epsilon + i\delta \mathrm{sign}(\epsilon)} \end{aligned} \tag{8.132}$$

and $N(\epsilon)$ is the density of states. A high-energy cut-off has been introduced to guarantee the convergence of the integral. Physically, such a cut-off corresponds to the energy scale, beyond which ,the scattering potential no longer behaves as a point potential. At low energies, $F(\omega) < 0$, so that if $U < 0$, there is the possibility of poles in the t-matrix, corresponding to bound-states.

As we have derived it, our scattering t-matrix describes scattering in the presence of a Fermi sea. To recover free particle behavior, we imagine that the Fermi sea is empty, so that the chemical potential is zero so that

$$\epsilon_{\mathbf{k}} = \frac{k^2}{2m} \tag{8.133}$$

In d-dimensions, the density of states is given by

$$N(\epsilon) \propto k^{d-1} \frac{dk}{d\epsilon} \propto \epsilon^{\frac{d}{2}-1} \tag{8.134}$$

The low energy behavior of $F(\omega)$ is then given by

$$F(\omega) \propto -\omega^{d/2-1} \tag{8.135}$$

This quantity diverges in dimensions $d \leq 2$, so that for there will be bound-states for arbitrarily small attractive potentials. In two dimensions, the density of states is $N(\omega) = N(0)$and $F(\omega) = -N(0)\ln\frac{\Lambda}{-\omega}$, so that for attractive $U = -|U|$,

$$t(\omega) = -\frac{|U|}{1 - |U|N(0)\ln\frac{\Lambda}{-\omega}} = \frac{1}{N(0)\ln\left(\frac{\omega_o}{-\omega}\right)} \tag{8.136}$$

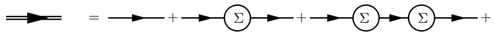
where $\omega_o = \Lambda e^{-\frac{1}{|U|N(0)}}$, giving rise to a bound-state at energies $\omega = -\omega_o$.
Remarks

- The energy scale ω_o can not be written as a power-series in U, and as such, is an elementary example of a "non-perturbative" result. The bound-state appears because an infinite class of Feynman diagrams have been resummed.
- The appearance of a bound-state for electrons scattering off an arbitrarily weak attractive potential is similar to the Cooper instability.

8.5 The self-energy

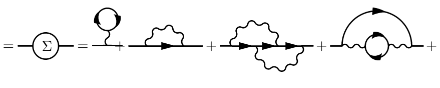
The concept of the self-energy enables us to understand the feedback of the interacting environment on a propagating particle. This is one of the most important examples of the power of Feynman diagram resummation.

Let us consider the Greens function of a fermion in an interacting environment. Every diagram contributing to the propagator consists of free propagators, separated by various scattering processes are "inserted". If we lump all of these scattering processes into one quantity, called the self-energy, the propagator has the structure



(8.137)

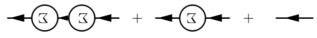
where

$\Sigma(\mathbf{k}, \omega) =$


(8.138)

denotes the self-energy: the sum of all scattering processes that can not be separated into two by cutting a single propagator.

The one-particle propagator can be written in terms of the self-energy as follows

$G(\mathbf{k}, \omega) =$


$$\begin{aligned} &= G^o + G^o\Sigma G^o + G^o(\Sigma G^o)^2 + \ldots \\ &= \tfrac{1}{(G^o)^{-1} - \Sigma} \end{aligned} \tag{8.139}$$

So that

$$\boxed{G(\mathbf{k}, \omega) = \frac{1}{\omega - \epsilon_{\mathbf{k}} - \Sigma(\mathbf{k}, \omega)}} \tag{8.140}$$

Physically, the self-energy describes the cloud of particle-hole excitations that form the wake which accompanies the propagating electron. In general, the self-energy has both a real, and an imaginary component.

$$\Sigma(\mathbf{k}, \omega - i\delta) = \Sigma'(\mathbf{k}, \omega) + i\Gamma(\mathbf{k}, \omega) \tag{8.141}$$

If we use this expression to evaluate the one-particle spectral function, we obtain

$$A(\mathbf{k}, \omega) = \frac{1}{\pi}\mathrm{Im}G(\mathbf{k}, \omega - i\delta) = \frac{\Gamma(\mathbf{k}, \omega)}{[\omega - \epsilon_{\mathbf{k}} - \Sigma'(\mathbf{k}, \omega)]^2 + \Gamma(\mathbf{k}, \omega)^2} \tag{8.142}$$

If the self-energy is small, we see that this corresponds to a Lorentzian of centered around a renormalized energy $\epsilon^*_{\mathbf{k}} = \epsilon_{\mathbf{k}} + \Sigma'(\mathbf{k}, \epsilon^*_{\mathbf{k}})$. If we expand the Lorentzian around this point, we must be careful to write $\omega - \epsilon_{\mathbf{k}} - \Sigma'(\mathbf{k}, \omega) = (\omega - \epsilon^*_{\mathbf{k}})Z_{\mathbf{k}}$ where $Z^{-1}_{\mathbf{k}} = (1 - \partial_\omega\Sigma'(\mathbf{k}, \omega))|_{\omega=\epsilon^*_{\mathbf{k}}}$. Near the renormalized energy,

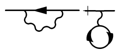
$$G(\mathbf{k}, \omega - i\delta) = \frac{Z_{\mathbf{k}}}{\omega - \epsilon^*_{\mathbf{k}} - i\Gamma^*_{\mathbf{k}}} \tag{8.143}$$

corresponding to a "quasiparticle" excitation with a finite lifetime. The finite width reflects the fact that an electron can now decay into combinations of electrons, plus electron-hole pairs. The reduced weight reflects the finite overlap between the bare electron, and the renormalized excitation:

$$\begin{array}{rcll} \epsilon^*_{\mathbf{k}} &=& \epsilon_{\mathbf{k}} + \Sigma'(\mathbf{k}, \epsilon^*_{\mathbf{k}}), & \text{renormalized energy} \\ \tau^{-1} &=& Z_{\mathbf{k}}\Gamma(\mathbf{k}, \epsilon^*_{\mathbf{k}}), & \text{Lifetime} \\ Z_{\mathbf{k}} &=& |\langle \text{q.ptcle } \mathbf{k}\sigma | c^\dagger{}_{\mathbf{k}\sigma} | \phi \rangle|^2 & \text{``Wavefunction renormalization''} \end{array} \tag{8.144}$$

8.5.1 Hartree-Fock Self-energy

The simplest example of the self-energy is the Hartree-Fock self energy, given by the two diagrams

$\Sigma_{HF}(\mathbf{p}, \omega) =$


$$= i\int_{\mathbf{p}'} \{-(2S+1)V_{\mathbf{q}=0} + V_{\mathbf{p}-\mathbf{p}'}\} \int \frac{d\omega}{2\pi} G^o(k) e^{i\omega 0^+} \tag{8.145}$$

Here we see a case where we must include a convergence factor, associated with the normal ordering of the operators inside the interaction. Identifying $\int d\omega G^o(k) e^{i\omega 0^+} = 2\pi i f_{\mathbf{p}'}$, we obtain

$$\Sigma_{HF}(\mathbf{p}) = \int_{|\mathbf{p}'|<k_F} \frac{d^3k'}{(2\pi)^3}\Big[(2S+1)V_{\mathbf{q}=0} - V_{\mathbf{p}-\mathbf{p}'}\Big] \tag{8.146}$$

In the Hartree-Fock approximation, the electron acquires a renormalized energy

$$\epsilon^*_{\mathbf{p}} = \epsilon_{\mathbf{p}} + \Sigma_{HF}(\mathbf{p}) \tag{8.147}$$

but since the Hartree-Fock self-energy is completely static, in this approximation, the quasiparticle has an infinite lifetime. The mass of the quasiparticle is nevertheless renormalized. Suppose we write

$$\frac{\mathbf{p}}{m^*} = \nabla_{\mathbf{p}}\epsilon^*_{\mathbf{p}} = \left[\frac{\mathbf{p}}{m} + \nabla_{\mathbf{p}}\Sigma_{HF}(\mathbf{p})\right] \tag{8.148}$$

then integrating by parts,

$$\nabla_{\mathbf{p}}\Sigma_{HF}(\mathbf{p}) = -\int_{\mathbf{p}'} V_{\mathbf{p}-\mathbf{p}'}\nabla_{\mathbf{p}'}f_{\mathbf{p}'} \tag{8.149}$$

Writing $\nabla_{\mathbf{p}}f_{\mathbf{p}} = \nabla_{\mathbf{p}}\epsilon^*_{\mathbf{p}}\partial f/\partial\epsilon^* = \frac{\mathbf{p}}{m^*}\delta(\epsilon^*_{\mathbf{p}})$, we then obtain

$$\nabla_{\mathbf{p}}\Sigma_{HF}(\mathbf{p}) = \frac{\mathbf{p}}{3m^*}F^s_1 \tag{8.150}$$

where, by analogy with Fermi liquid theory, we have written,

$$F^s_1 = -N(0)\int \frac{d\Omega_{\hat{\mathbf{p}}'}}{4\pi} V_{\mathbf{p}-\mathbf{p}'}\cos(\hat{\mathbf{p}} \cdot \hat{\mathbf{p}}'). \tag{8.151}$$

where $N(0) = m^* p_F/(\pi^2\hbar^3)$ is the renormalized density of states, and we have included the minus sign in the definition in keeping with the exchange origin of this term. The renormalized mass is then

$$\frac{m^*}{m} = 1 + \frac{1}{3}F^s_1 \tag{8.152}$$

Formally, this result is the same as that derived in Landau Fermi liquid theory. However, a more realistic theory would take into account the screening and modification of the interactions by the medium, a subject which we touch on in as our next topic.

8.6 Large-N electron gas

Although the Feynman diagram approach gives us a way to generate all perturbative corrections, we still need a way to selecting the physically important diagrams. In general, as we have seen from the last examples, it is important to resum particular classes of diagrams to obtain a physical result. What principles, other than pragmatism govern the choice of diagrams?

In general, one hopes for a small parameter which selects out the most important diagrams. Frequently however, there is no obvious choice of small parameter, in which case, one needs an alternative strategy. One way to select Feynman diagrams in a system with no natural small parameter is to take the so-called "large-N" limit. This involves generalizing some internal degree of freedom so that it has N components. Examples include:

- The Hydrogen atom in N-dimensions.
- The electron gas with $N = 2S + 1$ spin components
- Spin systems, with spin S in the limit that S becomes large.
- Quantum Chromodynamics, with N, rather than three colours.

In each of these cases, the limit $N \to \infty$ corresponds to a new kind of semiclassical limit, where certain variables cease to undergo quantum fluctuations. The parameter $1/N$ plays the role of an effective $\hbar$

$$\frac{1}{N} \sim \hbar \tag{8.153}$$

This does not however mean that quantum effects have been lost, merely that their macroscopic consequences can be lumped into certain semi-classical variables. We shall now examine the second of these two examples. The idea is to take an interacting Fermi gas where each fermion has $N = 2S+1$ possible spin components. The interacting Hamiltonian is still written

$$H = \sum_{\mathbf{k},\sigma} \epsilon_{\mathbf{k}} c^{\dagger}{}_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} + \frac{1}{2}\sum V_{\mathbf{q}} c^{\dagger}{}_{\mathbf{k}+\mathbf{q}\sigma} c^{\dagger}{}_{\mathbf{k}'-\mathbf{q}\sigma'} c_{\mathbf{k}'\sigma'} c_{\mathbf{k}\sigma} \tag{8.154}$$

but now, the spin summations run over $N = 2S + 1$ values, rather than just two. As N is made very large, it is important that both the kinetic and the interaction energy scale extensively with N, and for this reason, the original interaction $V_{\mathbf{q}}$ is rescaled, writing

$$V_{\mathbf{q}} = \frac{1}{N}\mathcal{V}_{\mathbf{q}} \tag{8.155}$$

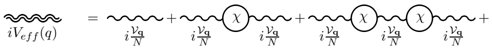
where it is understood that as $N \to \infty$, U is to be kept fixed. The idea is to now calculate quantities as an expansion in powers of $1/N$, and at the end of the calculation, to give N

the value of specific interest, in our case, $N = 2$. For example, if we are interested in a Coulomb gas of spin 1/2 electrons, then study the family of problems where

$$V_{\mathbf{q}} = \frac{1}{N}\frac{4\pi\tilde{e}^2}{q^2} \tag{8.156}$$

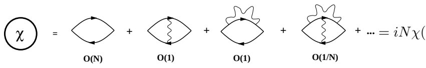
and $\tilde{e}^2 = 2e^2$. At the end, we set $N = 2$, hoping that the key features of the solution around $N = 2$ will be shared by the entire family of models.

With the above substitution, the Feynman rules are unchanged, excepting that now we associate a factor $1/N$ with each interaction vertex. Let us examine how the fermions interact in this large-N fermi gas. We can expand the effective interaction as follows



(8.157)

The "self-energy" diagram for the interaction line is called a "polarization bubble", and has the following diagramatic expansion.

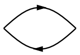


(8.158)

By summing the geometric series that appears in (8.157) we obtain

$$V_{eff} = \frac{1}{N}\frac{\mathcal{V}(q)}{1 + \mathcal{V}(q)\chi(q)} \tag{8.159}$$

This modification of the interaction by the polarization of the medium is an example of "screening". In the large-N limit, the higher-order Feynman diagrams for $\chi(q)$ are smaller by factors of $1/N$., so in the large-N limit, these terms can be neglected giving

$i\chi_0(q)N =$  (8.160)

In the case of a Coulomb interaction, where the screened interaction becomes

$$V_{eff}(\mathbf{q},\omega) = \frac{1}{N}\frac{4\pi\tilde{e}^2}{q^2\epsilon(\mathbf{q},\omega)} \tag{8.161}$$

where we have identified

$$\epsilon(\mathbf{q},\omega) = 1 + \mathcal{V}(q)\chi(q) = 1 + \frac{4\pi\tilde{e}^2}{q^2}\chi_o(q) \tag{8.162}$$

as the dielectric function of the charged medium. Notice how, in the interacting medium, the interaction between the fermions has become frequency dependent, indicating that the

interactions between the particles are now *retarded*. Using the Feynman rules, we can calculate $\chi_o(q)$, as follows

$$iN\chi_o(q) = (-N)\int \frac{d^4k}{(2\pi)^4} G_o(k+q)G_o(k) \tag{8.163}$$

where the factor $-N$ comes from the fermion loop, and the sum over the N spin indices. Written out explicitly, this is

$$\chi_o(\mathbf{q},\nu) = i\int_{\mathbf{k}}\int_{-\infty}^{\infty}\frac{d\omega}{(2\pi)}\frac{1}{\omega + \nu - \epsilon_{\mathbf{k}+\mathbf{q}} + i\delta_{\mathbf{k}+\mathbf{q}}}\frac{1}{\omega - \epsilon_{\mathbf{k}} + i\delta_{\mathbf{k}}} \tag{8.164}$$

We can do the frequency integral by closing the contour integral in the upper half-plane, whereupon we pick up a pole contribution $if_{\mathbf{k}}$ and $if_{\mathbf{k}+\mathbf{q}}$ for the poles in the two Green's functions. The result of this calculation is then

$$\chi_o(\mathbf{q},\nu) = \int_{\mathbf{k}}\frac{f_{\mathbf{k}+\mathbf{q}} - f_{\mathbf{k}}}{\nu - (\epsilon_{\mathbf{k}+\mathbf{q}} - \epsilon_{\mathbf{k}}) + i\delta_{\mathbf{k},\mathbf{q}}} \tag{8.165}$$

where $\delta_{\mathbf{k},\mathbf{q}} = \delta\mathrm{sign}(\epsilon_{\mathbf{k}+\mathbf{q}} - \epsilon_{\mathbf{k}})$ guarantees that positive frequency poles are below the real axis, and negative frequency poles are above the real axis. From our earlier discussion, the corresponding response function- the charge susceptibility of the non-interacting electron gas, is given by $N\chi_o(\mathbf{q},\nu + i\delta)$, the same function, but with all poles moved just below the real axis. This function has a number of fascinating properties

- $\chi_o(\mathbf{q},\nu+i\delta) = \chi'(\mathbf{q},\nu)+i\chi''(\mathbf{q},\nu)$ has both a real, and an imaginary component. The imaginary component

  $$\chi''(\mathbf{q},\nu) = \int_{\mathbf{k}}\pi\delta[\nu - (\epsilon_{\mathbf{k}+\mathbf{q}} - \epsilon_{\mathbf{k}})](f_{\mathbf{k}} - f_{\mathbf{k}+\mathbf{q}}), \tag{8.166}$$

  arises because of dissipation associated with the creation of particle-hole pairs in the Fermi sea. $\chi''(\mathbf{q},\nu)$ defines the density of states of particle-hole pair excitations, a quantity which is finite within a band of wavevectors spanning the Fermi surface, as shown in Figure ???. Outside this region, $\chi_o(\mathbf{q},\nu)$ is purely real.

- In the low frequency limit, the susceptibility is given by

  $$\chi_o(\mathbf{q}) = 2N(0)F(\frac{q}{2k_F}) \tag{8.167}$$

  where $N(0)$ is the density of states per spin at the Fermi surface and

  $$F(x) = \frac{1}{4x}(1 - x^2)\ln\left|\frac{1+x}{1-x}\right| + \frac{1}{2} \tag{8.168}$$

  is called the Lindhard function. This function is maximal at $x = 0$, but has a weak singularity at $x = 1$, which is when the wavevector exceeds the diameter of the Fermi surface. If the bare interaction is a Coulomb interaction, then at low momentum, the effective interaction becomes

  $$V_{eff}(\mathbf{q},\nu) = \frac{1}{N}\frac{4\pi\tilde{e}^2}{q^2 + \kappa^2} \tag{8.169}$$

  where $\kappa = \sqrt{4\pi\tilde{e}^2N(o)}$ can be identified as an inverse screening length. $\kappa^{-1} = a$ is the "Thomas Fermi" screening length of a classical charge plasma. In this way, the long-range part of the interaction is screened out by the Fermi sea. You would however be mistaken in thinking that the effective interaction is of the Yukawa type, for the weak singularity in $\chi_o(\mathbf{q},\nu)$ around $q = 2k_F$ induces a long-range, albeit weaker interaction between the particles of the form

  $$V_{eff}(r) \propto \frac{\cos 2k_F r}{r^3} \tag{8.170}$$

  This long-range oscillatory interaction gives rise to oscillations in the charge density called "Friedel oscillations".

- In the low momentum limit, $\chi_o(\mathbf{q},\nu) \propto -q^2/\nu^2$, and

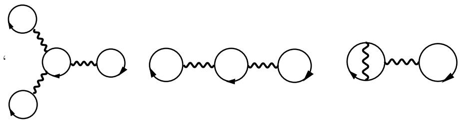
  $$\epsilon_o(\mathbf{q},\nu) = 1 - \frac{\omega_p^2}{\nu^2} \tag{8.171}$$

  where

  $$\omega^2 = \frac{4\pi\tilde{e}^2\tilde{n}}{m} \tag{8.172}$$

  is the plasma frequency. Here where $\tilde{n} = n/N$ is the density of electrons per spin. The appearance of this zero in the dielectric function indicates the presence of collective plasma oscillations in the medium at frequency ω_p.

Let us now examine the linked cluster expansion of the ground-state energy. First, note that all diagrams which involve insertions to zero-momentum interaction lines, other than the basic Hartree diagram, such as



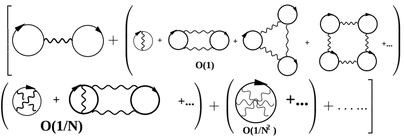
, (8.173)

identically vanish. This is because, these diagrams involve a power of the propagator higher than one, inside integrals of the form

$$\int d\omega G(\mathbf{k},\omega)^n = o, \qquad (n > 1) \tag{8.174}$$

which are zero, because there is no other ω dependent function inside the integral. The only nonzero diagrams are then:

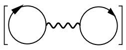
$$\frac{\Delta E}{V} = i$$



(8.175)

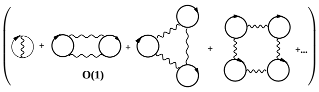
We shall select the two leading contributions,

$$\frac{\Delta E_{cl}}{V} = i$$



, (O(N)) (8.176)

which corresponds to the classical repulsive energy between particles, and the sum



(8.177)

These diagrams are derived from the zero the zero-point fluctuations in charge density, which modify the ground-state energy $E \rightarrow E_o + E_{zp}$. Now the nth diagram in this series has a symmetry factor $p = 2n$, and a contribution $(-\chi_o(q)\mathcal{V}(q))^n$ associated with the n polarization bubbles and interaction lines. The energy per unit volume associated with this series of diagrams is thus

$$E_{zp} = i\sum_{n=1}^{\infty}\frac{1}{2n}\int\frac{d^4q}{(2\pi)^4}(-\chi_o(q)\mathcal{V}(q))^n. \qquad (8.178)$$

By interchanging the sum and the integral, we see that we obtain a series of the form $\sum_n \frac{(-x)^n}{n} = -\ln(1+x)$, so that the zero-point correction to the ground-state energy is

$$E_{zp} = -i\frac{1}{2}\int\frac{d^4q}{(2\pi)^4}ln[1+\mathcal{V}_{\mathbf{q}}\chi_o(q)]$$

Now the logarithm has a branch cut just below the real axis, for positive frequency, but just above the real axis for negative frequency. If we carry out the frequency integral by completing the contour in the lower half plane, we can distort the contour integral around the branch cut at positive frequency, to obtain

$$E_{zp} \;=\; -\frac{i}{2}\int_{\mathbf{q}}\int_0^{\infty}\frac{d\omega}{2\pi}\left[\ln[1+\chi_o(\mathbf{q},\nu+i\delta)\mathcal{V}_{\mathbf{q}}]-\ln[1+\chi_o(\mathbf{q},\nu-i\delta)\mathcal{V}_{\mathbf{q}}]\right]$$

$$= \frac{1}{2}\int_{\mathbf{q}}\int_0^{\infty}\frac{d\omega}{\pi}\arctan\left(\frac{\mathcal{V}_{\mathbf{q}}\chi''(\mathbf{q},\nu)}{[1+\mathcal{V}_{\mathbf{q}}\chi'(\mathbf{q},\nu)]}\right) \qquad (8.179)$$

If we associate a "phase shift"

$$\delta(\mathbf{q},\omega) = \arctan\left(\frac{\mathcal{V}_{\mathbf{q}}\chi''(\mathbf{q},\nu)}{[1+\mathcal{V}_{\mathbf{q}}\chi'(\mathbf{q},\nu)]}\right) \qquad (8.180)$$

then we can the zero-point fluctuation energy can also be written in the form

$$\Delta E_{zp} = \int\frac{d^3q}{(2\pi)^3}\int_0^{\infty}d\omega\Lambda(\omega)\left[\frac{\omega}{2}\right] \qquad (8.181)$$

where

$$\Lambda(\omega) = \frac{1}{\pi}\frac{\partial\delta(\mathbf{q},\omega)}{\partial\omega}. \qquad (8.182)$$

We can interpret $\Lambda(\omega)$ as the "density of states" of charge fluctuations at an energy ω. When the interactions are turned on, each charge fluctuation mode in the continuum experiences a scattering phase shift $\delta(\vec{q},\omega)$ which has the effect of changing the density of states of charge fluctuations. The zero-point energy describes the change in the energy of the continuum due to these scattering effects.

Example: Compute the rms quantum fluctuations $\Delta\rho = \sqrt{\langle(\rho-\rho_o)^2\rangle}$ in the charge density of the electron gas about its average density, ρ_o, in the large-N limit. Show that $\Delta\rho/\rho_o \sim O(1/N)$, so that the density behaves as a semiclassical variable in the large N limit.

Example: Show that the dynamical charge susceptibility of an interacting electron gas in the large N limit, defined by

$$\chi(\mathbf{q},\nu+i\delta) = \int d^x\int_0^{\infty} i\langle\phi|[\rho(\mathbf{x},t),\rho(0,0)]|\phi\rangle e^{-i(\mathbf{q}\cdot\mathbf{x}-\omega t)} \qquad (8.183)$$

contains a pole at frequencies

$$\omega_q = \omega_p(1+\frac{3}{10}qv_F) \qquad (8.184)$$

where $\omega_p = \sqrt{4\pi\tilde{e}^2\tilde{n}/m}$ is the Plasma frequency and $v_F = p_F/m$ is the Fermi velocity.

8.7 Exercises for chapter 8

1. Consider a gas of particles with interaction

$$\hat{V} = 1/2\sum_{\vec{k}\vec{k}'\vec{q}\sigma\sigma'} V_q c^{\dagger}{}_{\vec{k}-\vec{q}\sigma}c^{\dagger}{}_{\vec{k}'+\vec{q}\sigma'}c_{\vec{k}'\sigma'}c_{\vec{k}\sigma}$$

(a) Let $|\phi\rangle$ represent a filled Fermi sea, i.e. the ground state of the non interacting problem. Use Wick's theorem to evaluate an expression for the expectation value of the interaction energy $\langle\phi|\hat{V}|\phi\rangle$ in the non-interacting ground state. Give a physical interpretation of the two terms that arise and draw the corresponding Feynman diagrams.

(b) Suppose $|\tilde{\phi}\rangle$ is the full ground-state of the interacting system. If we add the the interaction energy $\langle\tilde{\phi}|\hat{V}|\tilde{\phi}\rangle$ to the non-interacting ground-state energy, do we obtain the full ground-state energy? Please explain your answer.

(c) Draw the Feynman diagrams corresponding to the second order corrections to the ground-state energy. Without calculation, write out each diagram in terms of the electron propagators and interaction V_q, being careful about minus signs and overall pre-factors.

2. Consider a d-dimensional system of fermions with spin-degeneracy $n_s = 2S+1$, mass m and total density $n_s\rho$, where ρ is the density per spin component. The fermions attract one-another via the two-body potential

$$V(\mathbf{r}_i-\mathbf{r}_j) = -\alpha\delta^{(d)}(\mathbf{r}_i-\mathbf{r}_j), \qquad (\alpha > 0) \qquad (8.185)$$

(a.) Calculate the *total* energy *per particle*, $\epsilon_s(n_s,\rho)$ to first order in α.

(b.) Beyond some critical value α_c, the attraction between to the particles becomes so great that the gas becomes unstable, and may collapse. Calculate the dependence of α_c on the density per spin ρ. To what extent do you expect the gas to collapse in $d = 1,2,3$ when α_c is exceeded?

(c.) In addition to the above two-body interaction nucleons are also thought to interact via a repulsive three-body interaction. Write the three-body potential $V(\mathbf{r}_i,\mathbf{r}_j,\mathbf{r}_k) = \beta\delta^{(d)}(\mathbf{r}_i-\mathbf{r}_j)\delta^{(d)}(\mathbf{r}_j-\mathbf{r}_k)$, in second-quantized form.

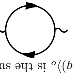
(d.) Use Feynman diagrams to calculate the ground-state energy *per particle*, $\epsilon_s(n_s,\rho)$ to leading order in both β and α. How does your result compare with that obtained in (a) when $n_s = 2$?

(e.) If we neglect Coulomb interactions, why is the case $n_s = 4$ relevant to nuclear matter?

3. (a.)Consider a system of fermions interacting via a momentum-dependent interaction $V(\mathbf{q}) = \frac{1}{n_s}U(\mathbf{q})$, where $n_s = 2S+1$ is the spin degeneracy. When n_s is large, the interactions in this fluid can be treated exactly. Draw the Feynman diagram expansion for the ground-state energy, identifying the leading and subleading terms in the $1/n_s$ expansion.

(b) Certain classes of Feynman diagrams in the linked-cluster expansion of the ground-state energy identically vanish. Which ones, and why?

(c.) If $n_s\chi^{(o)}(q) = \langle\delta\rho(q)\delta\rho(-q)\rangle_o$ is the susceptibility of the non-interacting Fermi gas, i.e



$$= in_s\chi^{(o)}(q), \qquad (8.186)$$

where $q = (\mathbf{q},\nu)$, what is the effective interaction between the fermions in the large n_s limit? Suppose that in real space, $U(r) = e^2/r$ is a long-range Coulomb interaction, explain in detail what happens to the effective interaction at long-distances.

(d.) Consider the rms size of the quantum density fluctuations,

$$\Delta\rho = \sqrt{\langle(\rho-\rho_o)^2\rangle}, \qquad (8.187)$$

where ρ_o is the equilibrium density of fermions. What happens to the ratio $\Delta\rho/\rho_o$ as $n_s \rightarrow \infty$? Comment on the significance of your answer. Write down an expression for the rms amplitude of the density fluctuations.

Chapter 9

Finite Temperature Many Body Physics

For most purposes in many body theory, we need to know how to include the effects of temperature. At first sight, this might be thought to lead to undue extra complexity in the mathematics, for now we need to average the quantum effects over an ensemble of states, weighted with the Boltzmann average

$$p_\lambda = \frac{e^{-\beta E_\lambda}}{Z} \qquad (9.1)$$

It is here that some of the the most profound aspects of many body physics come to our aid.

Remarkably, finite temperature Many Body physics is no more difficult than its zero temperature partner, and in many ways, the formulation is easier to handle. The essential step that makes this possible is due to the Japanese physicist Kubo, who noticed in the early fifties that the quantum-mechanical partition function can be regarded as a time-evolution operator in *imaginary time*:

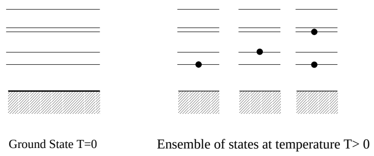
$$\hat{\rho} \propto e^{-\beta \hat{H}} = U(-i\hbar\beta),$$

where $U(t) = e^{-i\frac{tH}{\hbar}}$ is the time-evolution operator, and by convention, we write $H = H_0 - \mu N$ to take into account of the chemical potential. Kubo's observation led him to realize that finite temperature many body physics can be compactly reformulated using an imaginary, rather than a real time to time-evolve all states

$$\frac{it}{\hbar} \longrightarrow \tau.$$

Kubo's observation was picked up by Matsubara, who wrote down the first imaginary time formulation of finite temperature many body physics. In the imaginary time approach, the partition function of a quantum system is simply the trace of the time-evolution operator, evaluated at imaginary time t = -i $\hbar\beta$,

$$Z{=}\, Tr e^{-\ \beta H}{=}\, TrU(-i\hbar\beta),$$



$$p_\lambda = \frac{e^{-\beta E_\lambda}}{Z}$$

Figure 9.1: At zero temperature, the properties of a system are determined by the ground-state. At finite temperature, we must average the properties of the system over an ensemble which includes the ground-state and excited states, averaged with the Boltzmann probability weight $\frac{e^{-\beta E_\lambda}}{Z}$.

whilst the expectation value of a quantity A in thermal equilibrium is given by

$$\langle A \rangle = \frac{Tr\,[U(-i\hbar\beta)A]}{Tr\,[U(-i\hbar\beta)]},$$

an expression reminiscent of the Gell-Mann Lowe formula excepting that now, the S-matrix is replaced by time-evolution over the *finite* interval $t \in [0, -i\hbar\beta]$: The imaginary time universe is of finite extent in the time direction! We will see that physical quantities turn out to be periodic in imaginary time, over this finite interval $\tau \in [0, \hbar\beta]$. This can loosely understood as a consequence of the incoherence induced by thermal fluctuations: thermal fluctuations lead to an uncertainty k_BT in energies, so

$$\tau_T = \frac{\hbar}{k_BT}$$

represents a characteristic time of a thermal fluctuation. Processes of duration longer than τ_T loose their phase coherence, so coherent quantum processes are limited within a world of finite temporal extent, $\hbar\beta$.

One of the most valuable aspects of finite temperature quantum mechanics, first explored by Kubo concerns the intimate relationship between response functions and correlation functions in both real and imaginary time, which are mathematically quantified via the "fluctuation dissipation theorem".

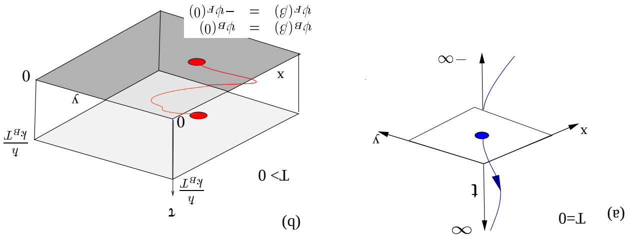


Figure 9.2: (a) Zero temperature field theory is carried out in a space that extends infinitely from $t = -\infty$ to $t = \infty$. (b) Finite temeprature field theory is carried out in a space that extends over a finite time, from $\tau = 0$ to $\tau = \hbar\beta$. Bosonic fields (ψ_B) are periodic over this interval whereas Fermionic fields (ψ_F) are antiperiodic over this interval.

Quantum/thermal Fluctuations ↔ Dynamic Response

"Fluctuation dissipation"

These relationships, first exploited in detail by Kubo, and now known as the "Kubo formalism", enable us to calculate correlation functions in imaginary time, and then, by analytically continuing the Fourier spectrum, to obtain the real-time response and correlation functions at a finite temperature.

Most theoretical many body physics is conducted in the imaginary time formalism, and theorists rarely give the use of this wonderful method a moments use. It is probably fair to say that we do not understand the deep reasons why the imaginary time formalism works. Feynman admits in his book on Statistical mechanics, that he has sought, but not found a reason for why imaginary time and thermal equilibrium are so intimately intertwined. In relativity, it turns out that thermal density matrices are always generated in the presence of an event horizon, which excludes any transmission of information between the halves of the universe of different sides of the horizon. It would seem that a complete understanding of imaginary time may be bound-up with a more complete understanding of information

theory and quantum mechanics than we currently possess. What-ever the reason, it is a very pragmatic and beautiful approach, and it is this which motivates us to explore it further!

9.1 Imaginary time

The key step in making the jump from zero temperature, to finite temperatures many body physics, is the replacement

$$\boxed{\frac{it}{\hbar} \to \tau. \qquad (9.2)}$$

With this single generalization, we can generalize almost everything we have done at zero temperature. In zero temperature quantum mechanics, we introduced the idea of the Schrödinger, Heisenberg and interaction representations. We went on to introduce the concept of the Greens function, and developed a Feynman diagram expansion of the S-matrix. We shall now repeat this exact procedure in imaginary time, reinterpreting the various entities which appear in terms of finite temperature statistical mechanics. Table 1. summarizes the key analogies between real time zero temperature, and imaginary time, finite temperature many body physics.

9.1.1 Representations

The imaginary time generalization of the Heisenberg and interaction representations precisely parallels the development in real time, but there are some minor differences that require us to go through the details here. After making the substitution $t \to -i\tau\hbar$, the real time Schrödinger equation

$$H|\psi_s\rangle = i\hbar\frac{\partial}{\partial t}|\psi_s\rangle, \qquad (9.3)$$

becomes

$$H|\psi_s\rangle = -\frac{\partial}{\partial \tau}|\psi_s\rangle. \qquad (9.4)$$

so the time-evolved wavefunction is given by

$$|\psi_s(\tau)\rangle = e^{-H\tau}|\psi_s(0)\rangle. \qquad (9.5)$$

The Heisenberg representation removes all time-dependence from the wavefunction, so that $|\psi_H\rangle = |\psi_s(0)\rangle$ and all time-evolution is transfered to the operators,

$$A_H(\tau) = e^{iH(-i\tau)}A_S e^{-iH(-i\tau)} = e^{H\tau}A_S e^{-H\tau}. \qquad (9.6)$$

so that the Heisenberg equation of motion becomes

$$\frac{\partial A_H}{\partial \tau} = [H, A_H]$$

Table. 9.0 The link between real and imaginary time formalisms.

Schrödinger eqn	$\vert\psi_s(t)\rangle = e^{-itH}\vert\psi_s(0)\rangle$	$\vert\psi_s(\tau)\rangle = e^{-\tau H}\vert\psi_s(0)\rangle$
Heisenberg rep	$A_h = e^{itH}A_s e^{-itH}$	$A_H = e^{\tau H}A_s e^{-\tau H}$
Interaction rep	$\vert\psi_I(t)\rangle = e^{-itH_0}\vert\psi_I(t)\rangle$	$\vert\psi_I(\tau)\rangle = e^{-\tau H_0}\vert\psi_I(\tau)\rangle$
Perturbation Expansion	$S = \langle -\infty\vert Te^{-i\int V dt}\vert\infty\rangle$	$\frac{Z}{Z_0} = Tr\left[e^{-\int_0^\beta V d\tau}\right]$
Wick's Theorem	$\overbrace{\psi(1)\psi^\dagger}(2) = \langle 0\vert T\psi(1)\psi^\dagger(2)\vert 0\rangle$	$\overbrace{\psi(1)\psi^\dagger}(2) = \langle T\psi(1)\psi^\dagger(2)\rangle$
Green's function	$G_{\lambda\lambda'}(t) = -i\langle 0\vert T\psi_\lambda(\tau)\psi^\dagger{}_{\lambda'}(0)\vert 0\rangle$	$\mathcal{G}_{\lambda\lambda'}(\tau) = -\langle T\psi_\lambda(\tau)\psi^\dagger{}_{\lambda'}(0)\rangle$
Feynman Diagrams	$\ln S = TV\sum$ [linked clusters] $= -iT\Delta E$	$\ln\frac{Z}{Z_o} = \beta V\sum$ [linked clusters] $= -\beta\Delta F$

If we apply this to the free particle Hamiltonian

$$H = \sum \epsilon_k c^\dagger{}_k c_k$$

we obtain

$$\begin{aligned}\frac{\partial c_k}{\partial\tau} &= [H, c_k] = -\epsilon_k c_k\\ \frac{\partial c^\dagger{}_k}{\partial\tau} &= [H, c^\dagger{}_k] = \epsilon_k c^\dagger{}_k\end{aligned} \tag{9.7}$$

so that

$$\left.\begin{aligned}c_k(\tau) &= e^{-\epsilon_k\tau}c_k\\ c^\dagger{}_k(\tau) &= e^{\epsilon_k\tau}c^\dagger{}_k\end{aligned}\right\} \quad (\text{p.s} \quad c^\dagger{}_k(\tau) \neq (c_k(\tau))^\dagger \quad). \tag{9.8}$$

Notice a key difference to the real-time formalism: in the imaginary time Heisenberg representation, creation and annihilation operator are no longer Hermitian conjugates.

We go on next, to develop the Interaction representation, which freezes time-evolution from the non-interacting part of the Hamiltonian H_0, so that

$$|\psi_I(\tau)\rangle = e^{H_0\tau}|\psi_s(\tau)\rangle = e^{H_0\tau}e^{-H\tau}|\psi_H\rangle = U(\tau)|\psi_H\rangle$$

where $U(\tau) = e^{H_0\tau}e^{-H\tau)}$ is the time evolution operator. The relationship between the Heisenberg and the interaction representation of operators is given by

$$A_H(\tau) = e^{H\tau}A_S e^{-H\tau} = U^{-1}(\tau)A_I(\tau)U(\tau)$$

In the interaction representation, states can be evolved between two times as follows

$$|\psi_I(\tau_1)\rangle = U(\tau_1)U^{-1}(\tau_2))|\psi_I(\tau_2)\rangle = S(\tau_1,\tau_2)|\psi_I(\tau_2)\rangle$$

The equation of motion for $U(\tau)$ is given by

$$\begin{aligned}-\frac{\partial}{\partial\tau}U(\tau) &= -\frac{\partial}{\partial\tau}\left[e^{H_o\tau}e^{-H\tau}\right]\\ &= e^{H_o\tau}Ve^{-H\tau}\\ &= e^{H_o\tau}Ve^{-H_o\tau}U(\tau)\\ &= V_I(\tau)U(\tau)\end{aligned} \tag{9.9}$$

and a similar equation applies to $S(\tau_1,\tau_2)$,

$$-\frac{\partial}{\partial\tau}S(\tau_1,\tau_2) = V_I(\tau_1)S(\tau_1,\tau_2). \tag{9.10}$$

These equations parallel those in real time, and following exactly analogous procedures, we deduce that the imaginary time evolution operator in the interaction representation is given by a time-ordered exponential, as follows

$$\begin{aligned}U(\tau) &= T\exp\left[-\int_0^\tau V_I(\tau)d\tau\right]\\ S(\tau_1,\tau_2) &= T\exp\left[-\int_{\tau_1}^{\tau_2} V_I(\tau)d\tau\right].\end{aligned} \tag{9.11}$$

One of the immediate applications of these results, is to provide a perturbation expansion for the partition function. We can relate the partition function to the time-evolution operator in the interaction representation as follows

$$\begin{aligned}Z &= \text{Tr}\left[e^{-\beta H}\right] = \text{Tr}\left[e^{-\beta H_o}U(\beta)\right]\\ &= \overbrace{\text{Tr}\left[e^{-\beta H_0}\right]}^{Z_0}\overbrace{\left(\frac{\text{Tr}\left[e^{-\beta H_o}U(\beta)\right]}{\text{Tr}\left[e^{-\beta H_0}\right]}\right)}^{\langle U(\beta)\rangle_0}\\ &= Z_0\langle U(\beta)\rangle_0\end{aligned} \tag{9.12}$$

enabling us to write the ratio of the interacting, to the non-interacting partition function as the expectation value of the time-ordered exponential in the non-interacting system.

$$\boxed{\frac{Z}{Z_0} = e^{-\beta\Delta F} = \langle T\exp\left[-\int_0^\beta V_I(\tau)d\tau\right]\rangle} \tag{9.13}$$

Notice how the logarithm of this expression gives the shift in Free energy resulting from interactions. The perturbative expansion of this relation in powers of V is basis for the finite temperature Feynman diagram approach.

9.2 Imaginary Time Green Functions

The finite temperature Green function is defined to be

$$\mathcal{G}_{\lambda\lambda'}(\tau-\tau') = -\langle T\psi_\lambda(\tau)\psi_{\lambda'}{}^\dagger(\tau')\rangle = -Tr\left[e^{-\beta(H-F)}\psi_\lambda(\tau)\psi_{\lambda'}{}^\dagger(\tau')\right] \tag{9.14}$$

where ψ_λ can be either a fermionic or bosonic field, evaluated in the Heisenberg representation, $F = -T\ln Z$ is the Free energy. The T inside the angle brackets the time-ordering operator. Provided H is time independent, time-translational invariance insures that $\mathcal{G}$ is solely a function of the time difference $\tau - \tau'$. In most cases, we will refer to situations where the quantum number λ is conserved, which will permit us to write

$$\mathcal{G}_{\lambda\lambda'}(\tau) = \delta_{\lambda\lambda'}\mathcal{G}_\lambda(\tau).$$

For the case of continuous quantum numbers λ, such as momentum, it is convention to promote the quantum number into the argument of the Green function, writing $\mathcal{G}(\mathbf{p},\tau)$ rather than $\mathcal{G}_{\mathbf{p}}(\tau)$.

As an example, consider a non-interacting system with Hamiltonian

$$H = \sum \epsilon_\lambda\psi^\dagger{}_\lambda\psi_\lambda, \tag{9.15}$$

where $\epsilon_\lambda = E_\lambda - \mu$ is the one-particle energy, shifted by the chemical potential. Here, the equal time expectation value of the fields is

$$\langle\psi_{\lambda'}{}^\dagger\psi_\lambda\rangle = \delta_{\lambda\lambda'}\begin{cases} n(\epsilon_\lambda) & \text{(Bosons)}\\ f(\epsilon_\lambda) & \text{(Fermions)}\end{cases} \tag{9.16}$$

where

$$\begin{aligned}n(\epsilon_\lambda) &= \frac{1}{e^{\beta\epsilon_\lambda - 1}}\\ f(\epsilon_\lambda) &= \frac{1}{e^{\beta\epsilon_\lambda + 1}}\end{aligned} \tag{9.17}$$

are the Bose and Fermi functions respectively. Similarly,

$$\langle\psi_\lambda\psi^\dagger{}_{\lambda'}\rangle = \delta_{\lambda\lambda'} \pm \langle\psi_{\lambda'}{}^\dagger\psi_\lambda\rangle = \delta_{\lambda\lambda'}\begin{cases} 1 + n(\epsilon_\lambda) & \text{(Bosons)}\\ 1 - f(\epsilon_\lambda) & \text{(Fermions)}\end{cases} \tag{9.18}$$

Using the time evolution of the operators,

$$\begin{aligned}\psi_\lambda(\tau) &= e^{-\epsilon_\lambda\tau}\psi_\lambda(0)\\ \psi^\dagger{}_\lambda(\tau) &= e^{\epsilon_\lambda\tau}\psi^\dagger{}_\lambda(0)\end{aligned} \tag{9.19}$$

we deduce that

$$\mathcal{G}_{\lambda\lambda'}(\tau-\tau') = -\left[\theta(\tau-\tau')\langle\psi_{\lambda'}{}^\dagger\psi_\lambda\rangle + \zeta\theta(\tau'-\tau)\langle\psi_{\lambda'}{}^\dagger\psi_\lambda\rangle\right]e^{-\epsilon_\lambda(\tau-\tau')} \tag{9.20}$$

where we have re-introduced $\zeta = 1$ for Bosons and -1 for fermions, from Chapter 8. If we now write $\mathcal{G}_{\lambda\lambda'}(\tau-\tau') = \delta_{\lambda\lambda'}\mathcal{G}_\lambda(\tau-\tau')$, then

$$\mathcal{G}_\lambda(\tau) = -e^{-\epsilon_\lambda\tau}.\begin{cases}[(1+n(\epsilon_\lambda))\theta(\tau) + n(\epsilon_\lambda)\theta(-\tau)] & \text{(Bosons)}\\ [(1-f(\epsilon_\lambda))\theta(\tau) - f(\epsilon_\lambda)\theta(-\tau)] & \text{(Fermions)}\end{cases} \tag{9.21}$$

There are several points to notice about this Green's function:

- Apart from prefactors, at zero temperature the imaginary time Green's function $\mathcal{G}_\lambda(\tau)$ is equal to zero-temperature Green's function $G_\lambda(t)$, evaluated at a time $t = -i\tau$, $\mathcal{G}_\lambda(\tau) = -iG_\lambda(-i\tau)$.
- If $\tau < 0$ the Green function satisfies the relation

  $$\mathcal{G}_{\lambda\lambda'}(\tau+\beta) = \zeta\mathcal{G}_{\lambda\lambda'}(\tau)$$

  so that the bosonic Green function is periodic in imaginary time, while the fermionic Green function is antiperiodic in imaginary time, with period β.

9.2.1 Periodicity and Antiperiodicity

The (anti) periodicity observed in the last example is actually a general property of finite temperature Green functions. To see this, take $-\beta < \tau < 0$, then we can expand the Green function as follows

$$\begin{aligned}\mathcal{G}_{\lambda\lambda'}(\tau) &= \zeta\langle\psi^\dagger{}_{\lambda'}(0)\psi_\lambda(\tau)\rangle\\ &= \zeta\text{Tr}\left[e^{-\beta(H-F)}\psi^\dagger{}_{\lambda'}e^{\tau H}\psi_\lambda e^{-\tau H}\right]\end{aligned} \tag{9.22}$$

Now we can use the periodicity of the trace $\text{Tr}(AB) = \text{Tr}(BA)$ to cycle the operators on the left of the trace over to the right of the trace, as follows

$$\begin{aligned}\mathcal{G}_{\lambda\lambda'}(\tau) &= \zeta\text{Tr}\left[e^{\tau H}\psi_\lambda e^{-\tau H}e^{-\beta(H-F)}\psi^\dagger{}_{\lambda'}\right]\\ &= \zeta\text{Tr}\left[e^{-\beta F}e^{\tau H}\psi_\lambda e^{-(\tau+\beta)H}\psi^\dagger{}_{\lambda'}\right]\\ &= \zeta\text{Tr}\left[e^{-\beta(H+F)}e^{\tau+\beta H}\psi_\lambda e^{-(\tau+\beta)H}\psi^\dagger{}_{\lambda'}\right]\\ &= \zeta\text{Tr}\langle\psi_\lambda(\tau+\beta)\psi^\dagger{}_{\lambda'}(0)\rangle\\ &= \zeta\mathcal{G}_{\lambda\lambda'}(\tau+\beta)\end{aligned} \tag{9.23}$$

This periodicity, or antiperiodicity was noted by Matsubara. In the late 1950's, Abrikosov, Gorkov and Dzyalozinski observed that we are infact at liberty to extend the function outside $G(\tau)$ outside the range $\tau \in [-\beta,\beta]$ by assuming that this periodicity, or antiperiodicity extends indefinitely along the entire imaginary time axis. In otherwords, there need be no constraint on the value of τ in the periodic or antiperiodic boundary conditions

$$\mathcal{G}_{\lambda\lambda'}(\tau+\beta) = \pm\mathcal{G}_{\lambda\lambda'}(\tau)$$

With this observation, it becomes possible to carry out a Fourier expansion of the Green function in terms of discrete, so called „Matsubara" frequencies.

9.2.2 Matsubara Representation

The Matsubara frequencies are defined as

$$\begin{aligned}\nu_n &= 2\pi n k_B T && \text{(Boson)}\\ \omega_n &= \pi(2n+1)k_B T && \text{(Fermion).}\end{aligned} \tag{9.24}$$

where by convention, ν_n is reserved for Bosons and ω_n for fermions. These frequencies have the property that

$$\begin{aligned}e^{i\nu_n(\tau+\beta)} &= e^{i\nu_n\tau}\\ e^{i\omega_n(\tau+\beta)} &= -e^{i\omega_n\tau}\end{aligned} \tag{9.25}$$

The periodicity or antiperiodicity of the Green function is then captured by expanding it as a linear sum of these functions:

$$\mathcal{G}_{\lambda\lambda'}(\tau) = \begin{cases} T\sum_n \mathcal{G}_{\lambda\lambda'}(i\nu_n)e^{-i\nu_n\tau} & \text{Boson}\\ T\sum_n \mathcal{G}_{\lambda\lambda'}(i\omega_n)e^{-i\omega_n\tau} & \text{Fermion}\end{cases} \tag{9.26}$$

and the inverse of these relations is given by

$$\mathcal{G}_{\lambda\lambda'}(i\alpha_n) = \int_0^\beta d\tau \mathcal{G}_{\lambda\lambda'}(\tau)e^{i\alpha_n\tau}, \qquad (\alpha_n = \{\text{Matsubara frequency}\}) \tag{9.27}$$

Example : Free Fermions and Free Bosons

For example, let us use (9.27) to derive the propagator for non-interacting fermions or bosons with $H = \sum \epsilon_\lambda \psi^\dagger{}_\lambda \psi_\lambda$. For fermions, the Matsubara frequencies are $i\omega_n = \pi(2n+1)k_B T$ so using the real time propagator(9.21), we obtain

$$\begin{aligned}\mathcal{G}_\lambda(i\omega_n) &= -\int_0^\beta d\tau e^{(i\omega_n-\epsilon_\lambda)\tau}\overbrace{(1-f(\epsilon_\lambda))}^{[1+e^{-\beta\epsilon_\lambda}]^{-1}}\\ &= -\frac{1}{i\omega_n-\epsilon_\lambda}\frac{\overbrace{(e^{(i\omega_n-\epsilon_\lambda)}-1)}^{-1}}{1+e^{-\beta\epsilon_\lambda}}\end{aligned} \tag{9.28}$$

so that

$$\boxed{\mathcal{G}_\lambda(i\omega_n) = \frac{1}{i\omega_n-\epsilon_\lambda} \qquad \textbf{Free Fermions}} \tag{9.29}$$

In a similar way, for Free Bosons, where the Matsubara frequencies are $i\nu_n = \pi 2nk_BT$, using (9.27) and (9.21), we obtain

$$\mathcal{G}_\lambda(i\nu_n) = -\delta_\lambda\int_0^\beta d\tau e^{(i\nu_n-\epsilon_\lambda)\tau}\overbrace{(1+n(\epsilon_\lambda))}^{[1-e^{-\beta\epsilon_\lambda}]^{-1}}$$

$$= -\frac{1}{i\nu_n-\epsilon_\lambda}\frac{\overbrace{(e^{(i\nu_n-\epsilon_\lambda)}-1)}^{-1}}{1-e^{-\beta\epsilon_\lambda}} \tag{9.30}$$

so that

$$\boxed{\mathcal{G}_\lambda(i\nu_n) = -\frac{1}{i\nu_n-\epsilon_\lambda} \qquad \textbf{Free Bosons}} \tag{9.31}$$

Remarks

- Notice how the finite temperature propagators (9.29) and (9.31) are essentially identical for free fermions and bosons. All the information about the statistics is encoded in the Matsubara frequencies.
- With the replacement $\omega \to i\omega_n$ the finite temperature propagator for Free fermions (9.29) is essentially identical to the zero temperature propagator, but notice that the inconvenient $i\delta\text{sign}(\epsilon_\lambda)$ in the denominator has now disappeared.

Example: Finite temperature Propagator for the Harmonic Oscillator

As a second example, let us calculate the finite temperature Green function

$$D(\tau) = -\langle Tx(\tau)x(0)\rangle \tag{9.32}$$

and its corresponding propagator

$$D(i\nu) = \int_0^\beta e^{i\nu_n\tau}D(\tau) \tag{9.33}$$

for the simple harmonic oscillator

$$\begin{aligned}H &= \hbar\omega(b^\dagger b + \frac{1}{2})\\ x &= \sqrt{\frac{\hbar}{2m\omega}}(b+b^\dagger)\end{aligned} \tag{9.34}$$

Expanding the Green function in terms of the creation and annihilation operators, we have

$$\begin{aligned}D(\tau) &= -\frac{\hbar}{2m\omega}\langle T(b(\tau)+b^\dagger(\tau))(b(0)+b^\dagger(0))\rangle\\ &= -\frac{\hbar}{2m\omega}\left(\langle Tb(\tau)b^\dagger(0)\rangle + \langle Tb^\dagger(\tau)b(0)\rangle\right),\end{aligned} \tag{9.35}$$

where terms involving two creation or two annihilation operators vanish. Now using the derivations that led to (9.21)

$$-\langle Tb(\tau)b^\dagger(0)\rangle = \mathcal{G}(\tau) = -[(1+n(\omega))\theta(\tau)+n(\omega)\theta(-\tau)]e^{-\omega\tau}. \tag{9.36}$$

and

$$\begin{aligned}-\langle Tb^\dagger(\tau)b(0)\rangle &= -[n(\omega)\theta(\tau)+(1+n(\omega))]e^{\omega\tau}\\ &= [(1+n(-\omega))\theta(\tau)+n(-\omega)\theta(-\tau)]e^{\omega\tau}.\end{aligned} \tag{9.37}$$

which corresponds to $-\mathcal{G}(\tau)$ with the sign of ω inverted. With this observation,

$$D(\tau) = \frac{\hbar}{2m\omega}\left[G(\tau) - \{\omega\to-\omega\}\right]. \tag{9.38}$$

When we Fourier transform the first term inside the brackets, we obtain $\frac{1}{i\nu_n-\omega}$, so that

$$\begin{aligned}D(i\nu_n) &= \frac{\hbar}{2m\omega}\left[\frac{1}{i\nu_n-\omega}-\frac{1}{i\nu_n+\omega}\right]\\ &= \frac{\hbar}{2m\omega}\left[\frac{2\omega}{(i\nu_n)^2-\omega^2}\right].\end{aligned} \tag{9.39}$$

This expression is identical to the corresponding zero temperature propagator, evaluated at frequency $z = i\nu_n$.

Example: Consider a system of non-interacting Fermions, described by the Hamiltonian $H = \sum_\lambda \epsilon_\lambda c^\dagger{}_\lambda c_\lambda$ where $\epsilon_\lambda = E_\lambda - \mu$ and E_λ is the energy of a one-particle eigenstate and μ is the chemical potential.

Show that the total number of particles in equilibrium is

$$N(\mu) = T\sum \mathcal{G}_\lambda(i\omega_n)e^{i\omega_n O^+}$$

where $G_\lambda(i\omega_n) = (i\omega_n - \epsilon_\lambda)^{-1}$ is the Matsubara propagator. Using the relationship $N = -\partial F/\partial\mu$ show that that Free energy is given by

$$F(T,\mu) = -k_BT\sum_{\lambda,i\omega_n}\ln\left[-\mathcal{G}_\lambda(i\omega_n)^{-1}\right]e^{i\omega_n O^+} + C(T) \tag{9.40}$$

<u>*Solution:*</u> The number of particles in state λ can be related to the equal time Green's function as follows

$$N_\lambda = \langle c^\dagger{}_\lambda c_\lambda\rangle = -\langle Tc_\lambda(0^-)c^\dagger{}_\lambda\rangle = \mathcal{G}_\lambda(0^-).$$

Rewriting $G_\lambda(\tau) = T\sum_{i\omega_n}\mathcal{G}_\lambda e^{-i\omega_n\tau}$, we obtain

$$N(\mu) = \sum_\lambda N_\lambda = T\sum_{\lambda,i\omega_n}\mathcal{G}_\lambda(i\omega_n)e^{i\omega_n 0^+}$$

Now since $-\partial F/\partial\mu = N(\mu)$, it follows that

$$\begin{aligned}F &= -\int^\mu d\mu N(\mu) = -T\sum_{\lambda,i\omega_n}\int^\mu d\mu\frac{e^{i\omega_n O^+}}{i\omega_n - E_\lambda+\mu}\\ &= -T\sum_{\lambda,i\omega_n}\ln\left[\epsilon_\lambda - i\omega_n\right]e^{i\omega_n O^+}\\ &= -T\sum_{\lambda,i\omega_n}\ln\left[-\mathcal{G}_\lambda(i\omega_n)^{-1}\right]e^{i\omega_n O^+} + C(T).\end{aligned} \tag{9.41}$$

We shall shortly see that $C = 0$ using Contour integral methods.

Example: Consider the an electron gas where the spins are coupled to a magnetic field, so that $\epsilon_\lambda \equiv \epsilon_{\mathbf{k}} - \mu_B\sigma B$. Write down an expression for the magnetization and by differentiating w.r.t the field B, show that the temperature dependent magnetic susceptibility is given by

$$\chi(T) = \frac{\partial M}{\partial B} = -2\mu_B^2 k_BT\sum_{\mathbf{k},i\omega_n}G(k)^2$$

where $\mathcal{G}(k) \equiv G(\mathbf{k}, i\omega_n)$ is the Matsubara propagator.

<u>*Solution:*</u> The magnetization is given by

$$M = \mu_B\sum_{\lambda,\sigma}\sigma\langle c^\dagger{}_{\mathbf{k}\sigma}c_{\mathbf{k}\sigma}\rangle = \mu_BT\sum_{\mathbf{k}\sigma,\mathbf{i}\omega_\mathbf{n}}\sigma\mathcal{G}_\sigma(\mathbf{k}, i\omega_n)e^{i\omega_n 0^+}$$

Differentiating this w.r.t. B and then setting $B = 0$, we obtain

$$\begin{aligned}\chi &= \frac{\partial M}{\partial B}\bigg| B = 0 = -\mu_B^2T\sum_{\mathbf{k}\sigma\mathbf{i}\omega_\mathbf{n}}\sigma^2\mathcal{G}_\sigma(\mathbf{k}, i\omega_n)^2\bigg|_{B=0}\\ &= -2\mu_B^2k_BT\sum_{\mathbf{k},i\omega_n}G(k)^2\end{aligned} \tag{9.42}$$

9.3 The contour integral method

In practice, we shall do almost all of our finite temperature calculations in the frequency domain. To obtain practical results, we will need to be able to sum over the Matsubara frequencies, and this forces us to make an important technical digression. As an example of the kind of tasks we might want to carry out, consider how we would calculate the occupancy of a given momentum state in a Fermi gas at finite temperature, using the Matsubara propagator $G(\mathbf{p}, i\omega_n)$. This can be written in terms of the equal time Green function, as follows

$$\langle c^\dagger{}_{\mathbf{p}\sigma}c_{\mathbf{p}\sigma}\rangle = \mathcal{G}(\mathbf{p}, 0^-) = T\sum_n\frac{1}{i\omega_n - \epsilon(\mathbf{p})}e^{i\omega_n O^+}. \tag{9.43}$$

A more involved example, is the calculation of the finite temperature dynamical spin susceptibility $\chi(q)$ of the Free electron gas at wavevector and frequency $q \equiv (\mathbf{q}, i\nu_n)$. We shall see that this quantity derives from a Feynman polarization bubble diagram which gives

$$\chi(q) = -2\mu_B^2 T\sum_p \mathcal{G}(p+q)\mathcal{G}(p) = 2\mu_B^2\sum_{\mathbf{p}}\left(k_BT\sum_r G(\mathbf{p}+\mathbf{q}, i\omega_r + i\nu_n)G(\mathbf{p}, i\omega_r)\right).(9.44)$$

where the -1 derives from the Fermion loop. In both cases, we need to know how to do the sum over he discrete Matsubara frequencies, and to do this, we use the method of contour integration. To make this possible, observe that the Fermi function $f(z) = 1/[e^{z\beta}+1]$ has poles of strength $-k_BT$ at each discrete frequency $z = i\omega_n$, because

$$f(i\omega_n + \delta) = \frac{1}{e^{\beta(i\omega_n+\delta)}+1} = -\frac{1}{\beta\delta} = -\frac{k_BT}{\delta}$$

so that for a general function $F(i\omega_n)$, we may write

$$k_BT\sum_n F(i\omega_n) = -\int_C \frac{dz}{2\pi i}F(z)f(z) \tag{9.45}$$

where the contour integral C is to be taken anticlockwise around the poles at $z = i\omega_n$ as shown in Fig. 9.3 (a)

Once we have cast the sum as a contour integral, we may introduce "null" contours (Fig. 9.3 (b)) which allow us to distort the original contour C into the modified contour C' shown in Fig. 9.3 (c), so that now

$$k_BT\sum_n F(i\omega_n) = -\int_{C'} \frac{dz}{2\pi i}F(z)f(z) \tag{9.46}$$

where C' runs *clockwise* around all the poles and branch-cuts in $F(z)$. Here we have used "Jordan's lemma" which guarantees that the contribution to the integral from the contour at infinity vanishes, provided the function $F(z)\times f(z)$ dies away faster than $1/|z|$ over the whole contour.

For example, in case (9.43), $F(z) = \frac{e^{z0^+}}{z-\epsilon_{\mathbf{p}}}$, so that $F(z)$ has a single pole at $z = \epsilon_{\mathbf{p}}$, and hence

$$\begin{aligned}\langle n_{\mathbf{p}\sigma}\rangle &= T\sum_n \frac{1}{i\omega_n - \epsilon(\mathbf{p})}e^{i\omega_n O^+} = -\int_{C'}\frac{dz}{2\pi i}\frac{1}{z-\epsilon_{\mathbf{p}}}e^{z0^+}f(z)\\ &= f(\epsilon_{\mathbf{p}}),\end{aligned} \tag{9.47}$$

recovering the expected result. In this example, the convergence factor e^{z0^+} that results from the small negative time increment in the Green function, plays an important role inside the Contour integral, where it gently forces the function $F(z)$ to die away faster than $1/|z|$ in the negative half-plane. Of course the original contour C integral could have been made by arbitrarily replacing $f(z)$ with $f(z)-$constant. However, the requirement that the function dies away in the positive half plane forces us to set the constant term here to zero.

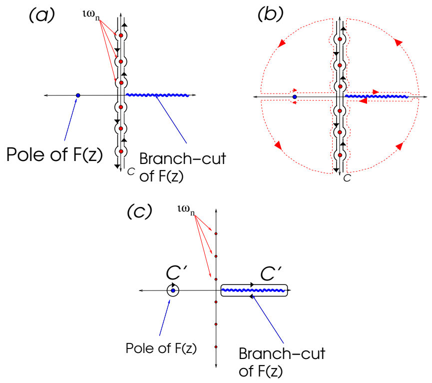


Figure 9.3: (a) Contour integration around the poles in the Fermi function enables us to convert a discrete Matsubara sum $T\sum F(i\omega_n)$ to a continuous integral (b) The integral can be distorted around the poles and branch-cuts of $F(z)$ provided that $F(z)$ dies away faster than $1/|z|$ at infinity.

In the second example (9.44)

$$F(z) = G(\mathbf{p}+\mathbf{q}, i\nu_n + z)G(\mathbf{p}, z) = \frac{1}{i\nu_n + z - \epsilon_{\mathbf{p}+\mathbf{q}}}\frac{1}{z-\epsilon_{\mathbf{p}}}$$

which has two poles at $z = \epsilon_{\mathbf{p}}$ and $z = -i\nu_n + \epsilon_{\mathbf{p}+\mathbf{q}}$. The integral for this case is then given by

$$\begin{aligned}\chi(q) &= 2\mu_B^2\sum_{\mathbf{p}}\int_{C'}\frac{dz}{2\pi i}G(\mathbf{p}+\mathbf{q}, z+i\nu_n)G(\mathbf{p}, z)f(z)\\ &= -\sum_{\mathbf{p}}\left(G(\mathbf{p}, -i\nu_n + \epsilon_{\mathbf{p}+\mathbf{q}})f(-i\nu_n + \epsilon_{\mathbf{p}+\mathbf{q}}) + G(\mathbf{p}+\mathbf{q}, \epsilon_{\mathbf{p}})f(\epsilon_{\mathbf{p}})\right)\end{aligned} \tag{9.48}$$

The first term in the above expression deserves some special attention. In this term we

shall make use the periodicity of the Fermi function to replace

$$f(-i\nu_n + \epsilon_{\mathbf{p}+\mathbf{q}}) = f(\epsilon_{\mathbf{p}+\mathbf{q}}).$$

This replacement may seem obvious, however, later, when we analytically extending $i\nu_n \to z$ we will keep this quantity *fixed*, i.e, we will not analytically extend $f(-i\nu_n + \epsilon_{\mathbf{p}+\mathbf{q}}) \to f(-z+\epsilon_{\mathbf{p}+\mathbf{q}})$. In other words, the Matsubara sum and the replacement $i\nu_n \to z$ are not to be commuted. With this understanding, we continue, and find that the resulting expression is given by

$$\chi(\mathbf{q}, i\nu_n) = 2\mu_B^2\sum_{\mathbf{p}}\left(\frac{f_{\mathbf{p}+\mathbf{q}} - f_{\mathbf{p}}}{i\nu_n - (\epsilon_{\mathbf{p}+\mathbf{q}} - \epsilon_{\mathbf{p}})}\right) \tag{9.49}$$

where we have used the shorthand $f_{\mathbf{p}} \equiv f(\epsilon_{\mathbf{p}})$. The analytic extension of this quantity is then

$$\chi(\mathbf{q}, z) = 2\mu_B^2\sum_{\mathbf{p}}\left(\frac{f_{\mathbf{p}+\mathbf{q}} - f_{\mathbf{p}}}{z - (\epsilon_{\mathbf{p}+\mathbf{q}} - \epsilon_{\mathbf{p}})}\right) \tag{9.50}$$

A completely parallel set of procedures can be carried for summation over Matsubara boson frequencies $i\nu_n$, by making the observation that the Bose function $n(z) = \frac{1}{e^{\beta z}-1}$ has a string of poles at $z = i\nu_n$ of strength k_BT. Using a completely parallel procedure to the fermions, we obtain

$$k_BT\sum_n P(i\nu_n) = \int_C \frac{dz}{2\pi i}P(z)n(z) = \int_{C'}\frac{dz}{2\pi i}P(z)n(z)$$

where C is an anticlockwise integral around the imaginary axis and C' is a clockwise integral around the poles and branch-cuts of $F(z)$. (See problem 9.1.)

Example: Starting with the expression

$$F = -T\sum_{\lambda i\omega_n}\ln[(\epsilon_\lambda - i\omega_n)e^{i\omega_n 0^+} + C(T)$$

derived in example (9.1), use the contour integration method to show that

$$F = -T\sum_\lambda \ln\left[1 + e^{-\beta\epsilon_\lambda}\right] + C(T)$$

so that $C(T) = 0$.

Solution: Writing the Free energy as a contour integral around the poles of the imaginary axis, we have

$$F = \sum_\lambda\int_P \frac{dz}{2\pi i}f(z)\ln\left[\epsilon_\lambda - z\right]e^{z0^+} + C(T)$$

where the path P runs anticlockwise around the imaginary axis. There is a branch cut in the function $F(z) = \ln[\epsilon_\lambda - z]$ running from $z = \epsilon_\lambda$ to $z = +\infty$. If we distort the contour P around this branch-cut, we obtain

$$F = \sum_\lambda\int_{P'}\frac{dz}{2\pi i}f(z)\ln\left[\epsilon_\lambda - z\right]e^{z0^+} + C(T)$$

where P' runs clockwise around the branch cut, so that

$$\begin{aligned}F &= \sum_\lambda\int_{\epsilon_\lambda}^\infty \frac{d\omega}{\pi}f(\omega) + C(T)\\ &= \sum_\lambda -T\ln(1+e^{-\beta\epsilon_\lambda}) + C(T)\end{aligned} \tag{9.51}$$

so that $C(T) = 0$, to reproduce the standard expression for the Free energy of a set of non-interacting fermions.

9.4 Generating Function and Wick's theorem

The zero temperature generating functions for Free fermions or bosons, derived in chapter 7. can be generalized to finite temperatures. Quite generally we can consider adding a source term to a free particle Hamiltonian to form $H(\tau) = H_0 + V(\tau)$,

$$\left.\begin{aligned}H_0 &= \sum\epsilon{\psi^\dagger}_\lambda\psi_\lambda\\ V(\tau) &= -\textstyle\sum_\lambda \bar{z}(\tau)\psi_\lambda + {\psi^\dagger}_\lambda z(\tau)\end{aligned}\right\} \tag{9.52}$$

The corresponding finite temperature Generating functional is actually the partition function in the presence of the perturbation V. Using a simple generalization of (9.13), we have

$$\begin{aligned}Z_0[\bar{z}, z] &= Z_0\langle Te^{-\int_0^\beta V_I(\tau)d\tau}\rangle_0\\ &= Z_0\langle T\exp\left[\int_0^\beta d\tau\sum_\lambda\left(\bar{z}_\lambda(\tau)\psi_\lambda(\tau) + {\psi^\dagger}_\lambda(\tau)z_\lambda(\tau)\right)\right]\rangle_0\end{aligned} \tag{9.53}$$

where the driving terms are complex numbers for bosons, but are anticommuting C-numbers or Grassman numbers, for fermions. For free fields, the Generating functional is given by

$$\boxed{\begin{aligned}\frac{Z_0[\bar{z}, z]}{Z_0} &= \exp\left[-\sum_\lambda\int_0^\beta d\tau_1 d\tau_2\bar{z}_\lambda(1)G_\lambda(\tau_1-\tau_2)z_\lambda(2)\right]\\ G_\lambda(\tau_1-\tau_2) &= -\langle T\psi_\lambda(\tau_1){\psi^\dagger}_\lambda(\tau_2)\rangle \qquad (9.54)\end{aligned}}$$

A detailed proof of this result is given in Appendix A of this chapter. However, a heuristic proof is obtained by appealing to the "Gaussian" nature of the underlying Free fields. As at zero temperature, we expect the the physics to be entirely Gaussian, that is, that the amplitudes of fluctuation of the free fields are entirely independent of the driving terms. The usefulness of the generating function, is that we can convert partial derivatives with respect to the source terms into field operators inside the expectation values,

$$\begin{aligned}\frac{\delta}{\delta\bar z(1)} &\rightarrow \psi_{\lambda_1}{}^{\dagger}(1),\\ \frac{\delta}{\delta z(2)} &\rightarrow \psi^{\dagger}(2)\end{aligned}\tag{9.55}$$

(where we have used the short-hand notation $z(1)\equiv z_\lambda(\tau_1)$, $\psi(1)\equiv\psi_\lambda(\tau_1)$), so that in particular

$$\frac{\delta\ln Z_0[\bar z,z]}{\delta z_\lambda(2)} = \langle\psi^\dagger(2)\rangle\tag{9.56}$$

where the derivative of the logarithm of $Z_0[\bar z,z]$ is required to place a $Z_0[\bar z,z]$ in the denominator for the correctly normalized expectation value. Likewise,

$$\begin{aligned}\frac{\delta^2\ln Z_0[\bar z,z]}{\delta\bar z(1)\delta z(2)} &= \frac{1}{Z_0[\bar z,z]}\frac{\delta}{\delta\bar z(1)}\left[\frac{1}{Z_0[\bar z,z]}\frac{\delta Z_0[\bar z,z]}{\delta z(2)}\right]\\ &= \frac{1}{Z_0[\bar z,z]}\frac{\delta^2 Z_0[\bar z,z]}{\delta\bar z(1)\delta z(2)} - \frac{1}{Z_0[\bar z,z]}\left[\frac{\delta Z_0[\bar z,z]}{\delta\bar z(1)}\right]\frac{1}{Z_0[\bar z,z]}\left[\frac{\delta Z_0[\bar z,z]}{\delta z(2)}\right]\\ &= \langle\psi(1)\psi^\dagger(2)\rangle - \langle\psi(1)\rangle\langle\psi^\dagger(2)\rangle\\ &= \langle(\psi(1)-\langle\psi(1)\rangle)\left(\psi^\dagger(2)-\langle\psi^\dagger(2)\rangle\right)\rangle\end{aligned}\tag{9.57}$$

which represents the fluctuation of the field ψ around its mean value. If this quantity is independent of the source terms, then it follows that the fluctuations must be equal to their value in the absence of any source field, i.e.

$$\frac{\delta^2\ln Z_0[\bar z,z]}{\delta\bar z_\lambda(\tau_1)\delta z_\lambda(\tau_2)} = -\mathcal{G}_\lambda(\tau_1-\tau_2).$$

A more detailed, algebraic rederivation of this result is given in Appendix A. One of the immediate corollaries of (**??**) is that the multi-particle Green functions can be entirely decomposed in terms of one-particle Green functions, i.e., the imaginary time Green functions obey a Wick's theorem. If we decompose the original generating function (9.126) into a power series, we find that the general coefficient of the source terms is given by

$$(-1)^n\mathcal{G}(1,2,\dots n;1',2',\dots n') = \langle T\psi(1)\dots\psi(n)\psi^\dagger(n')\dots\psi(1')\rangle$$

by contrast, if we expand the right-hand side of (9.127) in the same way, we find that the same coefficient is given by

$$(-1)^n\sum_P(\zeta)^p\prod_{r=1}^n\mathcal{G}(r-P_r)$$

where p is the number of pairwise permutations required to produce the permutation P. Comparing the two results, we obtain the imaginary time Wick's theorem

$$\boxed{\mathcal{G}(1,2,\dots n;1',2',\dots n') = \sum_P(-1)^p\prod_{r=1}^n\mathcal{G}(r-P_r)}$$

Although this result is the precise analog of the zero-temperature Wick's theorem, notice that that unlike its zero-temperature counterpart, we can not easily derive this result for simple cases by commuting the destruction operators operators so that they annihilate against the vacuum, since there is no finite temperature vacuum.

Just as in the zero temperature case, we can define a "contraction" as the process of connecting two free -field operators inside the correlation function,

$$\langle T[\dots\psi(\mathbf{1})\dots\psi^\dagger(\mathbf{2})\dots]\rangle \longrightarrow \langle T[\psi(\mathbf{1})\psi^\dagger(\mathbf{2})]\rangle = -G(\mathbf{1}-\mathbf{2})$$

$$\langle T[\dots\psi^\dagger(\mathbf{2})\dots\psi(\mathbf{1})\dots]\rangle \longrightarrow \langle T[\psi^\dagger(\mathbf{2})\psi(\mathbf{1})]\rangle = -\zeta G(\mathbf{1}-\mathbf{2})$$

so that as before,

$$\begin{aligned}&(-1)^n\langle T[\psi(\mathbf{1})\psi(\mathbf{2})\dots\psi(\mathbf{n})\dots\psi^\dagger(\mathbf{P'_2})\dots\psi^\dagger(\mathbf{P'_1})\dots\psi^\dagger(\mathbf{P'_n})]\rangle\\ &= \zeta^P G(\mathbf{1}-P'_1)G(\mathbf{2}-P'_2)\dots G(\mathbf{n}-P'_n).\end{aligned}\tag{9.58}$$

Example:

Use Wick's theorem to calculate the interaction energy of a dilute Bose gas of spin S bosons particles interacting via a the interaction

$$\hat V = \frac{1}{2}\sum_{q,k\sigma,k',\sigma'}V(q)b^\dagger{}_{k+q\sigma}b^\dagger{}_{k'\sigma'}b_{k'+q\sigma'}b_{k\sigma}$$

at a temperature above the Bose Einstein condensation temperature.

Solution: To leading order in the interaction strength, the interaction energy is given by

$$\langle V\rangle = \sum_{q,k,k',\sigma,\sigma'}V(q)\langle b^\dagger{}_{k+q,\sigma}b^\dagger{}_{k',\sigma'}b_{k'+q,\sigma'}b_{k\sigma}\rangle$$

Using Wick's theorem, we evalute

$$\begin{aligned}\langle b^\dagger{}_{k+q,\sigma}b^\dagger{}_{k',\sigma'}b_{k'+q,\sigma'}b_{k,\sigma}\rangle &= \langle b^\dagger_{k+q,\sigma}b^\dagger_{k',\sigma'}b_{k'+q,\sigma'}b_{k,\sigma}\rangle + \langle b^\dagger_{k+q,\sigma}b^\dagger_{k',\sigma'}b_{k'+q,\sigma'}b_{k,\sigma}\rangle\\ &= n_k n_{k'}\delta_{q,0} + n_k n_{k+q}\delta_{k,k'}\delta_{\sigma\sigma'}\end{aligned}\tag{9.59}$$

so that

$$\langle\hat V\rangle = \frac{1}{2}\int_{\mathbf{k},\mathbf{k}'}n_k n_{k'}\left[(2S+1)^2V_{q=0} + (2S+1)V_{k-k'}\right]$$

where $n_{\mathbf{k}} = \frac{1}{e^{\beta(\epsilon_{\mathbf{k}}-\mu)}-1}$.

9.5 Feynman diagram expansion

We are now ready to generalize the Feynman approach to finite temperatures. Apart from a very small change in nomenclature, almost everything we learnt for zero temperature in chapter 8 now generalizes to finite temperature. Whereas previously, we began with a Wick expansion of the S matrix, now we must carry out a Wick expansion of the partition function

$$Z = e^{-\beta F} = Z_0\langle T\exp\left[-\int_0^\beta\hat V(\tau)d\tau\right]\rangle_0 =$$

All the combinatorics of this expansion are unchanged at finite temperatures.

Now we are at finite temperature, the Free energy $F = E-ST-\mu N$ replaces the energy. The main results of this procedure can almost entirely be guessed by analogy. In particular:

- The partition function

$$Z = Z_0\sum\{\text{Unlinked Feynman diagrams }\}$$

- The change in the Free energy due to the perturbation V is given by

$$\Delta F = F-F_0 = -k_BT\ln\left[\frac{Z}{Z_0}\right] = -k_BT\sum\{\text{Linked Feynman diagrams}\}$$

  This is the finite temperature version of the linked cluster theorem.

- Matsubara one-particle Green's functions

$$\mathcal{G}(1-2) = \sum\{\text{Two-legged Feynman diagrams}\}$$

, and the main changes are

(i) the replacement of a $-i\longrightarrow -1$ in the time-ordered exponential.

(ii) the finite range of integration in time

$$\int_{-\infty}^{\infty}dt\longrightarrow\int_0^\beta d\tau$$

which leads to the discrete Matsubara frequencies.

The effect of these changes on the real-space Feynman rules is summarized in Table 9.1.

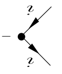
The book-keeping that leads to these diagrams now involves the redistribution of a "-1" associated with each propagator

$$\psi(2)\dots\psi^\dagger(1) \longrightarrow (i)^2\times\mathcal{G}(2-1).\tag{9.60}$$

where as before,

$$\mathcal{G}(2-1) = 2 \longleftarrow 1\tag{9.61}$$

represents the propagation of a particle from "1" to "2", but now we must redistribute an i (rather than a $\sqrt{-i}$) to each end of the progator. When these terms are redistributed onto one-particle scattering vertices, they cancel the -1 from the time-ordered exponential



$$-U(x) \quad = (i)^2\times -U(x)\equiv U(x)\tag{9.62}$$

whereas for a two-particle scattering potential $V(1-2)$, the four factors of i give a $(i)^4=1$, so that the two-particle scattering amplitude is $-V(1-2)$.

$$= (i)^4\times -V(1-2)\equiv -V(1-2).\tag{9.63}$$

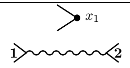
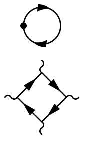
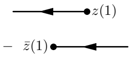
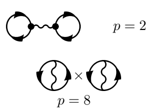
Apart from these small changes, the real-time Feynman rules are basically the same as those at zero temperature.

9.5.1 Feynman rules from Functional Derivative

As in chapter 8, we can formally derive the Feynman rules from a functional derivative formulation. Using the notation

$$\int d1d2\bar z(1)\mathcal{G}(1-2)z(2) = \bar z \longleftarrow z\tag{9.64}$$

Table. 9.1 Real Space Feynman Rules: Finite Temperature .

	$G(\mathbf{2}-\mathbf{1})$
	$U(x_1)$ $-V(\mathbf{1}-\mathbf{2})$
$\prod_i \int d^3x_i \int_0^\beta d\tau$	Integrate over all intermediate times and positions.
	$-(2S+1)G(\vec{0},0^-)$ $[-(2S+1)]^F,$ $F=$ no. Fermion loops.
	$z(1)$ $-\bar{z}(1)$
	$\frac{1}{p}$ $p=$ order of symmetry group.

where $d1$ and $d2$ implies the integration over the space-time variables $(\vec{1},\tau_1)$ and $(\vec{2},\tau_2)$ and a sum over suppressed spin variables σ_1 and σ_2, we can write the non-interacting generating functional as

$$\frac{Z_0[\bar{z},z]}{Z_0} = \langle\hat{S}\rangle_0 = \exp\Big[-\bar{z} \longleftarrow z\Big] \tag{9.65}$$

where we have used the short-hand

$$\hat{S} = T\exp\left[\int_0^\beta d1[\bar{z}(1)\psi(1)+\psi^\dagger(1)z(1)]\right]$$

Now each time we differentiate $\hat{S}$ with respect to its source terms, we bring down an additional field operator, so that

$$\begin{aligned}\frac{\delta}{\delta\bar{z}(1)}\langle T\ldots\hat{S}\rangle_0 &= \langle\ldots\psi(1)\ldots\hat{S}\rangle_0,\\ \frac{\delta}{\delta z(2)}\langle T\ldots\hat{S}\rangle_0 &= \langle T\ldots\psi^\dagger(2)\ldots\hat{S}\rangle_0\end{aligned} \tag{9.66}$$

we can formally evaluate the time-ordered expectation value of any operator $F[\psi^\dagger,\psi]$ as

$$\langle TF\left[\psi^\dagger,\psi\right]\hat{S}\rangle_0 = F[\frac{\delta}{\delta z},\frac{\delta}{\delta\bar{z}}]\exp\Big[-\bar{z} \longleftarrow z\Big]$$

so that

$$\begin{aligned}\frac{Z[\bar{z},z]}{Z_0} &= \langle Texp\left[-\int_0^\beta \hat{V}(\tau)d\tau\right]\hat{S}\rangle_0\\ &= \langle\exp\left[-\int_0^\beta d\tau V\left(\frac{\delta}{\delta z},\frac{\delta}{\delta\bar{z}}\right)\right]\exp\Big[-\bar{z} \longleftarrow z\Big]\end{aligned}$$

The formal expansion of this functional derivative generates the Feynman diagram expansion. Changing variables to $(\alpha,\bar{\alpha}) = (z,-\bar{z})$, we can remove the minus-sign associated with each propagator, to obtain

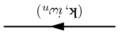
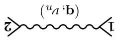
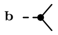
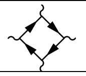
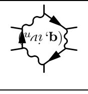
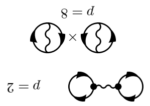
$$\frac{Z[-\bar{\alpha},\alpha]}{Z_0} = \exp\left[(-1)^n\int_0^\beta d\tau V\left(\frac{\delta}{\delta\alpha},\frac{\delta}{\delta\bar{\alpha}}\right)\right]\exp\Big[\bar{\alpha} \longleftarrow \alpha\Big] \tag{9.67}$$

for an $n-$ body interaction. The appearance of the $(-1)^n$ in the exponent indicates that we should associate a $(-1)^n$ with the corresponding scattering amplitude.

As in the case of zero temperature, we may regard (**??**) as a machine for generating a series of Feynman diagrams- both linked and unlinked, so that formally,

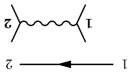
$$Z[\bar{\alpha},\alpha] = Z_0\sum\{\text{Unlinked Feynman diagrams}\}.$$

Table. 9.2 Momentum Space Feynman Rules: Finite Temperature .

	$G_o(\mathbf{k},i\omega_n)$	Fermion propagator
	$-V(q)$ $-g_q^2D_o(\mathbf{q},i\nu_n)$ $= -g_{\mathbf{q}}^2\left[\frac{2\omega_q}{(i\nu_n)^2-\omega_{\mathbf{q}}^2}\right]$	Interaction Exchange Boson.
	$U(\mathbf{q})$	Scattering potential
	$[-(2S+1)]^F,$	F= no. Fermion loops
	$T\sum_n\int\frac{d^dq}{(2\pi)^d}e^{i\alpha_n0^+}$	Sum over internal loop frequency and momenta.
	$\frac{1}{p}$	$p=$ order of symmetry group.

9.5.2 Feynman rules in frequency/momentum space

As at zero temperature, it is generally more convenient to work in Fourier space. The transformation to Fourier transform space follows precisely parallel lines to that at zero temperature, and the Feynman rules which result are summarized in Table 9.2. We first re-write each interaction line and Green's function in a Feynman diagram in terms of their Fourier transformed variables



$$\begin{aligned} &= G(X_1-X_2) = \sum_n\int\frac{d^{d-1}p}{(2\pi)^{d-1}}G(p)e^{ip(X_1-X_2)}\\ &= V(X_1-X_2) = T\sum_n\int\frac{d^{d-1}q}{(2\pi)^{d-1}}V(q)e^{iq(X_1-X_2)}\end{aligned} \tag{9.68}$$

where we have used a short-hand notation $p = (\mathbf{p},i\alpha_n)$ (where $\alpha_n = \omega_n$ for fermions, $\alpha_n = \nu_n$ for bosons), $q = (\mathbf{q},i\nu_n)$, $X = (\mathbf{x},i\tau)$, $ip.X = i\mathbf{p}\cdot\mathbf{x} - i\omega_n\tau$ and $iq.X = i\mathbf{q}\cdot\mathbf{x} - i\nu_r\tau$). As an example, consider a screened Coulomb interaction

$$V(r) = \frac{e^2}{r}e^{-\kappa r}$$

In our space time notation, we write the interaction as

$$V(X) = V(\mathbf{x},\tau) = \frac{e^2}{|\mathbf{x}|}e^{-\kappa|\mathbf{x}|}\times\tilde{\delta}(\tau)$$

Where the delta function in time arises because the interaction is instantaneous. (Subtle point: we will infact inforce periodic boundary conditions by taking the delta function to be a periodic delta function $\tilde{\delta}(\tau) = \sum_n\delta(\tau-n\beta)$). When we Fourier transform this interaction, we obtain

$$\begin{aligned}V(Q) = V(\mathbf{q},i\nu_r) &= \int d^4XV(X)e^{-iQ.X}\\ &= \int d^3x\int_0^\beta d\tau V(\mathbf{x})\tilde{\delta}(\tau)e^{-i(\mathbf{q}\cdot\mathbf{x}-\nu_r\tau)}\\ &= V(\mathbf{q}) = \frac{4\pi e^2}{q^2+\kappa^2}\end{aligned} \tag{9.69}$$

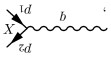
and the delta function in time translates to an interaction that is frequency independent.

We can also transform the source terms in a similar way, writing

$$\begin{aligned}z(X) &= T\sum_n\int\frac{d^{d-1}p}{(2\pi)^{d-1}}e^{ipX}z(p)\\ \bar{z}(X) &= T\sum_n\int\frac{d^{d-1}p}{(2\pi)^{d-1}}e^{-ipX}\bar{z}(p)\end{aligned}$$

(9.70)

where, $ipX = i\vec{p}\cdot\vec{x} - i\alpha_n\tau$. With these transformations, the space-time co-ordinates associated with each scattering vertex now only appear as "phase factors". By making the integral over space-time co-ordinates at each such vertex, we impose the conservation of momentum and (discrete) Matsubara frequencies at each vertex



$$= \int d^dXe^{i(p_1-p_2-q)X} = (2\pi)^3\beta\delta^{(d-1)}(\mathbf{p}_1-\mathbf{p}_2-\mathbf{q})\delta_{\alpha_1+\alpha_2-\nu_r} \quad (9.71)$$

Since momentum and frequency are conserved at each vertex, this means that there is one independent energy and frequency per loop in the Feynman diagram. To be sure that this really works, let us count the number of independent momenta that are left over after imposing a constraint at each vertex in the diagram. Consider a diagram with V vertices and P propagators. Each propagator introduces $P\times d$, momenta. When we integrate over the space-time co-ordinates of the V vertices, we must be careful to split the integral up into the integral over the $V-1$ relative co-ordinates $\tilde{X}_j = X_{j+1}-X_j$ and the center of mass co-ordinates:

$$\int\prod_{j=1}^{V}d^dX_j = \int d^dX_{CM}\int\prod_{j=1}^{V-1}d^d\tilde{X}_j$$

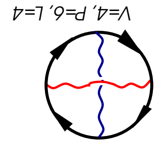
This imposes $(V-1)$ constraints per dimension, so the number of independent momenta are then

$$\text{no. of independent momenta } = d[P-(V-1)]$$

Now in a general Feynman graph, the apparent number of momentum loops is the same as the number of facets in the graph, and this is given by

$$L = \mathcal{E} + (P-V)$$

where $\mathcal{E}$ is the Euler characteristic of the object. The Euler characteristic is equal to one for planar diagrams, and equal to one plus the number of "handles" in a non-planar diagram. For example, the diagram

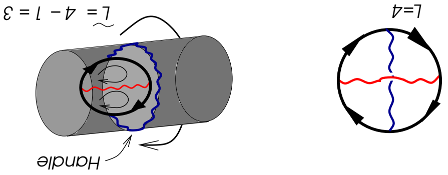


(9.72)

has $V=4$ vertices, $P=6$ propagators and it has one handle with Euler characteristic $E=2$, so that $L=6-4+2=4$ as expected. So from the above, we deduce that the number of independent momenta is given by

$$d[L-(E-1)]$$

This result needs a moments pause. One might have expected number of independent momentum loops to be equal to L. However, when there are handles, this overcounts the number of independent momentum loops - for each handle added to the diagram adds only one additional momentum loop, but L increases by 2. If you look at our one example, this diagram can be embedded on a cylinder, and the interaction propagator which loops around the cylinder only counts as one momentum loop, giving a total of $4-(2-1)=3$ independent momentum loops.



(9.73)

In this way, we see that $\tilde{L} = L + (E-1)$ *is* the correct number of independent momentum loops. Indeed, our momentum constraint does indeed convert the diagram from an integral over V space-time co-ordinates to $\tilde{L}$ independent momentum loops.

In this way, we see that the transformation from real-space, to momentum space Feynman rules is effected by replacing the sum over all internal space-time co-ordinates by an integral/sum over all loop momenta and frequencies. A convergence factor

$$e^{i\alpha_n 0^+}$$

is included in the loop integral. This term guarantees that if the loop contains a single propagator which propagates back to the point from which it eminated, then the corresponding contraction of field operators is normal ordered.

9.5.3 Linked Cluster Theorem

The linked cluster theorem for imaginary time follows from the replica trick, as at zero temperature. In this case, we wish to compute the logarithm of the partition function

$$ln(\frac{Z}{Z_0}) = \lim_{n\to 0}\frac{1}{n}\left[\left(\frac{Z}{Z_0}\right)^n - 1\right]$$

It is worth mentioning here that the replica trick was infact originally invented by Edwards as a device for dealing with disorder- we shall have more to say about this in chapter 11.

We now write the term that contains $(Z/Z_0)^n$ as the product of contributions from n replica systems, so that

$$\left(\frac{Z}{Z_0}\right)^n = \left\langle \exp\left[-\int_0^\beta d\tau\sum_{\lambda=1}^{n}V^{(\lambda)}(\tau)\right]\right\rangle_0$$

When we expand the right-hand side as a sum over unlinked Feynman diagrams, each separate Feynman diagram has a replica index that must be summed over, so that a single linked diagram is of order $O(n)$, whereas a group of k unlinked diagrams is of order $O(n^k)$. In this way, as $n\to 0$, only the unlinked diagrams survive, so that. The upshot of this result is that the shift in the Free energy ΔF produced by the perturbation $\hat{V}$, is given by

$$-\beta\Delta F = \ln(Z/Z_0) = \sum\{\text{Closed link diagrams in real space}\}$$

Notice that unlike the zero temperature proof, here we do not have to appeal to adiabaticity to extract the shift in Free energy from the closed loop diagrams.

When we convert to momentum space, Fourier transforming each propagator and interaction line, an overall integral over the center of mass co-ordinates factors out of the entire diagram, giving rise to a prefactor

$$\int d^dX_{cm} = \beta(2\pi)^{d-1}\delta^{(d-1)}(0) \equiv V\beta$$

where V is the spatial volume. Consequently, expressed in momentum space, the change in Free energy is given by

$$\frac{\Delta F}{V} = -\sum\{\text{Closed linked diagrams in momentum space}\}\,.$$

Finally, let us say a few words about Green-functions Since the $n-th$ order coefficients of α and $\bar{\alpha}$ are the irreducible n-point Green-functions,

$$\begin{aligned}\ln Z[\bar{\alpha},\alpha] &= -\beta\Delta F + \int d1d2\bar{\alpha}(1)\mathcal{G}(1-2)\alpha(2)\\ &+ \frac{1}{(2!)^2}\int d1d2d3d4\bar{\alpha}(1)\bar{\alpha}(2)\alpha(3)\alpha(4)\mathcal{G}_{irr}(1,2;3,4)+\ldots. \qquad (9.74)\end{aligned}$$

n-particle irreducible Green functions are simply the n-particle Green functions in which all contributions from $n-1$ particle Green functions have been subtracted. Now since the n-th order coefficients in the Feynman diagram expansion of $\ln Z[\bar{\alpha},\alpha]$ are the connected $2n$-point diagrams, it follows that the n-paricle irreducible Green functions are given by the sum of all $2n$ point diagrams

$$\mathcal{G}_{irr}(1,2,\ldots n;1',2',\ldots n') = \sum\{\text{Connected n-point diagrams}\}.$$

The main links between finite temperature Feynman diagrams and physical quantities are given in table 9.3.

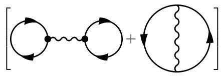
9.6 Examples of the application of the Matsubara Technique

To illustrate the Matsubara technique, we shall examine three examples. In the first, we will see briefly how the Hartree Fock approximation is modified at finite temperatures. This will give some familiarity with the techniques. In the second, we shall examine the effect of disorder on the electron propagator. Surprisingly, the spatial fluctuations in the electron potential that arise in a disordered medium behave like a highly retarded potential, and the scattering created by these fluctuations is responsible for the Drude lifetime in a disordered medium. As our third introductory example, we will examine an electron moving under the retarded interaction effects produced by the exchange of phonons, examining for the first time how inelastic scattering generates an electron lifetime.

9.6.1 Hartree Fock at a finite temperature.

As a first example, consider the Hartree-Fock correction to the Free energy,

$$\frac{\Delta F_{HF}}{V} = -\Bigg[\qquad\qquad\Bigg] \qquad (9.75)$$



These diagrams are precisely the same as those encountered in chapter 8, but now to evaluate them, we implement the finite temperature rules, which give,

$$\frac{\Delta F_{HF}}{V} = \frac{1}{2}\sum_k G(k)\sum_{k'}G(k')\left\{[-(2S+1)]^2V(k-k') - (2S+1)V(q=0)\right\} \qquad (9.76)$$

where the prefactor is the $p=2$ symmetry factor for these diagrams and

$$\sum_k G(k) \equiv \int_{\mathbf{k}} T\sum\frac{1}{i\omega_n - \epsilon_{\mathbf{k}}}e^{i\omega_n 0^+}$$

Using the contour integration method introduced in section (9.3), following (9.47), we have

$$T\sum\frac{1}{i\omega_n-\epsilon_{\mathbf{k}}}e^{i\omega_n 0^+} = \int_C\frac{dz}{2\pi i}\frac{1}{z-\epsilon_{\mathbf{k}}}e^{z0^+}f(z) = f(\epsilon_{\mathbf{k}}),$$

where the contour C runs anticlockwise around the pole at $z=\epsilon_{\mathbf{k}}$, so that the first order shift in the Free energy is

$$\Delta F_{HF} = \frac{1}{2}\int_{\mathbf{k},\mathbf{k}'}\left[(2S+1)^2(V_{\mathbf{q}=\mathbf{0}}) - (2S+1)(V_{\mathbf{k}-\mathbf{k}'})\right]f_{\mathbf{k}}f_{\mathbf{k}'}.$$

This is formally exactly the same as at zero temperature, excepting that now $f_{\mathbf{k}}$ refers to the finite temperature Fermi Dirac. Notice that we could have applied exactly the same method to bosons, the main result being a change in sign of the second Fock term.

9.6.2 Electron in a disordered potential

As a second example of the application of finite temperature methods, we shall consider the propagator for an electron in a disordered potential. This will introduce the concept of an "impurity average".

Our interest in this problem is driven ultimately by a desire to understand the bulk properties of a disordered metal. The problem of electron transport is almost as old as our knowledge of the electron itself. Already, within the first ten years of the discovery of the electron in 1897, Lorentz had derived his famous force law, and Drude had argued, based on the idea of a classical gas of charged electrons, that the electrons would exhibit a mean-free path $l = v_{\text{electron}}\tau$, where τ is the scattering rate an l the average distance between scattering events. In Drude's theory electrons were envisioned as diffusing through the metal, and he was able to derive his famous formula for the conductivity σ

$$\sigma = \frac{ne^2\tau}{m}.$$

Missing from Drude's pioneering picture, was any notion of the Fermi-Dirac statistics of the electron fluid. He had for example, no notion that the characteristic velocity of the electrons was given by the Fermi velocity, $v_{\text{electron}} \sim v_F$ a vastly greater velocity at low temperatures than could ever be expected on the grounds of a Maxwell Boltzman fluid of particles. This raises the question - how - in a fully quantum mechanical picture of the electron fluid, can we rederive Drude's basic model?

A real metal contains both disorder and electron-electron interactions - in this course we shall only touch on the simpler problem of disorder in an otherwise free electron gas. We shall actually return to this problem in earnest in the next chapter. Our task here in our first example will be to examine the electron propagator in a disordered medium of elastically scattering impurities. We shall consider an electron in a disordered potential

$$\boxed{\begin{aligned} H &= \sum_{\mathbf{k}} \epsilon_{\mathbf{k}} c^{\dagger}{}_{\mathbf{k}} c_{\mathbf{k}} + V_{\text{disorder}} \\ V_{\text{disorder}} &= \int d^3x U(\vec{x})\psi^{\dagger}(\mathbf{x})\psi^{\dagger}(\mathbf{x}) \qquad (9.77) \end{aligned}}$$

where $U(\mathbf{x})$ represents the scattering potential generated by a random array of N_i impurities located at positions $\mathbf{R_j}$, each with atomic potential $\mathcal{U}(\mathbf{x} - \mathbf{R_j})$,

$$U(\mathbf{x}) = \sum_j \mathcal{U}(\mathbf{x} - \mathbf{R_j})$$

An important aspect of this Hamiltonian, is that it contains no interactions between electrons, and as such the energy of each individual electron is conserved: all interactions are elastic.

We shall not be interested in calculating the value of a physical quantity for a *specific* location of impurities, but rather on the value of that quantity after we have averaged over the locations of the impurities, i.e.

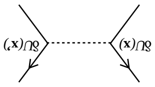
$$\overline{\langle A \rangle} = \int \prod_j \frac{1}{V} d^3R_j \langle \hat{A}[\{\mathbf{R}_j\}]\rangle$$

This is an elementary example of a "quenched average", in which the "impurity average" takes place *after* the Thermodynamic average. Here, we'll calculate the impurity averaged Green function. To do this we need to know something about the fluctuations of the impurity scattering potential about its average. It is these fluctuations that scatter the electrons.

Electrons will in general scatter off the fluctuations in the potential. The average impurity potential $\overline{U(\mathbf{x})}$ plays the roll of a kind of shifted chemical potential. Indeed, if we shift the chemical potential by an amount $\Delta\mu$, the scattering potential becomes $U(\mathbf{x}) - \Delta\mu$, and we can always choose $\Delta\mu$ so that $\overline{U(\mathbf{x})} - \mu = 0$. The more important quantity are the fluctuations about the average potential $\delta U(\mathbf{x}) = U(\mathbf{x}) - \overline{U(\mathbf{x})}$. These fluctuations are spatially correlated, with variance

$$\overline{\delta U(\mathbf{x})\delta U(\mathbf{x'})} = \int_q e^{i\mathbf{q}\cdot(\mathbf{x}-\mathbf{x'})} n_i \,|u(\mathbf{q})|^2 \qquad (9.78)$$

where $u(\mathbf{q}) = \int d^3x \mathcal{U}(\mathbf{x})e^{-i\mathbf{q}\cdot\mathbf{x}}$ is the Fourier transform of the scattering potential and $n_i = N_i/V$ is the concentration of impurities. It is these fluctuations that scatter the electrons, and when we come to draw the impurity averaged Feynman diagrams, we'll see that the spatial correlations in the potential fluctuations induce a sort of "attractive interaction", denoted by the diagram



$$\int n_i |u(\mathbf{q})|^2 e^{i\mathbf{q}\cdot(\mathbf{x}-\mathbf{x'})} = -V_{\text{eff}}(\mathbf{x}-\mathbf{x'}) \qquad (9.79)$$

Although in principle, we should keep all higher moments of the impurity scattering potential, in practice, the leading order moments are enough to extract a lot of the basic physics in weakly disordered metals. Notice that the fluctuations in the scattering potential are short-range - they only extend over the range of the scattering potential. Indeed, if we neglect the momentum dependence of $u(\mathbf{q})$, assuming that the impurity scattering is dominated by low energy s-wave scattering, then we can writie $u(\mathbf{q}) = u_0$. In this situation, the fluctuations in the impurity scattering potential are entirely local,

$$\overline{\delta U(\mathbf{x})\delta U(\mathbf{x'})} = n_i u_0^2 \delta(\mathbf{x} - \mathbf{x'}) \qquad \text{white noise potential}$$

In our discussion today, we will neglect the higher order moments of the scattering potential, effectively assuming that it is purely Gaussian.

To prove (9.78), we first Fourier transform the potential

$$U(\mathbf{q}) \;=\; \sum_j e^{-i\mathbf{q}\cdot\mathbf{R_j}} \int d^3x\, \mathcal{U}(\mathbf{x} - \mathbf{R_j})\mathbf{e}^{-\mathbf{i}\mathbf{q}\cdot(\mathbf{x}-\mathbf{R_j})} = \mathbf{u}(\mathbf{q})\sum_{\mathbf{j}} \mathbf{e}^{-\mathbf{i}\mathbf{q}\cdot\mathbf{R_j}}, \qquad (9.80)$$

so that the locations of the impurities are encoded in the phase shifts which multiply $u(\mathbf{q})$. If we now carry out the average,

$$\begin{aligned} \overline{\delta U(\mathbf{x})\delta U(\mathbf{x'})} \;&=\; \int_{\mathbf{q},\mathbf{q'}} e^{i(\mathbf{q}\cdot\mathbf{x}-\mathbf{q}\cdot\mathbf{x'})} \left(\overline{U(\mathbf{q})U(-\mathbf{q'})} - \overline{U(\mathbf{q})}\;\; \overline{U(-\mathbf{q'})}\right) \\ = \int_{\mathbf{q},\mathbf{q'}} e^{i(\mathbf{q}\cdot\mathbf{x}-\mathbf{q}\cdot\mathbf{x'})} \quad & u(\mathbf{q})u(-\mathbf{q'}) \sum_{i,j} \left(\overline{e^{-i\mathbf{q}\cdot\mathbf{R_i}} e^{i\mathbf{q'}\cdot\mathbf{R_j}}} - \overline{e^{-i\mathbf{q}\cdot\mathbf{R_i}}}\;\; \overline{e^{i\mathbf{q'}\cdot\mathbf{R_j}}}\right) \qquad (9.81) \end{aligned}$$

Now since the phase terms are independent at different sites, the variance of the random phase term in the above expression vanishes unless $i = j$, so

$$\begin{aligned} \sum_{i,j} \left(\overline{e^{-i\mathbf{q}\cdot\mathbf{R}_i} e^{i\mathbf{q'}\cdot\mathbf{R}_j}} - \overline{e^{-i\mathbf{q}\cdot\mathbf{R_i}}}\;\; \overline{e^{i\mathbf{q'}\cdot\mathbf{R_j}}}\right) \;&=\; N_i \times \int \frac{1}{V} d^3R_j e^{-i(\mathbf{q}-\mathbf{q'})\cdot\mathbf{R}_j} \\ &=\; n_i (2\pi)^3 \delta^{(3)}(\mathbf{q} - \mathbf{q'}) \qquad (9.82) \end{aligned}$$

from which

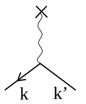
$$\overline{U(\mathbf{q})U(-\mathbf{q'})} - \overline{U(\mathbf{q})}\;\; \overline{U(-\mathbf{q'})} = n_i |u(\mathbf{q})|^2 (2\pi)^3 \delta^{(3)}(\mathbf{q} - \mathbf{q'})$$

and (9.78) follows.

Now let us examine how electrons scatter off these fluctuations. If we substitute $\psi^{\dagger}(\mathbf{x}) = \int_{\mathbf{k}} c^{\dagger}{}_k e^{-i\mathbf{k}\cdot\mathbf{x}}$ into $\hat{V}_{\text{disorder}}$, we obtain

$$\hat{V}_{\text{disorder}} = \int_{\mathbf{k},\mathbf{k'}} c^{\dagger}{}_{\mathbf{k}} c_{\mathbf{k'}} \delta U(\mathbf{k} - \mathbf{k'})$$

We shall represent the scattering amplitude for scattering once



$$\delta U(\mathbf{k} - \mathbf{k'}) = \left(u(\mathbf{k} - \mathbf{k'}) \sum_j e^{i(\mathbf{k}-\mathbf{k'})\cdot\mathbf{R_j}}\right) - \Delta\mu\delta_{\mathbf{k}-\mathbf{k'}}. \qquad (9.83)$$

where we have subtracted the scattering off the average potential. The potential transfers momentum, but does not impart any energy to the electron, and for this reason frequency is conserved along the electron propagator. Let us now write down, in momentum space the Greens function of the electron

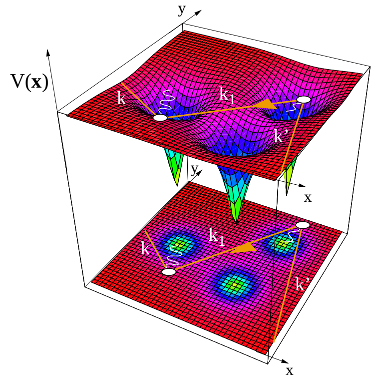
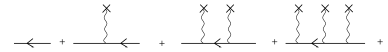


Figure 9.4: Double scattering event in the random impurity potential.

$$\mathcal{G}(\mathbf{k},\mathbf{k'},i\omega_n) \;=$$



$$\begin{aligned} &=\; \mathcal{G}^0(\mathbf{k},i\omega_n)\delta_{\mathbf{k},\mathbf{k'}} + \mathcal{G}^0(\mathbf{k},i\omega_n)\delta U(\mathbf{k}-\mathbf{k'})\mathcal{G}^0(\mathbf{k'},i\omega_n) \\ &+\; \int_{\mathbf{k}_1} \mathcal{G}^0(\mathbf{k},i\omega_n)\delta U(\mathbf{k}-\mathbf{k}_1)\mathcal{G}^0(\mathbf{k}_1,i\omega_n)\delta U(\mathbf{k}_1-\mathbf{k'})\mathcal{G}^0(\mathbf{k'},i\omega_n) + ..(9.84) \end{aligned}$$

where the frequency $i\omega_n$ is constant along the electron line. Notice that $\mathcal{G}^0$ is actually a function of each impurity position! Fig. 9.4 illustrates one of the scattering events contributing to the third diagram in this sum. We want to calculate the quenched avaerage $\overline{\mathcal{G}(\mathbf{k},\mathbf{k'},i\omega_n)}$, and to do this, we need to average each Feynman diagram in the above series.

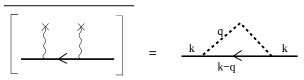
When we impurity average the single scattering event, it vanishes:

$$\overline{\mathcal{G}^0(\mathbf{k},i\omega_n)\delta U(\mathbf{k}-\mathbf{k'})\mathcal{G}^0(\mathbf{k'},i\omega_n)} = \mathcal{G}^0(\mathbf{k},i\omega_n)\overbrace{\overline{\delta U(\mathbf{k}-\mathbf{k'})}}^{=0}\mathcal{G}^0(\mathbf{k'},i\omega_n)$$

but the average of a double scattering event is

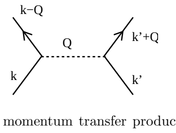
$$\sum_{\mathbf{k}_1}\mathcal{G}^0(\mathbf{k},i\omega_n)\mathcal{G}^0(\mathbf{k}_1,i\omega_n)\mathcal{G}^0(\mathbf{k}',i\omega_n)\times\overbrace{\overline{\delta U(\mathbf{k}-\mathbf{k}_1)\delta U(\mathbf{k}_1-\mathbf{k}')}}^{n_i|u_{\mathbf{k}-\mathbf{k}'}|^2\delta_{\mathbf{k}-\mathbf{k}'}}$$
$$= \delta_{\mathbf{k}-\mathbf{k}'}\times\mathcal{G}^0(\mathbf{k},i\omega_n)^2 n_i\sum_{\mathbf{k}_1}u(\mathbf{k}-\mathbf{k}_1)^2\mathcal{G}^0(\mathbf{k}_1,i\omega_n)\mathcal{G}^0(\mathbf{k},i\omega_n) \quad (9.85)$$

Notice something fascinating - after impurity averating, momentum is now conserved. We can denote the impurity averaged double scattering event Feynman diagram



(9.86)

where we have introduced the Feynman diagram



$$n_i|u(\mathbf{q})|^2 = -V_{\rm eff}(Q) \quad (9.87)$$

to denote the momentum transfer produced by the quenched fluctuations in the random potential. In writing the diagram this way, we bring out the notion that quenched disorder can be very loosely thought of as an interaction with an effective potential

$$V_{\rm eff}(\mathbf{q},i\nu_n) = \int_0^\beta d\tau e^{i\nu_n\tau}\overbrace{V_{\rm eff}(\mathbf{q},\tau)}^{-n_i|u(\mathbf{q})|^2} = -\beta\delta_{n0}n_i|u(\mathbf{q})|^2$$

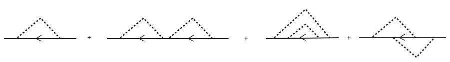
where the $\beta\delta_{n0}\equiv\int d\tau e^{i\nu_n\tau}$ is derived from the fact that the interaction $V_{\rm eff}(\mathbf{q},\tau)$does not depend on the time difference guarantees that there is no energy transferred by the quenched scattering events. In otherwords, quenched disorder induces a sort of infinitely retarded, but "*attractive*" potential between electrons. (Our statement can be made formally correct in the language of replicas - this interaction takes place between electrons of the same, or different replica index. In the $n\to 0$ limit, the residual interaction only acts on one electron in the same replica.) The notion that disorder induces interactions is an interesting one, for it motivate the idea that disorder can lead to new kinds of collective behavior.

After the impurity averaging, we notice that momentum is now conserved, so that the impurity averaged Green function is now diagonal in momentum space,

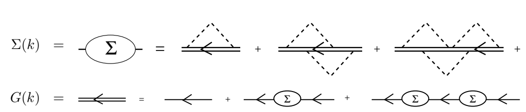
$$\overline{\mathcal{G}(\mathbf{k},\mathbf{k}',i\nu_n)} = \delta_{\mathbf{k}-\mathbf{k}'}\mathcal{G}(\mathbf{k},i\nu_n).$$

If we now carry out the impurity averaging on multiple scattering events, only repeated scattering events at the same sites will give rise to non-vanishing contributions. If we take account of all scattering events induced by the Gaussian fluctuations in the scattering potential, then we generate a series of diagrams of the form

$G(k) =$



In the Feynman diagrams, we can group all scatterings into connected self-energy diagrams, as follows:

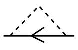


$$= [i\omega_n - \epsilon_{\mathbf{k}} - \Sigma(k)]^{-1} \quad (9.88)$$

In the case of s-wave scattering, all momentum dependence of the scattering processes is lost, so that in this case $\Sigma(k) = \Sigma(i\omega_n)$ only depends on the frequency. In the above diagram, the double line on the electron propagator indicates that all self-energy corrections have been included. From the above, you can see that the self-energy corrections calculated from the first expression are fed into the electron propagator, which in turn is used in a self-consistent way inside the self-energy

We shall begin by trying to calculate the first order above diagrams for the self-energy without imposing any self-consistency. This diagram is given by

$\Sigma(i\omega_n) =$



$$= n_i\sum_{\mathbf{k}'}|u(\mathbf{k}-\mathbf{k}')|^2 G(\mathbf{k}',i\omega_n)$$
$$= n_i\sum_{\mathbf{k}'}|u(\mathbf{k}-\mathbf{k}')|^2\frac{1}{i\omega_n-\epsilon_{\mathbf{k}'}} \quad (9.89)$$

Now we can replace the summation over momentum inside this self-energy by an integration over solid angle and energy, as follows

$$\sum_{\mathbf{k}'}\to\int\frac{d\Omega_{\mathbf{k}'}}{4\pi}d\epsilon' N(\epsilon')$$

where $N(\epsilon)$ is the density of states. With this replacement,

$$\Sigma(i\omega_n) = n_i u_0^2\int d\epsilon N(\epsilon)\frac{1}{i\omega_n-\epsilon}$$

where

$$u_0^2 = \int\frac{d\Omega_{\mathbf{k}'}}{4\pi}|u(\mathbf{k}-\mathbf{k}')|^2 = \frac{1}{2}\int_{-1}^{1}d\cos\theta|u(\theta)|^2$$

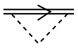
is the angular average of the squared scattering amplitude. To a good approximation, this expression can be calculated by replacing the energy dependent density of states by its value at the Fermi energy. In so doing, we neglect a small real part to the self-energy, which can, in any case be absorbed by the chemical potential. This kind of approximation is extremely common in many body physics, in cases where the key physics is dominated by electrons close to the Fermi energy. The deviations from constancy in $N(\epsilon)$, will in practice affect the real part of $\Sigma(i\omega_n)$, and these small changes can be accomodated by a shift in the chemical potential. The resulting expression for $\Sigma(i\omega_n)$ is then

$$\Sigma(i\omega_n) = n_i u_0^2 N(0)\int_{-\infty}^{\infty}d\epsilon\frac{1}{i\omega_n-\epsilon} = -i\frac{1}{2\tau}{\rm sgn}(\omega_n) \quad (9.90)$$

where we have identified $\frac{1}{\tau} = 2\pi n_i u_0^2$ as the electron elastic scattering rate. We notice that this expression is entirely imaginary, and it only depends on the sign of the Matsubara frequency. Notice that in deriving this result we have extended the limits of integration to infinity, an approximation that involves neglecting terms of order $1/(\epsilon_F\tau)$.

We can now attempt to recompute $\Sigma(i\omega_n)$ with self-consistency. In this case,

$\Sigma(i\omega_n) =$



$$= n_i u_0^2\sum_{\mathbf{k}'}\frac{1}{i\omega_n-\epsilon_{\mathbf{k}'}-\Sigma(i\omega_n)} \quad (9.91)$$

If carry out the energy integration again, we see that the imposition of self-consistency has no effect on the scattering rate

$$\Sigma(i\omega_n) = n_i u_0^2 N(0)\int_{-\infty}^{\infty}d\epsilon\frac{1}{i\omega_n-\epsilon-\Sigma(i\omega_n)}$$
$$= -i\frac{1}{2\tau}{\rm sgn}(\omega_n). \quad (9.92)$$

Our result for the electron propagator, ignoring the "vertex corrections" to the scattering self-energy is given by

$$G(\mathbf{k},z) = \frac{1}{z-\epsilon_{\mathbf{k}}+i\frac{1}{2\tau}{\rm sgn}Im(z)}$$

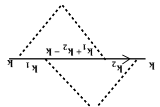
where we have boldly extended the Green function into the complex plane. We may now make a few remarks:

- The original pole of the Green function has been broadened. The electron "spectral function",
$$A(\mathbf{k},\omega) = \frac{1}{\pi}\Im G(\mathbf{k},\omega-i\delta) = \frac{1}{\pi}\frac{(2\tau)^1}{(\omega-\epsilon_{\mathbf{k}})^2+(2\tau)^{-2}}$$

is a Lorentzian of width $1/\tau$. The electron of momentum $\mathbf{k}$ now has a lifetime τ due to elastic scattering effects.

- Although the electron has a mean-free path, $l = v_F\tau$the electron propagator displays no features of diffusion. The main effect of the finite scattering rate is to introduce a decay length into the electron propagation. The electron propagator does not bear any resemblance to the "diffusion propagator" $\chi = 1/(i\nu - Dq^2)$ that is the Greens function for the diffusion equation $(\partial_t - D\nabla^2)\chi = -\delta(x,t)$. The physics of diffusion and Ohm's law do not appear until we are able to examine the charge and spin response functions, and for this, we have to learn how to compute the density and current fluctuations in thermal equilibrium. (Chapter 10).
- The scattering rate that we have computed is often called the "classical" electron scattering rate. The neglected higher order diagrams with vertex corrections are actually smaller than the leading order contribution by an amount of order
$$\frac{1}{\epsilon_F\tau} = \frac{1}{k_F l}$$

This small parameter defines the size of "quantum corrections" to the Drude scattering physics, which are the origin of the physics of electron localization. To understand how this small number arises in the self-energy, consider the first vertex correction to the impurity scattering,



(9.93)

This diagram is given by

$$\Sigma_2 = \overbrace{N(0)\int\frac{d\epsilon_1}{i\omega_n-\epsilon_1}}^{-i\frac{1}{2\tau}}\overbrace{N(0)\int\frac{d\epsilon_2}{i\omega_n-\epsilon_2}}^{-i\frac{1}{2\tau}}\overbrace{\int\frac{d\Omega_1 d\Omega_2}{(4\pi)^2}\frac{1}{i\omega_n-\epsilon_{\mathbf{k}_1+\mathbf{k}_2-\mathbf{k}}}}^{\sim\frac{-i}{k_F v_F}}$$
$$\sim i\frac{1}{\tau}\times\frac{1}{k_F l} \quad (9.94)$$

where the last term in the integral derives from the central propagator in the self-energy. In this self-energy, the momentum of the central propagator is entirely determined by the momentum of the two other internal legs, so that the energy associated with this propagator is $\epsilon_{-\mathbf{k}+\mathbf{k}_1+\mathbf{k}_2}$. This energy is only close to the Fermi energy when $\mathbf{k}_1\sim-\mathbf{k}_2$, so that only a small fraction $1/(k_F l)$ of the possible directions of k_2 give a large contribution to the scattering processes.

9.7 Interacting electrons and phonons

The electron phonon interaction is one of the earliest successes of many body physics in condensed matter. In many ways, it is the condensed matter analog of quantum-electrodynamics - and the early work on the electron phonon problem was carried out by physicists who had made their early training in the area of quantum electrodynamics.

When an electron passes through a crystal, it attracts the nearby ions, causing a local build-up of positive charge. Perhaps a better analogy, is with a supersonic aircraft, for indeed, an electron is a truly supersonic particle inside crystals, moving at many times the velocity of sound. To get an idea of just how much faster the electron moves in comparison with sound, notice that the ratio of the sound velocity c_s to the Fermi velocity is determined by the ratio of the Debye frequency to the Fermi energy, for

$$\frac{v_s}{v_F} \sim \frac{\nabla_k \omega_k}{\nabla_k \epsilon_k} \sim \frac{\omega_D/a}{\epsilon_F/a} = \frac{\omega_D}{\epsilon_F}$$

where a is the size of the unit cell. Now an approximate estimate for the Debye frequency is given by $\omega_D^2 \sim k/M$, where M is the mass of an atomic nucleus and $k \sim \epsilon_F/a^2$ is the "spring constant" associated with atomic motions, thus

$$\omega_D^2 \sim \left(\frac{\epsilon_F}{a^2}\right)\frac{1}{M}$$

and

$$\frac{\omega_D^2}{\epsilon_F^2} \sim \underbrace{\frac{1}{(\epsilon_F a^2)}}_{\sim 1/m}\frac{1}{M} \sim \frac{m}{M}$$

so that the ratio

$$\frac{v_s}{v_F} \sim \sqrt{\frac{m}{M}} \sim \frac{1}{100}.$$

so an electron moves at around Mach 100. As it moves through the crystal, it leaves behind it a very narrow wake of "positively charged" distortion in the crystal lattice which attracts other electrons, long after the original disturbance has passed by. This is the origin of the weak attractive interaction produced by the exchange of virtual phonons. This attractive interaction is highly retarded, quite unlike the strongly repulsive Coulomb interaction that acts between electrons which is almost instantaneous in time. (The ratio of characteristic timescales being $\sim \frac{\epsilon_F}{\omega_D} \sim \sqrt{\frac{M}{m}} \sim 100$). Thus- whereas two electrons at the same place and time, feel a strong mutual Coulomb repulsion, two electrons which arrive at the same place, but at different times can be subject to an attractive electron phonon interaction. It is this interaction that is responsible for the development of superconductivity in many conventional metals.

In an electron fluid, we must take into account the quantum nature of the sound-vibrations. An electron can not continously interact with the surrounding atomic lattice - it must do so by the emission and absorption of sound quanta or "phonons". The basic

Hamiltonian to describe the electron phonon problem is the Frohlich Hamiltonian, derived by Fröhlich, a German emigré to Britain, who worked in Liverpool shortly after the second-world war. Fröhlich recognized that the electron-phonon interaction is closely analogous to the electron-photon interaction of QED. To introduce the Frohlich Hamiltonian, we will imagine we have a three phonon modes labelled by the index $\lambda = (1, 2, 3)$, with frequency $\omega_{\mathbf{q}\lambda}$. For the moment, we shall also ignore the Coulomb interaction between electrons. The Fröhlich Hamiltonian is then

$$\boxed{\begin{aligned} H_e &= \sum_{\mathbf{k}\sigma} \epsilon_{\mathbf{k}} c^\dagger{}_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} \\ H_p &= \sum_{\mathbf{q},\lambda} \omega_{\mathbf{q}\lambda}(a^\dagger{}_{\mathbf{q}\lambda} a_{\mathbf{q}\lambda} + \frac{1}{2}) \\ H_I &= \sum_{\mathbf{k},\mathbf{q},\lambda} g_{\mathbf{q}\lambda} c^\dagger{}_{\mathbf{k}+\mathbf{q}\sigma} c_{\mathbf{k}\sigma} \left[a_{\mathbf{q}\lambda} + a^\dagger{}_{-\mathbf{q}\lambda}\right] \qquad (9.95) \end{aligned}}$$

To understand the electron phonon coupling, let us consider how long-wavelength fluctuations of the lattice couple to the electron energies. Let $\vec{\Phi}(\mathbf{x})$ be the displacement of the lattice at a given point $\mathbf{x}$, so that the strain tensor in the lattice is given by

$$u_{\mu\nu}(\mathbf{x}) = \frac{1}{2}\left(\nabla_\mu \Phi_\nu(\mathbf{x}) + \nabla_\nu \Phi_\mu(\mathbf{x})\right)$$

In general, we expect a small change in the strain to modify the background potential of the lattice, modifying the energies of the electrons, so that locally,

$$\epsilon(\mathbf{k}) = \epsilon_0(\mathbf{k}) + C_{\mu\nu} u_{\mu\nu}(\mathbf{x}) + \dots$$

Consider the following, very simple model. In a free electron gas, the Fermi energy is related to the density of the electrons N/v by

$$\epsilon_F = \frac{1}{2m}\left(\frac{3\pi^2 N}{V}\right)^{\frac{2}{3}} \tag{9.96}$$

so that if we expand the lattice,

$$\frac{\delta\epsilon_F}{\epsilon_F} = -\frac{2}{3}\frac{dV}{V} \sim -\frac{2}{3}\vec{\nabla}\cdot\Phi$$

On the basis of this simple model, we expect the following coupling between the displacement vector and the electron field

$$\boxed{H_I = C\int d^3x \psi_\sigma{}^\dagger(\mathbf{x})\psi_\sigma(\mathbf{x}) \qquad C = -\frac{2}{3}\epsilon_F \qquad (9.97)}$$

The quantity C is often called the "deformation potential". Now the displacement of the the phonons was studied in Chapter 4. In a general model, it is given by

$$\Phi(\mathbf{x}) = -i\sum_{\mathbf{q}\lambda} \mathbf{e}^\lambda_{\mathbf{q}}\, \Delta x_{\mathbf{q}\lambda} \left[a_{\mathbf{q}\lambda} + a^\dagger{}_{-\mathbf{q}\lambda}\right] e^{i\mathbf{q}\cdot\mathbf{x}}$$

where we've introduced the shorthand

$$\Delta x_{\mathbf{q}\lambda} = \left(\frac{\hbar}{2mN\omega_{\mathbf{q}\lambda}}\right)^{\frac{1}{2}}$$

to denote the characteristic zero point fluctuation associated with a given mode. (N_s is the number of sites in the lattice.) The body of this expression is essentially identical to the displacement of a one-dimensional harmonic lattice (see (4.60)), dressed up with additional polarization indices. The unfamiliar quantity $\mathbf{e}^\lambda_{\mathbf{q}}$ is the polarization vector of the mode. For longitudinal phonons, for instance, $\mathbf{e}^L_{\mathbf{q}} = \hat{q}$. The "$-i$" infront of the expression has been introduced into the definition of the phonon creation and annihilation operators so that the requirement that the Hamiltonian is hermitian (which implies $(\mathbf{e}^\lambda_{\mathbf{q}})^* = -(\mathbf{e}^\lambda_{-\mathbf{q}})$) is consistent with the convention that $\mathbf{e}$ changes sign when the momentum vector $\mathbf{q}$ is inverted.

The divergence of the phonon field is then

$$\vec{\nabla}\cdot\Phi(\mathbf{x}) = \sum_{\mathbf{q}\lambda} \mathbf{q}\cdot\mathbf{e}^\lambda_{\mathbf{q}}\Delta x_{\mathbf{q}\lambda}\left[a_{\mathbf{q}\lambda} + a^\dagger{}_{-\mathbf{q}\lambda}\right] e^{i\mathbf{q}\cdot\mathbf{x}}$$

In this simple model, the electrons only couple to the longitudinal phonons, since these are the only phonons that change the density of the unit cell. When we now Fourier transform the interaction Hamiltonian, making the insertion $\psi_\sigma(\mathbf{x}) = \frac{1}{\sqrt{V}}\sum_{\mathbf{k}} c_{\mathbf{k}\sigma} e^{i\mathbf{k}\cdot\mathbf{x}}$ (9.97), we obtain

$$\begin{aligned} H_I &= C\int d^3x \psi_\sigma{}^\dagger(\mathbf{x})\psi_\sigma(\mathbf{x})\vec{\nabla}\vec{\Phi}(\mathbf{x}) \\ &= \sum_{\mathbf{k},\mathbf{k}',\mathbf{q},\lambda} c^\dagger{}_{\mathbf{k}'\sigma} c_{\mathbf{k}\sigma}\left[a_{\mathbf{q}\lambda} + a^\dagger{}_{-\mathbf{q}\lambda}\right]\overbrace{\frac{1}{V}\int d^3x e^{i(\mathbf{q}+\mathbf{k}-\mathbf{k}')\cdot\mathbf{x}}}^{\delta_{\mathbf{k}'-(\mathbf{k}+\mathbf{q})}} \times C\Delta x_{\mathbf{q}\lambda}(\mathbf{q}\cdot\mathbf{e}^\lambda_{\mathbf{q}}) \\ &= \sum_{\mathbf{q}\mathbf{k}\lambda} g_{\mathbf{q}\lambda} c^\dagger{}_{\mathbf{k}+\mathbf{q}\sigma} c_{\mathbf{k}\sigma}\left[a_{\mathbf{q}\lambda} + a^\dagger{}_{-\mathbf{q}\lambda}\right] \end{aligned} \tag{9.98}$$

where

$$g_{\mathbf{q}\lambda} = \begin{cases} C q \Delta x_{\mathbf{q}\lambda} = Cq\left(\frac{\hbar}{2mN_s\omega_{\mathbf{q}\lambda}}\right)^{\frac{1}{2}} & (\lambda = L) \\ 0 & (\text{otherwise }) \end{cases}$$

Our simple model captures the basic aspects of the electron phonon interaction, and it can be readily generalized. In a more sophisticated model,

- C becomes momentum dependent and should be replaced by the Fourier transform of the atomic potential. For example, if we compute the electron - phonon potential from

given by the change in the atomic potential V_{atomic} resulting from the displacement of atoms,

$$\delta V(\mathbf{x}) = \sum_j \delta V_{\text{atomic}}(\mathbf{x} - \mathbf{R}^0_j - \vec{\Phi}_j) = -\sum_j \vec{\Phi}_j\cdot\vec{\nabla}V_{\text{atomic}}(\mathbf{x} - \mathbf{R}^0_j)$$

we must replace interaction,

$$C \rightarrow V_{\text{atomic}}(\mathbf{q}) = \frac{1}{v_{cell}}\int d^3x V_{\text{atomic}}(\mathbf{x}) e^{-i\mathbf{q}\cdot\mathbf{x}}. \tag{9.99}$$

- When the plane-wave functions are replaced by the detailed Bloch wavefunctions of the electron band, the electron phonon coupling becomes dependent on both the incoming and outgoing electron momenta, so that

$$g_{\mathbf{k}'-\mathbf{k}\lambda} \rightarrow g_{\mathbf{k}',\mathbf{k}\lambda}.$$

Nevertheless, much can be learnt from our simplified model In the discussion that follows, we shall drop the polarization index, and assume that the phonon modes we refer to are exclusively longitudinal modes.

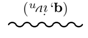
In setting up the Feynman diagrams for our Frohlich model, we need to introduce two new elements- a diagram for the phonon propagator, and a diagram to denote the vertex. If we denote $\phi_{\mathbf{q}} = a_{\mathbf{q}} + a^\dagger{}_{-\mathbf{q}}$, then the phonon Green function is given by

$$D(\mathbf{q}, \tau - \tau') = -\langle T\phi_{\mathbf{q}}(\tau)\phi_{\mathbf{q}}(\tau')\rangle = T\sum_{i\nu_n} D(q) e^{-i\nu_n(\tau-\tau')} \tag{9.100}$$

where the propagator

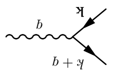
$$D(q) = \frac{2\omega_{\mathbf{q}}}{(i\nu_n)^2 - (\omega_{\mathbf{q}})^2}$$

is denoted by the diagram



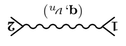
$$= D(\mathbf{q}, i\nu_n) \tag{9.101}$$

The interaction vertex between electrons and phonon is denoted by the diagram



$$= (i)^3 \times -g_{\mathbf{q}} = ig_{\mathbf{q}} \tag{9.102}$$

The factor i^3 arises because we have three propagators entering the vertex, each donating a factor of i. The $-1g_{\mathbf{q}}$ derives from the interaction Hamiltonian in the time-ordered exponential. Combining these two Feynman rules, we see that when two electrons exchange a boson, this gives rise to the diagram



$$= (ig_{\mathbf{q}})^2 D(q) = -(g_{\mathbf{q}})^2 D(q) \tag{9.103}$$

where we have taken the liberty of analytically extending the function into the complex plane. There is a remarkable amount of physics hidden in this expression.

The terms appearing in the electron phonon self-energy can be interpreted in terms of virtual and real phonon emission processes. Consider the zero temperature limit, when the Bose terms $n_{\mathbf{q}} = 0$. If we look at the first term in $\Sigma(k)$, we see that the numerator is only finite if the intermediate electron state is empty, i.e $|\mathbf{k}-\mathbf{q}| > k_F$. Furthermore, the poles of the first expression are located at energies $\omega_{\mathbf{q}} + \epsilon_{\mathbf{k}-\mathbf{q}}$, which is the energy of an electron of momentum $\mathbf{k}-\mathbf{q}$ and an emitted phonon of momentum $\omega_{\mathbf{q}}$, so the first process corresponds to phonon emission by an electron. If we look at the second term, then at zero temperature, the numerator is only finite if $|\mathbf{k}-\mathbf{q}| < k_F$, so the intermediate state is a hole. The pole in the second term occurs at $-z = -\epsilon_{\mathbf{k}-\mathbf{q}} + \omega_{\mathbf{q}}$, corresponding to a state of one hole and one phonon, so one way to interpret the second term as the energy shift that results from the emission of virtual phonons by holes. At zero temperature then,

$$\Sigma(\mathbf{k}, z) = \sum_{\mathbf{q}} g_{\mathbf{q}}^2 \left[\overbrace{\frac{1 - f_{\mathbf{k}-\mathbf{q}}}{z - (\epsilon_{\mathbf{k}-\mathbf{q}} + \omega_{\mathbf{q}})}}^{\text{virtual/real phonon emission by electron}} + \overbrace{\frac{f_{\mathbf{k}-\mathbf{q}}}{z - (\epsilon_{\mathbf{k}-\mathbf{q}} - \omega_{\mathbf{q}})}}^{\text{virtual/real phonon emission by hole}} \right]$$

As we shall discuss in more detail in the next chapter, the analytically extended Greens function

$$G(\mathbf{k}, z) = \frac{1}{z - \epsilon_{\mathbf{k}} - \Sigma(\mathbf{k}, z)}$$

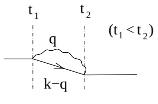
can be used to derive the real-time dynamics of the electron in thermal equilibrium. In general, $\Sigma(\mathbf{k}, \omega - i\delta) = Re\Sigma(\mathbf{k}, \omega - i\delta) + iIm\Sigma(\mathbf{k}, \omega - i\delta)$ will have a real and an imaginary part. The solution of the relation

$$\epsilon^*_{\mathbf{k}} = \epsilon_{\mathbf{k}} + Re\Sigma(\mathbf{k}, \epsilon^*_{\mathbf{k}})$$

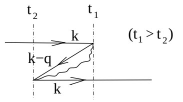
determines the renormalized energy of the electron due to virtual phonon emission. Lets consider the case of an electron, for which $\epsilon^*_{\mathbf{k}}$ is above the Fermi energy. The quasiparticle energy takes the form

$$\epsilon^*_{\mathbf{k}} = \epsilon_{\mathbf{k}} - \overbrace{\sum_{|\mathbf{k}-\mathbf{q}|>k_F} g_{\mathbf{q}}^2 \frac{1}{(\epsilon_{\mathbf{k}-\mathbf{q}} + \omega_{\mathbf{q}}) - \epsilon^*_{\mathbf{k}}}}^{\text{energy lowered by virtual phonon emission}} + \overbrace{\sum_{|\mathbf{k}-\mathbf{q}|<k_F} g_{\mathbf{q}}^2 \frac{1}{\epsilon^*_{\mathbf{k}} + |\epsilon_{\mathbf{k}-\mathbf{q}}| + \omega_{\mathbf{q}}}}^{\text{energy raised by blocking vacuum fluctuations}} .$$

If we approximate $\epsilon^*_{\mathbf{k}}$ by its unrenormalized value $\epsilon_{\mathbf{k}}$, we obtain the second-order perturbation correction to the electron quasiparticle energy, due to virtual phonon processes. To understand these two terms, it is helpful to redraw the Feynman diagram for the self energy so that the scattering events are explicitly time ordered, then we see that there are two virtual processes - depending on whether the intermediate electron line propagates forwards or backwards in time:



Virtual phonon emission



Virtual phonon and e−h pair

The first term is recognized as the effect of virtual scattering into an intermediate state with one photon and one electron. But what about the second term? This term involves the initial formation of an electron-hole pair and the subsequent reannihilation of the hole with the incoming electron. During the intermediate process, there seem to be *two* electrons (with the same spin) in the same momentum state **k**. Can it really be that virtual processes violate the exculsion principle? Fortunately, another interpretation can be given. Under close examination, we see that unlike typical virtual fluctuations to high energy states, which lower the total energy, this term actually raises the quasiparticle energy. These energy raising processes are a "blocking effect" produced by the exclusion principle, on the vacuum fluctuations. In the ground-state, there are virtual fluctuations

$$GS \rightleftharpoons \text{electron } (\mathbf{k}') + \text{hole } (-\mathbf{k}' - \mathbf{q}) + \text{phonon } (\mathbf{q})$$

which lower the energy of the ground-state. When a single electron occupies the state of momentum $\mathbf{k}$, the exclusion principle prevents vacuum fluctuations with $\mathbf{k}' = \mathbf{k}$, raising the energy of the quasiparticle. So time ordered diagrams that appear to violate the exclusion principle describe the suppression of vacuum fluctuations by the exclusion principle.

If we now extend our discussion to finite temperatures, for any given $\mathbf{k}$ and $\mathbf{q}$, both the first and the second terms in the phonon self-energy are presen. For phonon emission processes, the appearance of the additional Bose terms $n_{\mathbf{q}}$ is the the effect of stimulated emission, whereby the occupancy of phonon states enhances the emission of phonons. The terms which vanish at zero temperature can also be interpreted as the effect of phonon absorption of the now thermally excited phonons, i.e

$$\Sigma(\mathbf{k}, z) = \sum_{\mathbf{q}} g_{\mathbf{q}}^2 \left[\underbrace{\frac{1 - f_{\mathbf{k}-\mathbf{q}} + n_{\mathbf{q}}}{z - (\epsilon_{\mathbf{k}-\mathbf{q}} + \omega_{\mathbf{q}})}}_{\text{virtual/real phonon absorption by hole}} + \underbrace{\frac{f_{\mathbf{k}-\mathbf{q}} + n_{\mathbf{q}}}{z - (\epsilon_{\mathbf{k}-\mathbf{q}} - \omega_{\mathbf{q}})}}_{\text{virtual/real phonon absorption by electron}} \right]$$

By contrast, the imaginary part of the self-energy determines the decay rate of the electron due to real phonon emission, and the decay rate of the electron is related to the quantity

$$\Gamma_{\mathbf{k}} = 2Im\Sigma(\mathbf{k}, \epsilon^*_{\mathbf{k}} - i\delta) \approx 2Im\Sigma(\mathbf{k}, \epsilon_{\mathbf{k}} - i\delta)$$

If we use the Dirac relation

$$\left[\frac{1}{x - a - i\delta}\right] = P\frac{1}{x - a} + i\pi\delta(x - a)$$

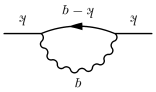
so that the exchange of a boson induces an effective interaction

$$\boxed{V_{\text{eff}}(\mathbf{q}, z) = g_{\mathbf{q}}^2 \frac{2\omega_{\mathbf{q}}}{(z)^2 - \omega_{\mathbf{q}}^2} \qquad (9.104)}$$

Notice two things about this interaction -

- It is strongly frequency dependent, reflecting the strongly retarded nature of the electron phonon interaction. The characteristic phonon frequency is the Debye frequency $\omega_D \sim$, and the characteristic "restitution" time associated with the electron phonon interaction is $\tau \sim 1/\omega_D$, whereas the corresponding time associated with the repulsive Coulomb interaction is of order $1/\epsilon_F$. The ratio $\epsilon_F/\omega_D \sim 20$ is a measure of how much more retarded the electron-phonon interaction is compared with the Coulomb potential.
- At frequencies below the Debye energy, $\omega \lesssim \omega_D$ the denominator in V_{eff} changes sign, and the residual low-energy interaction is actually attractive. It is this component of the interaction that is responsible for superconductivity in conventional superconductors.

We wish to now calculate the effect of the electron-phonon interaction on electron propagation. The main effect on the electron propagation is determined by the electron-phonon self energy. The leading order Feynman diagram for the self-energy is given by



$$\equiv \Sigma(k) = \sum_q (ig_{\mathbf{q}})^2 \mathcal{G}^0(k - q) D(q) \qquad (9.105)$$

or written out explicitly,

$$\begin{aligned}
\Sigma(\mathbf{k}, i\omega_n) &= -T \sum_{\mathbf{q}, i\nu_n} g_{\mathbf{q}}^2 \left[\frac{2\omega_{\mathbf{q}}}{(i\nu_n)^2 - \omega_{\mathbf{q}}^2}\right] \frac{1}{i\omega_n - i\nu_n - \epsilon_{\mathbf{k}-\mathbf{q}}} \\
&= -T \sum_{\mathbf{q}, i\nu_n} \left[\frac{1}{i\nu_n - \omega_{\mathbf{q}}} \frac{1}{i\omega_n - i\nu_n - \epsilon_{\mathbf{k}-\mathbf{q}}} - (\omega_{\mathbf{q}} \to -\omega_{\mathbf{q}})\right] \qquad (9.106)
\end{aligned}$$

where we have simplified the expression by splitting up the boson propagator into a positive and negative frequency component, the latter being obtained by reversing the sign on $\omega_{\mathbf{q}}$. We shall carry out the Matsubara sum over the bosonic frequencies by writing it as a contour integral with the Bose function:

$$-T \sum_{i\nu_n} F(i\nu_n) = -\int_C \frac{dz}{2\pi i} n(z) F(z) = \int_{C'} \frac{dz}{2\pi i} n(z) F(z) \qquad (9.107)$$

where C runs anti-clockwise around the imaginary axis and C' runs anticlockwise around the poles in $F(z)$. In this case, we choose

$$\begin{aligned}
F(z) &= \frac{1}{z - \omega_{\mathbf{q}}} \frac{1}{i\omega_n - z - \epsilon_{\mathbf{k}-\mathbf{q}}} \\
&= \left[\frac{1}{z - \omega_{\mathbf{q}}} - \frac{1}{z - (i\omega_n - \epsilon_{\mathbf{k}-\mathbf{q}})}\right] \frac{1}{i\omega_n - (\omega_{\mathbf{q}} + \epsilon_{\mathbf{k}-\mathbf{q}})} \qquad (9.108)
\end{aligned}$$

which has two poles, one at $z = \omega_{\mathbf{q}}$ and one at $z = i\omega_n - \epsilon_{\mathbf{k}-\mathbf{q}}$ (Fig. 9.5). Carrying out the

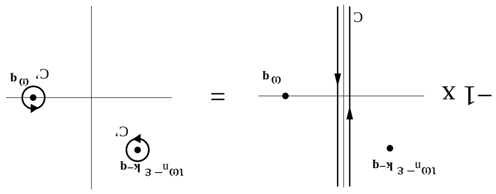


Figure 9.5: Contours C and C' used in evaluation of $\Sigma(\mathbf{k}, i\omega_n)$

contour integral, we then obtain

$$\begin{aligned}
\Sigma(k) &= \sum_{\mathbf{q}} g_{\mathbf{q}}^2 \left[\frac{n(\omega_{\mathbf{q}}) - \overbrace{n(i\omega_n - \epsilon_{\mathbf{k}-\mathbf{q}})}^{-(1 - f_{\mathbf{k}-\mathbf{q}})}}{i\omega_n - (\omega_{\mathbf{q}} + \epsilon_{\mathbf{k}-\mathbf{q}})} - \{\omega_{\mathbf{q}} \to -\omega_{\mathbf{q}}\}\right] \\
&= \sum_{\mathbf{q}} g_{\mathbf{q}}^2 \left[\frac{1 + n_{\mathbf{q}} - f_{\mathbf{k}-\mathbf{q}}}{i\omega_n - (\omega_{\mathbf{q}} + \epsilon_{\mathbf{k}-\mathbf{q}})} - \{\omega_{\mathbf{q}} \to -\omega_{\mathbf{q}}\}\right] \qquad (9.109)
\end{aligned}$$

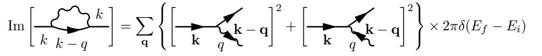
The second term in this expression is obtained by reversing the sign on $\omega_{\mathbf{q}}$ in the first term, which gives finally,

$$\boxed{\Sigma(\mathbf{k}, z) = \sum_{\mathbf{q}} g_{\mathbf{q}}^2 \left[\frac{1 + n_{\mathbf{q}} - f_{\mathbf{k}-\mathbf{q}}}{z - (\epsilon_{\mathbf{k}-\mathbf{q}} + \omega_{\mathbf{q}})} + \frac{n_{\mathbf{q}} + f_{\mathbf{k}-\mathbf{q}}}{z - (\epsilon_{\mathbf{k}-\mathbf{q}} - \omega_{\mathbf{q}})}\right]}$$

then we see that for a weak interaction, the decay rate of the electron is given by

$$\Gamma_{\mathbf{k}} = 2\pi \sum_{\mathbf{q}} g_{\mathbf{q}}^2 \Big[\overbrace{(1 + n_{\mathbf{q}} - f_{\mathbf{k}-\mathbf{q}})\delta(\epsilon_{\mathbf{k}} - (\epsilon_{\mathbf{k}-\mathbf{q}} + \omega_{\mathbf{q}}))}^{\text{phonon emission}} + \overbrace{(n_{\mathbf{q}} + f_{\mathbf{k}-\mathbf{q}})\delta(\epsilon_{\mathbf{k}} - (\epsilon_{\mathbf{k}-\mathbf{q}} - \omega_{\mathbf{q}}))}^{\text{phonon absorption}} \Big]$$

which we may identify as the contribution to the decay rate from phonon emission and absorption, respectively. Schematically, we may write



so that taking the imaginary part of the self-energy "cuts" the internal lines. The link between the imaginary part of the self-energy and the real decay processes of absorption and emission is sometimes refered to as the "optical theorem".

9.7.1 $\alpha^2 F$: the electron-phonon coupling function

One of the most important effects of the electron phonon interaction, is to give rise to a superconducting instability. Superconductivity is driven by the interaction of low-energy electrons very close to the Fermi surface, so the amount of energy transferred in an interaction is almost zero. For this reason, the effective interaction between the electrons is given by (9.104)

$$V_{\text{eff}}(\mathbf{q}, 0) = -\frac{2g_{\mathbf{q}}^2}{\omega_{\mathbf{q}}}$$

Now the momentum dependence of this interaction is very weak. In our simple model, for example, $g_{\mathbf{q}}^2/2\omega_q \sim \frac{q^2}{\omega_q^2} \sim$ constant, and a weak momentum dependence implies that to a first approximation then, the effective low energy interaction is local, extending over one unit cell and of approximate form

$$H_{eff} \approx -g \sum_{\sigma\sigma'} \int_{\mathbf{q},\mathbf{k},\mathbf{k}',(|\epsilon_k|,\ |\epsilon_{k'}|)<\omega_D)} {\psi^\dagger}_{\mathbf{k}+\mathbf{q}\sigma} {\psi^\dagger}_{\mathbf{k}'\sigma'} \psi_{\mathbf{k}'+\mathbf{q}\sigma'} \psi_{\mathbf{k}\sigma} \tag{9.110}$$

where the sum over electron momenta is restricted to within a narrow band of energies, within ω_D of the Fermi energy. (Which means that the interaction is only "instantaneous" to within a time-scale of $\delta t \sim 1/\omega_D$ and the effective coupling constant is the momentum average of $2g_{\mathbf{q}}^2/\omega_{bq}$,

$$g = \frac{1}{N_s} \sum_{\mathbf{q}} \frac{2g_{\mathbf{q}}^2}{\omega_{\mathbf{q}}} \tag{9.111}$$

We can make an order-of-magnitude estimate of g, by replacing

$$g \sim \frac{g_{2k_F}^2}{\omega_D} \sim \frac{1}{\omega_D} \overbrace{\left[\left(\frac{\hbar^2}{2M\omega_D} \right) \epsilon_F^2 (2k_F)^2 \right]}^{(g_{2k_F})^2} \sim \overbrace{\left(\frac{\epsilon_F^2}{\omega_D^2} \right)}^{\frac{M}{m}} \frac{\hbar^2 k_F^2}{2M} \sim \epsilon_F$$

The electron phonon interaction is defined as the product of the local interaction strength, times the electron density of states,

$$\lambda = N(0)g = \frac{1}{N_s} \sum_{\mathbf{q}} \frac{2N(0)g_{\mathbf{q}}^2}{\omega_{\mathbf{q}}} \tag{9.112}$$

This dimensionless quantity is not reduced by the small ratio of electron to atom mass, and in typical metals $\lambda \sim 0.1 - 0.2$. We'll now see that we relate the electron phonon self energy to this quantity.

The electron-phonon self-energy can be simplified by the introduction of a function we call "$\alpha^2 F$", that keeps track of the frequency dependence of the electron-phonon coupling constant, where $\alpha(\omega)$ is the typical energy dependent coupling constant and F is the phonon density of states. It turns out that $\alpha^2 F$ can be actually measured inside superconductors and F can be measured by neutron scattering.

The basic idea here, is that the frequency dependence of the electron-phonon self energy is far greater than the momentum dependence. The approximate dimensionless ratio of the momentum, to frequency dependence is given by the small ratio of the Debye frequency to the Fermi energy, ω_D/ϵ_F

$$\left(\frac{1}{v_F} |\nabla_k \Sigma| \right) / \left(\frac{\partial \Sigma}{\partial \omega} \right) \sim \frac{\omega_D}{\epsilon_F} << 1$$

To a good approximation then, the electron phonon self-energy can be averaged over the Fermi surface, writing

$$\Sigma(\omega) = \frac{\int dS \Sigma(\mathbf{k}, \omega)}{\int dS}$$

where $\int dS \equiv \int d^2k$ is an integral over the Fermi surface. Now the sum over $\mathbf{k}'$ inside the self-energy can be replaced by a combination of an energy integral, and a Fermi surface integral, as follows

$$\sum_{\mathbf{k}'} \rightarrow \int dS' dk'_{\text{perp}} = \int \frac{dS'}{|d\epsilon_{k'}/dk'|} d\epsilon' = \int \frac{dS'}{v_F(S')} d\epsilon'$$

where $dS' \equiv d^2k$ is a surface integral along the surface of constant energy and $v_F(S) = \mathbf{n} \cdot \nabla_{\mathbf{k}} \epsilon_{\mathbf{k}}$ is the local Fermi velocity normal to this surface. Making this substitution,

$$\Sigma(\omega) = \frac{1}{\int dS} \int \frac{dS dS'}{v'_F} d\epsilon' g_{\mathbf{k}-\mathbf{k}'}^2 \left[\frac{1 + n_{\mathbf{k}-\mathbf{k}'} - f(\epsilon')}{z - (\epsilon' + \omega_{\mathbf{k}-\mathbf{k}'})} + \frac{n_{\mathbf{k}-\mathbf{k}'} + f(\epsilon')}{z - (\epsilon' - \omega_{\mathbf{k}-\mathbf{k}'})} \right]$$

If we introduce a delta function in the phonon frequency into this expression, using the identity $1 = \int d\nu \delta(\nu - \omega_{\mathbf{q}\lambda})$, then we may rewrite it as follows

$$\Sigma(\omega) \quad = \quad \frac{1}{\int dS} \int d\epsilon' d\nu \int \frac{dS\ dS'}{v'_F} g_{\mathbf{k}-\mathbf{k}'}^2 \delta(\nu - \omega_{\mathbf{k}-\mathbf{k}'}) \left[\frac{1 + n(\nu) - f(\epsilon')}{z - (\epsilon' + \nu)} + \frac{n(\nu) + f(\epsilon')}{z - (\epsilon' - \nu)} \right]$$

$$= \quad \int d\epsilon' d\nu \alpha^2(\nu) F(\nu) \left[\frac{1 + n(\nu) - f(\epsilon')}{z - (\epsilon' + \nu)} + \frac{n(\nu) + f(\epsilon')}{z - (\epsilon' - \nu)} \right] \tag{9.113}$$

where the

$$F(\omega) = \sum_{\mathbf{q},\lambda} \delta(\omega - \omega_{\mathbf{q}\lambda})$$

is the phonon density of states, and

$$\alpha^2 F(\nu) = \frac{1}{\int dS} \int \frac{dS\ dS'}{v'_F} \delta(\omega - \omega_{\mathbf{k}-\mathbf{k}'}) g_{\mathbf{k}-\mathbf{k}'\lambda}^2$$

is the Fermi surface average of the phonon matrix element and density of states. With this definition, we may rewrite the self energy as

$$\boxed{\Sigma(z) = \int d\epsilon d\nu \alpha^2(\nu) F(\nu) \left[\frac{1 + n(\nu) - f(\epsilon)}{z - (\epsilon + \nu)} + \frac{n(\nu) + f(\epsilon)}{z - (\epsilon - \nu)} \right]}$$

where the energy dependence of the electron density of states has been neglected. This is a very practical form for the electron self-energy. In practice, most of the energy dependence in $\alpha^2 F$ is determined by the phonon density of states. As we shall see later, in a conventional electron-phonon superconductor, one may infer the function $\alpha^2 F$ using the density of electron states in the superconductor measured by tunneling in the superconducting state.

9.7.2 Mass Renormalization by the electron phonon interaction

Our simplified for of the self-energy enables us to examine how electron propagation is modified by the exchange of virtual phonons. Let us expand the electron-phonon self energy around zero frequency in the ground-state. In the ground-state,

$$\begin{aligned} \Sigma(\omega) \quad &= \quad \int d\epsilon d\nu \alpha^2(\nu) F(\nu) \left[\frac{\theta(\epsilon)}{z - (\epsilon + \nu)} + \frac{\theta(-\epsilon)}{z - (\epsilon' - \nu)} \right] \\ &= \quad \int d\epsilon d\nu \alpha^2(\nu) F(\nu) \ln \left[\frac{\nu - z}{\nu + z} \right] \end{aligned}$$

so that at low frequencies,

$$\Sigma(\omega) = \Sigma(0) - \lambda\omega$$

where

$$\begin{aligned} \lambda \quad &= \quad - \left. \frac{d\Sigma(\omega)}{d\omega} \right|_{\omega=0} \\ &= \quad 2 \int d\nu \frac{\alpha^2(\nu) F(\nu)}{\nu} \end{aligned} \tag{9.114}$$

If we look at our definition of $\alpha^2 F$, we see that this expression is the Fermi surface average of the electron phonon coupling constant defined in (9.112).

Now at low energies, we can write the electron propagator in terms of the quasiparticle energies, as follows

$$\begin{aligned} \mathcal{G}(\mathbf{k}, \omega - i\delta) \quad &= \quad \frac{1}{\omega - \epsilon_{\mathbf{k}} - \Sigma(\omega - i\delta)} \\ &= \quad \frac{1}{\omega - \underbrace{\epsilon_{\mathbf{k}} - \Sigma(\epsilon_k^* - i\delta)}_{\epsilon_{\mathbf{k}}^* - i\Gamma/2} + \lambda(\omega - \epsilon_k^*)}, \end{aligned} \tag{9.115}$$

or

$$\boxed{\mathcal{G}(\mathbf{k}, \omega - i\delta) = \frac{Z}{\omega - \epsilon_{\mathbf{k}}^* - i\Gamma^*/2}} \tag{9.116}$$

where

$$\begin{aligned} Z \quad &= \quad (1 + \lambda)^{-1} && \text{wavefunction renormalization} \\ \epsilon_{\mathbf{k}}^* \quad &= \quad \epsilon_{\mathbf{k}} + \Sigma(\epsilon_k^*) && \text{quasiparticle energy} \\ \Gamma^* \quad &= \quad 2ZIm\Sigma(\epsilon_{\mathbf{k}}^* - i\delta) && \text{quasiparticle decay rate.} \end{aligned} \tag{9.117}$$

We see that in the presence of the electron phonon interaction, electron quasiparticles are still well-defined at low temperatures. Indeed, at the Fermi surface, $\Gamma^* = 0$ in the ground-state, so that electron quasiparticles are infinitely long-lived. This is an example of a Landau Fermi liquid, discussed in chapter 8. If we differentiate $\epsilon_{\mathbf{k}}$ with respect to $\epsilon_{\mathbf{k}}^*$, we obtain

$$\frac{d\epsilon_{\mathbf{k}}}{d\epsilon_{\mathbf{k}}^*} = (1 + \lambda) = \left(\frac{m^*}{m} \right)$$

so that the effective mass of the electron is enhanced by the cloud of virtual phonons which trails behind it. The density of states is also renormalized in the same way

$$N(0)^* = \frac{d\epsilon_{\mathbf{k}}}{d\epsilon_{\mathbf{k}}^*} N(0) = N(0)(1 + \lambda)$$

while the electron group velocity is renormalized downwards according to

$$v_F^* = \nabla_{\mathbf{k}} \epsilon_{\mathbf{k}}^* = \frac{d\epsilon_{\mathbf{k}}^*}{d\epsilon_{\mathbf{k}}} \nabla_{\mathbf{k}} \epsilon_{\mathbf{k}} = Z v_F$$

Thus the electron phonon interaction drives up the mass of the electron, effect of squeezing the one-particle states more closely together and driving the electron group velocity downwards. This in turn will mean that the linear coefficient of the electronic specific heat $C_v = \gamma^* T$

$$\gamma^* = \frac{\pi^2 k_B^2}{3} N^*(0) = \gamma_0 (1 + \lambda)$$

is enhanced.

We can give the wavefunction renormalization another interpretation. Recall that using the method of contour integration, we can always rewrite the Matsubara representation of the Green function

$$G(\mathbf{k},\tau) = T\sum_n G(\mathbf{k}, i\omega_n)e^{-i\omega_n\tau}$$

as

$$G(\mathbf{k},\tau) = -\int \frac{d\omega}{\pi}\left[(1-f(\omega))\theta(\tau) - f(\omega)\theta(-\tau)\right]A(\mathbf{k},\omega)e^{-\omega\tau} \qquad (9.118)$$

where $A(\mathbf{k},\omega) = ImG(\mathbf{k},\omega - i\delta)$ is the spectral function. Now, from the normalization of the fermionic commutation relation $\{c_{\mathbf{k}\sigma}, c^\dagger{}_{\mathbf{k}\sigma}\} = 1$, we deduce that the spectral function is normalized:

$$\begin{aligned} 1 &= \langle\{c_{\mathbf{k}\sigma}, c^\dagger{}_{\mathbf{k}\sigma}\}\rangle = \overbrace{G(\mathbf{k},0^-)}^{\langle c^\dagger{}_{\mathbf{k}\sigma}c_{\mathbf{k}\sigma}\rangle} - \overbrace{G(\mathbf{k},0^+)}^{-\langle c_{\mathbf{k}\sigma}c^\dagger{}_{\mathbf{k}\sigma}\rangle} \\ &= \int \frac{d\omega}{\pi}A(\mathbf{k},\omega) \end{aligned} \qquad (9.119)$$

The quasiparticle part of the spectral function (9.116) is a Lorentzian of width $\Gamma^*_{\mathbf{k}}$, weight πZ, and since the width $\Gamma^*_{\mathbf{k}} \to 0$ as $\epsilon^*_{\mathbf{k}}$ gets closer to the Fermi energy, we deduce that for $k \sim k_F$, the quasiparticle part of the spectral function ever more closely represents a delta function of weight Z, so that

$$\frac{1}{\pi}A(\mathbf{k},\omega) \sim Z\delta(\omega - \epsilon^*_{\mathbf{k}}) + \text{incoherent background}$$

where the incoherent background is required so that the total frequency integral of the spectral function is equal to unity.

Now from (9.118), we see that the ground-state occupancy of the electron momentum state $\mathbf{k}$ is given by

$$\begin{aligned} n_{\mathbf{k}\sigma} &= \langle \hat{n}_{\mathbf{k}\sigma}\rangle_{T=0} = -G(\mathbf{k},0^-) = \int\frac{d\omega}{\pi}f(\omega)A(\mathbf{k},\omega)\Big|_{T=0} \\ &= \int_{-\infty}^{0}\frac{d\omega}{\pi}A(\mathbf{k},\omega), \qquad (T=0) \end{aligned} \qquad (9.120)$$

The presence of the quasiparticle pole in the spectral function means that at the Fermi surface, there is a discontinuity in the occupancy given by

$$n_{\mathbf{k}\sigma}|_{k=k_F^-} - n_{\mathbf{k}\sigma}|_{k=k_F^+} = Z = \frac{1}{1+\lambda}$$

as shown in Fig. 9.6

Remarks:

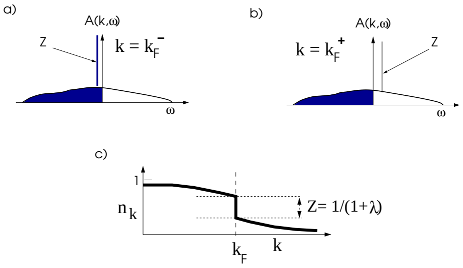


Figure 9.6: Illustrating the relationship between the coherent, quasiparticle component in the electron spectral function, and the discontinuity in the momentum-space occupancy at the Fermi surface due to the electron-phonon interaction. a) Spectral function just below the Fermi surface - quasiparticle peak occupied. b) Spectral function just above Fermi surface - quasiparticle peak unoccupied. c) Momentum space occupancy $n_{\mathbf{k}}$.

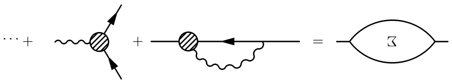
- *The survival of a sharp "coherent" delta-function peak in the quasiparticle spectral function, together with this sharp precipace-like discontinuity in the momentum-space occupancy, are one of the hallmark features of the Landau Fermi liquid. In an electron-phonon mediated superconductor, it is the coherent part of the spectral function which condenses into the pair condensate.*
- *At first sight, one might imagine that since the density of states $N^*(0) = (1+\lambda)N(0)$ is enhanced, the magnetic susceptibility will follow suit. In actual fact, the compression of the density of states produced by phonons is always located at the Fermi energy, and this means that if the electron phonon interaction is turned on adiabatically, it does not affect the Fermi momenta of either up, or down electrons, so that the magnetization, and hence the magnetic susceptibility are unaffected by the electron phonon interaction.*

9.7.3 Migdal's theorem.

At first sight, one might worry about the usefulness of our leading order self-energy correction. We have already seen that the size of the electron phonon interaction λ is of order unity. So what permits us to ignore the vertex corrections to the self energy?

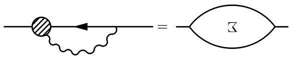
One of the classic early results in the electron phonon problem, is Migdal's theorem, according to which that the renormalization of the electron-phonon coupling by phonon exchange, is of order $\sqrt{\frac{m}{M}}$. Migdal's theorem is a result of the huge mismatch between the electron and phonon dispersion. Basically- when an electron scatters off a phonon, it moves away so fast that other phonons can not "catch up" with the outgoing electron.

Migdal's theorem concerns the correction to the electron-phonon vertex. Diagramatically, the electron self-energy can be expanded as follows



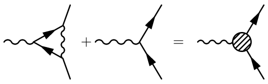
(9.121)

which we can denote by the shorthand



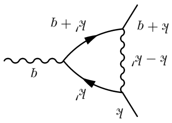
(9.122)

Here, the shaded circle denotes the vertex part, given by



$$+\ldots = ig(\mathbf{q})(1+\Lambda(q)) \qquad (9.123)$$

We shall discuss the leading order vertex correction,



$$= (ig_{\mathbf{q}})\Lambda(q) \qquad (9.124)$$

where the vertex function $\Lambda(q)$ is given by

$$\Lambda(q) = T\sum_{k'\equiv(i\omega'_n,\mathbf{k}')}(ig_{\mathbf{k}-\mathbf{k}'})^2G(k'+q)G(k')D(k-k') \qquad (9.125)$$

We are interested in an order of magnitude estimate of this quantity.

Now at low temperatures, we can replace the summation over the Matsubara frequency can be replaced by an integral,

$$T\sum_{\omega'_n} \to \int\frac{d\omega'_n}{2\pi}$$

so that

$$\Lambda(q) = -\int\frac{d\omega'_n}{2\pi}\int\frac{d^3k'}{(2\pi)^3}(g_{\mathbf{k}-\mathbf{k}'})^2G(k'+q)G(k')D(k-k')$$

Now the propogator

$$D(k-k') = -\frac{\omega_{\mathbf{k}-\mathbf{k}'}}{(\omega_n-\omega'_n)^2+\omega^2_{\mathbf{q}}}$$

vanishes as $1/(\omega'_n)^2$ in the region where $|\omega_n - \omega'_n| \gtrsim \omega_D$, so we restrict this integral, writing

$$\Lambda(q) = -\int_{-\omega_D}^{\omega_D}\frac{d\omega'_n}{2\pi}\int\frac{d^3k'}{(2\pi)^3}(g_{\mathbf{k}-\mathbf{k}'})^2D(k-k')G(k'+q)G(k')$$

Inside the restricted frequency integral, to obtain an estimate of this quantity, we shall replace $g^2_{\mathbf{k}-\mathbf{k}'}D(\mathbf{k}-\mathbf{k}') \sim g \times 2\omega_{\mathbf{k}-\mathbf{k}'}D(\mathbf{k}-\mathbf{k}') \sim -g$, since $2\omega_{\mathbf{k}-\mathbf{k}'}D(\mathbf{k}-\mathbf{k}') \sim -1$, thus Now to good approximation, the frequency integral may be replaced by a single factor ω_D, so that

$$\Lambda(q) \sim \omega_D g\overbrace{\int\frac{d^3k'}{(2\pi)^3}G(k'+q)G(k')\Big|_{\omega'_n=\omega_n}}^{\sim\frac{(k_Fa)^3}{\epsilon_F^2}}.$$

Now inside the momentum summation over $\mathbf{k}'$, the electron momenta are unrestricted so the energies $\epsilon_{\mathbf{k}'}$ and $\epsilon_{\mathbf{k}'+\mathbf{q}}$ are far from the Fermi energy and we may estimate this term as of order $\frac{(k_Fa)^3}{\epsilon_F^2}$. Putting these results together,

$$\Lambda \sim g\omega_D\frac{(k_Fa)^3}{\epsilon_F^2}$$

Now since $g \sim \lambda\epsilon_F$ and $(k_Fa)^3 \sim 1$, we see that

$$\Lambda \sim \lambda\frac{\omega_D}{\epsilon_F} \sim \sqrt{\frac{m}{M}}$$

In otherwords, even though the electron phonon interaction is of order unity, the large ratio of electron to ion mass leads to a very small vertex correction.

Remarks:

- *Perhaps the main difficulty of the Migdal argument, is that it provides a false sense of security to the theorist- giving the impression that one has "proven" that the perturbative treatment of the electron phonon interaction is always justified. Migdal's argument is basically a dimensional analysis. The weak-point of the derivation, is that the dimensional analysis does not work for those scattering events where the energies of the scattered electrons are degenerate. While such scattering events may make up a small contribution to the overall phase space contributing to the self-energy, they become important because the associated scattering amplitudes can develop strong singularities that ultimately result in a catastrophic instability of the Fermi liquid. The dimensional analysis in the Migdal argument breaks down when electrons inside the loop have almost degenerate energies. For example, the Migdal calculation, does not work for the case where* $\mathbf{q}$ *is close to a nesting vector of the Fermi surface, when* $\mathbf{q}$ *spans two nested Fermi surfaces, this causes* $\epsilon_{\mathbf{k}'}$ *and* $\epsilon_{\mathbf{k}'+\mathbf{q}}$ *to become degenerate, enhancing the size of the vertex by a factor of* $\epsilon_F/\omega_D \times \log(\omega_D/T)$*. The singular term ultimately grows to a point where an instability to a density wave takes place, producing a charge density wave. The other parallel instability is the Cooper instability, which is a singular correction to the particle-particle scattering vertex, caused by the degeneracy of electron energies for electrons of opposite momenta.*

9.8 Appendix A

In this appendix, we consider the Hamiltonian

$$H = \overbrace{\sum_\lambda \psi^\dagger{}_\lambda \psi_\lambda}^{H_0} - \overbrace{\sum_\lambda \left[\bar{z}_\lambda(\tau)\psi_\lambda + \psi^\dagger)_\lambda\right]}^{-V_I}$$

and show that the generating functional

$$\begin{aligned} Z_0[\bar{z}, z] &= Z_0 \langle T e^{-\int_0^\beta V_I(\tau) d\tau} \rangle_0 \\ &= Z_0 \langle T \exp\left[\int_0^\beta d\tau \sum_\lambda \left(\bar{z}_\lambda(\tau)\psi_\lambda(\tau) + \psi^\dagger{}_\lambda(\tau) z_\lambda(\tau)\right)\right] \rangle_0 \end{aligned} \qquad (9.126)$$

is explicitly given by

$$\boxed{\begin{aligned} \frac{Z_0[\bar{z}, z]}{Z_0} &= \exp\left[-\sum_\lambda \int_0^\beta d\tau_1 d\tau_2 \bar{z}_\lambda(1) G_\lambda(\tau_1 - \tau_2) z_\lambda(2)\right] \\ G_\lambda(\tau_1 - \tau_2) &= -\langle T \psi_\lambda(\tau_1) \psi^\dagger{}_\lambda(\tau_2) \rangle \end{aligned} \qquad (9.127)}$$

for both bosons and fermions.

We begin by evaluating the equation of motion of the fields in the Heisenberg representation:

$$\frac{\partial \psi_\lambda}{\partial \tau} = [H, \psi_\lambda] = -\epsilon_\lambda \psi_\lambda(\tau) + z_\lambda(\tau)$$

Multiplying this expression by the integrating factor $e^{\epsilon_\lambda \tau}$, we obtain

$$\frac{\partial}{\partial \tau}\left[e^{\epsilon_\lambda \tau}\psi_\lambda(\tau)\right] = e^{\epsilon_\lambda \tau} z_\lambda(\tau)$$

which we may integrate from $\tau' = 0$ to $\tau' = \tau$, to obtain

$$\psi_\lambda(\tau) = e^{-\epsilon_\lambda \tau}\psi_\lambda(0) + \int_0^\tau d\tau' e^{-\epsilon_\lambda(\tau - \tau')} z_\lambda(\tau') d\tau'$$

We shall now take expectation values of this equation, so that

$$\langle \psi_\lambda(\tau) \rangle = e^{-\epsilon_\lambda \tau}\langle \psi_\lambda(0) \rangle + \int_0^\tau d\tau' e^{-\epsilon_\lambda(\tau - \tau')} z_\lambda(\tau') d\tau' \qquad (9.128)$$

If we impose the boundary condition $\langle \psi_\lambda(\beta) \rangle = \zeta \langle \psi_\lambda(0) \rangle$, where $\zeta = 1$ for bosons and $\zeta = -1$ for fermions, then we deduce that

$$\langle \psi_\lambda(0) \rangle = \zeta n_\lambda \int_0^\beta e^{\epsilon_\lambda \tau'} z_\lambda(\tau') d\tau',$$

where $n_\lambda = 1/(e^{\beta \epsilon_\lambda} - \zeta)$ is the Bose ($\zeta = 1$), or Fermi function $\zeta = -1$. Inserting this into (9.128), we obtain

$$\langle \psi_\lambda(\tau) \rangle = \zeta n_\lambda \int_0^\beta e^{-\epsilon_\lambda(\tau - \tau')} z_\lambda(\tau') d\tau' + \int_0^\beta e^{-\epsilon_\lambda(\tau - \tau')} \theta(\tau - \tau') z_\lambda(\tau') d\tau', \qquad (9.129)$$

where we have introduced a theta function in the second term, in order to extend the upper limit of integration to β. Rearranging this expression, we obtain

$$\begin{aligned} \langle \psi_\lambda(\tau) \rangle &= \int_0^\beta d\tau' \overbrace{e^{-\epsilon_\lambda}(\tau - \tau')\left[(1 + \zeta n_\lambda)\theta(\tau - \tau') + \zeta n_\lambda \theta(\tau' - \tau)\right]}^{-\mathcal{G}_\lambda(\tau - \tau')} \\ &= -\int_0^\beta d\tau' \mathcal{G}_\lambda(\tau - \tau') z_\lambda(\tau') \end{aligned} \qquad (9.130)$$

so $\mathcal{G}_\lambda(\tau)$ is the imaginary time response of the field to the source term. We may repeat the same procedure for the expectation value of the creation operator. The results of these two calculations may be summarized as

$$\begin{aligned} \langle \psi_\lambda(\tau) \rangle &= \frac{\delta Z[\bar{z}, z]}{\delta \bar{z}(\tau)} = -\int_0^\beta d\tau' \mathcal{G}_\lambda(\tau - \tau') z_\lambda(\tau') \\ \langle \psi^\dagger{}_\lambda(\tau) \rangle &= \frac{\delta Z[\bar{z}, z]}{\delta z(\tau)} = -\int_0^\beta d\tau' \bar{z}(\tau) \mathcal{G}_\lambda(\tau - \tau'). \end{aligned} \qquad (9.131)$$

Notice how the creation field propagates backwards in time from the source. The common integral to these two expression is

$$\ln Z[\bar{z}, z] = \ln Z_0 - \int_0^\beta d\tau d\tau' \bar{z}_\lambda(\tau) G_\lambda(\tau - \tau') z_\lambda(\tau')$$

where the constant term $\ln Z_0$ has to be intependent of both z and $\bar{z}$. The exponential of this expression recovers the result (9.127).

9.9 Exercises for chapter 9

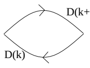
1. Use the method of complex contour integration to carry out the Matsubara sums in the following:

   (i) Derive the density of a spinless Bose Gas at finite temperature from the boson propagator $D(k) \equiv D(\mathbf{k}, \mathbf{i}\nu_\mathbf{n}) = [\mathbf{i}\nu_\mathbf{n} - \omega_\mathbf{k}]^{-\mathbf{1}}$, where $\omega_\mathbf{k} = E_\mathbf{k} - \mu$ is the energy of a boson, measured relative to the chemical potential.

   $$\rho(T) = \frac{N}{V} = V^{-1} \sum_\mathbf{k} \langle T b_\mathbf{k}(0^-) b^\dagger{}_\mathbf{k}(0) \rangle = -(\beta V)^{-1} \sum_{i\nu_n, \mathbf{k}} D(k) e^{i\nu_n 0^+}. \qquad (9.132)$$

   How do you need to modify your answer to take account of Bose Einstein condensation?

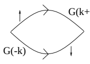
   (ii) The dynamic charge-susceptibility of a free Bose gas, i.e

   $\chi_c(q, i\nu_r) =$ 

   $= T \sum_{i\nu_n} \int \frac{d^3k}{(2\pi)^3} D(q + k) D(k).$ (9.133)

   where $q \equiv (\mathbf{q}, i\nu_r)$. Please analytically extend your final answer to real frequencies.

   (iii) The "pair-susceptibility" of a spin-1/2 free Fermi gas, i.e.

   $\chi_P(q, i\nu_n) =$ 

   $= T \sum_{i\omega_r} \int \frac{d^3k}{(2\pi)^3} G(q + k) G(-k)$ (9.134)

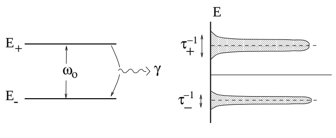
   where $G(k) \equiv G(\mathbf{k}, \mathbf{i}\omega_\mathbf{n}) = [\mathbf{i}\omega_\mathbf{n} - \epsilon_\mathbf{k}]^{-\mathbf{1}}$. (Note the direction of the arrows: why is there no minus sign for the Fermion loop?) Show that the static pair susceptibility, $\chi_P(0)$is given by

   $$\chi_P = \int \frac{d^3k}{(2\pi)^3} \frac{\tanh[\beta\epsilon_\mathbf{k}/2]}{2\epsilon_\mathbf{k}} \qquad (9.135)$$

   Can you see that this quantity diverges at low temperatures? How does it diverge, and why ?

2. A simple model an atom with two atomic levels coupled to a radiation field is described by the Hamiltonian

   $$H = H_o + H_I + H_{\rm photon}, \qquad (9.136)$$

   where

   $$H_o = \tilde{E}_- c^\dagger{}_- c_- + \tilde{E}_+ c^\dagger{}_+ c_+ \qquad (9.137)$$

   describes the atom, treating it as a *fermion*

   $$H_I = V^{-1/2} \sum_{\vec{q}} g(\omega_{\vec{q}}) \left(c^\dagger{}_+ c_- + c^\dagger{}_- c_+\right)\left[a^\dagger{}_{\vec{q}} + a_{-\vec{q}}\right] \qquad (9.138)$$

   describes the coupling to the radiation field (V is the volume of the box enclosing the radiation) and

   $$H_{photon} = \sum_{\vec{q}} \omega_{\vec{q}} a^\dagger{}_{\vec{q}} a_{\vec{q}}, \qquad (\omega_q = cq) \qquad (9.139)$$

   is the Hamiltonian for the electromagnetic field. The "dipole" matrix element $g(\omega)$ is weak enough to be treated by second order perturbation theory and the polarization of the photon is ignored.

   (i) Calculate the self-energy $\Sigma_+(\omega)$ and $\Sigma_-(\omega)$ for an atom in the + and − states.

   (ii) Use the self-energy obtained above to calculate the life-times $\tau_\pm$ of the atomic states, i.e.

   $$\tau_\pm^{-1} = 2{\rm Im}\Sigma_\pm(\tilde{E}_\pm - i\delta). \qquad (9.140)$$

   If the gas of atoms is non-degenerate, i.e the Fermi functions are all small compared with unity, $f(E_\pm) \sim 0$ show that

   $$\begin{aligned} \tau_+^{-1} &= 2\pi |g(\omega_o)|^2 F(\omega_o)[1 + n(\omega_o)] \\ \tau_-^{-1} &= 2\pi |g(\omega_o)|^2 F(\omega_o) n(\omega_o), \end{aligned} \qquad (9.141)$$

   where $\omega_o = \tilde{E}_+ - \tilde{E}_-$ is the separation of the atomic levels and

   $$F(\omega) = \int \frac{d^3q}{(\mathbf{2}\pi)^3} \delta(\omega - \omega_q) = \frac{\omega^2}{2\pi c^3} \qquad (9.142)$$

   is the density of state of the photons at energy ω. What do these results have to do with stimulated emission? Do your final results depend on the initial assumption that the atoms were fermions?

   (iii)Why is the decay rate of the upper state larger than the decay rate of the lower state by the factor $[1 + n(\omega_0)]/n(\omega_0)$?

Chapter 10

Fluctuation Dissipation Theorem and Linear Response Theory

10.1 Introduction

In this chapter we will discuss the deep link between fluctuations about equilibrium, and the response of a system to external forces. If the susceptibility of a system to external change is large, then the fluctuations about equilibrium are expected to be large. The mathematical relationship that quantifies this this connection is called the “fluctuation-dissipation” theorem. We shall discuss and derive this relationship in this chapter. It turns out that the link between fluctuations and dissipation also extends to imaginary time, enabling us to relate equilibrium correlation functions and response functions to the imaginary time Greens function of the corresponding variables.

To describe the fluctuations and response at a finite temperature we will introduce three related three types of Green function- the correlation function $S(t)$,

$$S(t-t') = \langle A(t)\ A(t')\rangle = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} e^{-i\omega(t-t')} S(\omega),$$

the dynamical susceptibility $\chi(t)$

$$\chi(t-t') = i\langle [A(t), A(t')]\rangle \theta(t-t'),$$

which determines the retarded response

$$\langle A(t)\rangle = \int_{-\infty}^{\infty} dt' \chi(t-t') f(t'), \quad \langle A(\omega)\rangle = \chi(\omega) f(\omega),$$

to a force $f(t)$ term coupled to A inside the Hamiltonian $H_I = -f(t)A(t)$, and lastly, the imaginary time response function $\chi(\tau)$

$$\chi(\tau-\tau') = \langle TA(\tau)A(\tau')\rangle$$

.

The fluctuation dissipation theorem relates the Fourier transforms of these quantities. according to

$$\boxed{\underbrace{S(\omega)}_{\text{Fluctuations}} = 2\hbar[\overbrace{1}^{\text{Quantum}} + \overbrace{n_B(\omega)}^{\text{Thermal}}] \underbrace{\chi''(\omega)}_{\text{Dissipation}},}$$

where $\chi''(\omega) = \text{Im}\ \chi(\omega)$ describes the dissipative part of the response function. In the limit, $\omega << k_B T$, when $n(\omega) \sim k_B T/\hbar\omega$, this result reverts to the classical fluctuation-dissipation theorem,

$$S(\omega) = \frac{2k_B T}{\omega} \chi''(\omega).$$

Thus in principle, if we know the correlation functions in thermal equilibrium, we can compute the response function of the system.

The dissipative response of the system also enters into the Kramer's Kronig expansion of the response function,

$$\chi(z) = \int \frac{d\omega}{\pi} \frac{1}{\omega - z} \chi''(\omega)$$

and this expression can be used to analytically extend $\chi(\omega)$ into the complex plane. In practice, the theorist takes advantage of a completely parallel fluctuation-dissipation theorem which exists in imaginary time. The imaginary time correlation function $\chi(\tau)$ is periodic in time. $\chi(\tau+\beta) = \chi(\tau)$, and has an discrete Matsubara Fourier expansion, given by

$$\chi(\tau) = \langle TA(\tau)A(0)\rangle = \frac{1}{\beta}\sum_n e^{-i\nu_n\tau}\chi_M(i\nu_n)$$

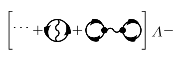
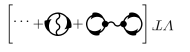
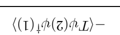
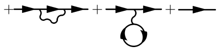
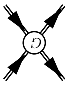
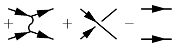
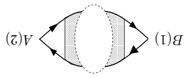
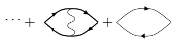
The key relation between this function and the physical response function is that

$$\chi_M(i\nu_n) = \chi(z).|_{z=i\nu_n}.$$

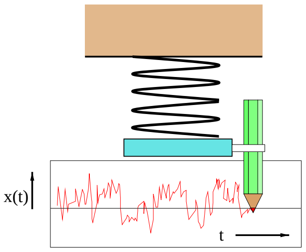
This relation permits us to compute the physical response function by analytically continuing the Fourier components of the imaginary-time correlation functions onto the real axis.

To understand these relations, we need first to understand the nature of the quantum mechanical response functions. We shall then carry out a “spectral decomposition” of each of the above functions, deriving the fluctuation dissipation theorem by showing that the same underlying matrix elements enter into each expression. A heuristic understanding of the relationship between fluctuations and dissipation, is obtained by examining a classical example. The main difference between the classical and the quantum fluctuation-dissipation theorem, is that in classical mechanics we are obliged to explicitly include the external sources of noise, whereas in the quantum case, the noise is intrinsic, and we can analyse the fluctuations without any specific reference to external sources of noise. Nevertheless, the classical case is highly pedagogocical, and it is this limit that we shall consider first.

Table. 9.3 Relationship With Physical Quantities: Finite Temperature

ΔF	$-V\sum\{\text{linked clusters}\}$	$-V$ 
$\ln Z/Z_o$	$V\beta\sum\{\text{linked clusters}\}$	VT 
 1 2 $-\langle T\psi(2)\psi^\dagger(1)\rangle$	$\sum\{\text{Two leg diagrams}\}$	
$(-1)^n\langle T\psi(1)\dots\psi^\dagger(2n)\rangle$  $n=2$	$\sum\{2n\text{- leg diagrams}\}$	
Response Functions $\langle\psi\|T[A(2)B(1)]\|\psi\rangle = \chi^T_{AB}$  $B(1)$ $A(2)$ $i\langle[A(2),B(1)]\rangle\theta(t_1-t_2) = \chi_{AB}$	$\chi_{AB} = \chi^T_{AB}(\omega - i\delta)$	

10.2 Fluctuation dissipation theorem for a classical harmonic oscillator



$$\overbrace{\langle x(t)x(0)\rangle}^{fluctuations} = 2k_BT\int\frac{d\omega}{2\pi}\underbrace{\frac{\chi''(\omega)}{\omega}}_{dissipation}e^{-i\omega t}$$

Figure 10.1: Fluctuations in a classical harmonic oscillator are directly related to the dissipative response function via the "fluctuation dissipation theorem".

In a classical system, to examine correlation functions we need to include an explicit source of external noise. To illustrate the procedure, consider a harmonic oscillator in thermal equilibrium inside a viscous medium. Suppose that thermal fluctuations give rise to a random force, acting on the oscillator, according to the quation of motion:

$$m(\ddot{x}+\omega_o^2x)+\eta\dot{x}=f(t)$$

If we Fourier transform this relationship, we obtain

$$\boxed{\begin{array}{rcl} x(\omega) & = & \chi(\omega)f(\omega)\\ \chi(\omega) & = & [m(\omega_0^2-\omega^2)-i\omega\eta]^{-1} \end{array}\qquad(10.1)}$$

Here $\chi(\omega)$ is the response function , or susceptibility to the external force. The imaginary part of the susceptibility governs the dissipation and is given by

$$\chi''(\omega)=\frac{\omega\eta}{m(\omega_0^2-\omega^2)+\omega^2\eta^2}=|\chi(\omega)|^2\omega\eta. \qquad (10.2)$$

Now let us consider the fluctuations in thermal equilibrium. Over long time periods, we expect the two-point correlation function to be purely a function of the time difference:

$$\langle x(t)x(t')\rangle=\langle x(t-t')x(0)\rangle$$

The power spectrum of fluctuations is defined as

$$\langle|x(\omega)|^2\rangle=\int dt\langle x(t)x(0)\rangle e^{i\omega t}$$

and the inverse relation gives

$$\langle x(t)x(t')\rangle=\int\frac{d\omega}{2\pi}e^{-i\omega(t-t')}\langle|x(\omega)|^2\rangle.$$

Now in thermal equilibrium, the equipartition theorem tells us that

$$\frac{m\omega_0^2}{2}\langle x^2\rangle=\frac{k_BT}{2},$$

or

$$\langle x^2\rangle=\int\frac{d\omega}{2\pi}\langle|x(\omega)|^2\rangle=\int\frac{d\omega}{2\pi}|\chi(\omega)|^2\langle|f(\omega)|^2\rangle=\frac{k_BT}{m\omega_0^2}$$

Since the integrand is very sharply peaked around $|\omega|=\omega_0$, we replace $\langle|f(\omega)|^2\rangle\rightarrow\langle|f(\omega_0)|^2\rangle$ in the above expression. Replacing $|\chi(\omega)|^2\rightarrow\frac{1}{\omega\eta}\chi''(\omega)$ we then obtain

$$\frac{k_BT}{m\omega_0^2}=\frac{\langle|f(\omega_0)|^2\rangle}{2\eta}\int\frac{d\omega}{\pi}\frac{\chi''(\omega)}{\omega}=\frac{|f(\omega_0)|^2}{2\eta m\omega_0^2}.$$

so that the spectrum of force fluctuations is determined by the viscosity η

$$\langle|f(\omega_0)|^2\rangle=2\eta k_BT.$$

Now if we assume that the noise spectrum it depends only on the properties of the viscous medium in which the oscillator is embedded, and that it does not depend on the properties of the oscillator, then we expect this expression holds for any frequency ω_0, and since it is *independent* of the frequency, we conclude that the power spectrum of the force is a flat function of frequency, enabling us to replace $\omega_0\rightarrow\omega$ in the above expression. This implies that in thermal equilibrium, the force coupling the system to the environment is a source of white noise of amplitude which depends on the viscosity of the medium

$$\langle f(t)f(t')\rangle=\int\frac{d\omega}{2\pi}e^{-i\omega(t-t')}\overbrace{\langle|f(\omega)|^2\rangle}^{2\eta k_BT}=2\eta k_BT\delta(t-t')$$

We can now compute the noise spectrum of fluctuations, which is given by

$$\boxed{S(\omega)=\langle|x(\omega)|^2\rangle=|\chi(\omega)|^2\langle|f(\omega)|^2\rangle=\langle|f(\omega)|^2\rangle\frac{\chi''(\omega)}{\omega\eta}=\frac{2k_BT}{\omega}\chi''(\omega).}$$

This expression relates the thermal fluctuations of a classical system to the dissipation, as described by the imaginary part of the response function, $\chi''(\omega)$.

10.3 Quantum Mechanical Response Functions.

Suppose we couple a force f to variable A. For later generality, it suits our need to consider a force in both in real and imaginary time, with Hamiltonian

$$\begin{array}{rcl} H & = & H_o-f(t)A\\ H & = & H_o-f(\tau)A. \end{array}\qquad(10.3)$$

We shall now show that the response to these forces are given by

$$\boxed{\begin{array}{rcll} \langle A(t)\rangle & = & \langle A\rangle+\int_{-\infty}^{\infty}\chi(t-t')f(t')dt' & \\ \langle A(\tau)\rangle & = & \langle A\rangle+\int_0^{\beta}\tilde{\chi}(\tau-\tau')f(\tau')d\tau' & (10.4)\\ \chi(t-t') & = & i\langle[A(t),\ A(t')]\rangle\theta(t-t') & \\ \tilde{\chi}(\tau-\tau') & = & \langle TA(\tau)A(\tau')]\rangle-\langle A\rangle^2 & (10.5) \end{array}}$$

where $\langle A\rangle$ is the value of A in thermal equilibrium. Let us begin in real time. Using the interaction representation, we know that

$$A_H(t)\ =U^{\dagger}(t)A_I(t)\,U(t),$$

where

$$U(t)=T\exp i\int_{-\infty}^{t}dt'A_I(t')f(t').$$

Remembering that the interaction representation corresponds to the Heisenberg representation for H_o, we can drop the subscript on $A_I(t)\equiv A(t)$, so that to linear order in $f(t)$,

$$\begin{array}{rcl} U(t) & = & 1+i\int_{-\infty}^{t}dt'A(t')f(t'),\\ U^{\dagger}(t) & = & 1-i\int_{-\infty}^{t}dt'A(t')f(t') \end{array}$$

so that

$$A_H(t)=A(t)+i\int_{-\infty}^{t}dt'[A(t),A(t')]\,f(t'),$$

In thermal equilibrium if $\langle A(t)\rangle=\langle A\rangle$, so the response to the applied force is given by

$$\langle A_H(t)\rangle=\langle A\rangle+\int_{-\infty}^{+\infty}dt'\ \chi(t-t')\,f(t'),$$

where

$$\boxed{\chi(t-t')=i\langle[A(t),A(t')]\,\rangle\theta(t-t')}$$

is the "retarded response function", also known as the "dynamical susceptibility". The above equation is particularly interesting, for it relates a quantum-mechanical response function to a correlation-function.

Let us now consider imaginary time. In this case, the partition function in the presence of the perturbation is

$$Z=Z_0\langle T\exp\int_0^{\beta}d\tau f(\tau)A_I(\tau)\rangle_0$$

The expectation value of $A(\tau)$ is then given by

$$\begin{array}{rcll} \langle A(\tau)\rangle & = & \frac{\delta\ln Z}{\delta f(\tau)}=\frac{\langle TA(\tau)\exp\int_0^{\beta}d\tau'f(\tau')A_I(\tau')\rangle}{\langle T\exp\int_0^{\beta}d\tau'f(\tau')A_I(\tau')\rangle} & \\ & = & \langle A\rangle+\int_0^{\beta}d\tau'\overbrace{\left[\langle TA(\tau)A(\tau')\rangle-\langle A\rangle^2\right]}^{\tilde{\chi}(\tau-\tau')}+O(f^2) & (10.6) \end{array}$$

so that

$$\begin{array}{rcll} \tilde{\chi}(\tau) & = & \langle TA(\tau)A(0)\rangle-\langle A\rangle^2 & \\ & = & \langle T(A(\tau)-\langle A\rangle)(A(0)-\langle A\rangle)\rangle & (10.7) \end{array}$$

where the expectation values are to be taken in thermal equilibrium for H_0.

10.3.1 Quantum Fluctuation-Dissipation Theorem

The quantum fluctuation dissipation theorem can be carried out in a much more mechanistic fashion by carrying out out a spectral decomposition of the various response and correlation functions. Surprisingly, one does not have to explicitly include the dissipation effects. The procedure is formally more direct that its classical analogue, but the algebra tends to hide the fact that the underlying physics holds precisely the same link between fluctuations- now both thermal and quantum in character- and dissipation. The procedure is basically the same for each function, but for completeness, we now carry out the complete procedure.

10.3.2 Spectral decomposition of $S(t-t')$

This is the easiest decomposition of the three to carry out. We begin by expanding the response function in terms of a complete set of energy eigenstates which satisfy

$$\begin{aligned} H\left|\lambda\right\rangle &= E_\lambda\left|\lambda\right\rangle, \\ \sum_\lambda \left|\lambda\right\rangle\left\langle\lambda\right| &= 1, \\ \left\langle\lambda\left|A(t)\right|\zeta\right\rangle &= \left\langle\lambda\left|e^{iHt}A\,e^{-iHt}\right|\zeta\right\rangle = e^{-i(E_\zeta-E_\lambda)(t-t')}\left\langle\lambda\left|A\right|\zeta\right\rangle. \end{aligned}$$

Using these key results, we make the expansion as follows,

$$\begin{aligned} S(t-t') &= \langle A(t)A(t')\rangle \\ &= \sum_{\lambda,\zeta} e^{-\beta(E_\lambda-F)}\left\langle\lambda\left|A(t)\right|\zeta\right\rangle\left\langle\zeta\left|A(t')\right|\lambda\right\rangle \\ &= \sum_{\lambda,\zeta} e^{-\beta(E_\lambda-F)}\left|\left\langle\zeta\left|A\right|\lambda\right\rangle\right|^2 e^{-i(E_\zeta-E_\lambda)(t-t')} \end{aligned} \tag{10.8}$$

If we now Fourier transform this expression, the frequency dependent correlation function can be written

$$\begin{aligned} S(\omega) &= \int_{-\infty}^{\infty} dt e^{i\omega t}S(t) \\ &= \sum_{\lambda,\zeta} e^{-\beta(E_\lambda-F)}\left|\left\langle\zeta\left|A\right|\lambda\right\rangle\right|^2 2\pi\delta(E_\zeta-E_\lambda-\omega). \end{aligned} \tag{10.9}$$

This is the frequency spectrum of the correlations.

10.3.3 Spectral decomposition of $\chi(t-t')$

We now use the same spectral decomposition approach for the response function. In this case, we need to take care of two operator orderings inside the commutator, which yield

$$\begin{aligned} \chi(t-t') &= i\sum_{\lambda,\zeta} e^{-\beta(E_\lambda-F)}\left\{\left\langle\lambda\left|A(t)\right|\zeta\right\rangle\left\langle\zeta\left|A(t')\right|\lambda\right\rangle - \left\langle\lambda\left|A(t')\right|\zeta\right\rangle\left\langle\zeta\left|A(t)\right|\lambda\right\rangle\right\}\theta(t-t') \\ &= i\sum_{\lambda,\zeta} e^{\beta F}(e^{-\beta E_\lambda}-e^{-\beta E_\zeta})\left|\left\langle\zeta\left|A\right|\lambda\right\rangle\right|^2 e^{-i(E_\zeta-E_\lambda)(t-t')}\theta(t-t'). \end{aligned}$$

By introducing the spectral function

$$\chi''(\omega) = \pi(1-e^{-\beta\omega})\sum_{\lambda,\zeta}\left|\left\langle\zeta\left|A\right|\lambda\right\rangle\right|^2\delta[\omega-(E_\zeta-E_\lambda)]e^{-\beta(E_\lambda-F)}, \tag{10.10}$$

we see that the retarded response function can be written,

$$\chi(t) = i\int d\omega\, e^{-i\omega t}\theta(t)\,\chi''(\omega). \tag{10.11}$$

Fourier transforming this result, using

$$i\int_0^\infty dt e^{i(\omega-\omega'+i\delta)\,t} = \frac{1}{\omega'-\omega-i\delta},$$

we obtain

$$\chi(\omega) = \int\frac{d\omega'}{\pi}\frac{1}{\omega'-\omega-i\delta}\chi''(\omega'). \tag{10.12}$$

This "Kramers-Krönig" relation can be used to extend the response function into the complex plane. Notice that because the response function is *retarded*, $\chi(\omega)$ is analytic in the upper-half complex plane and the poles lie just below the real axis, at $z=\omega'-i\delta$. Finally, taking the imaginary part of this expression, using the Dirac relation $Im[1/(\omega'-\omega-i\delta)=\pi\delta(\omega'-\omega)$, we are able to identify

$$\chi''(\omega) = Im\chi(\omega+i\delta)$$

as the dissipative part of the response function.

10.3.4 Quantum Fluctuation dissipation Theorem

If we compare the relations (10.10) and (10.9), we see that

$$S(\omega) = \frac{2}{1-e^{-\beta\omega}}\chi''(\omega).$$

If we restore $\hbar$, this becomes

$$S(\omega) = \frac{2\hbar}{1-e^{-\beta\hbar\omega}}\chi''(\omega) = 2\hbar\left[1+n_B(\hbar\omega)\right]\chi''(\omega). \tag{10.13}$$

Thus, by carrying out a spectral analysis, we have been able to directly link the correlation function $S(\omega)$ with the dissipative part of the response function $\chi(\omega)$.

10.3.5 Spectral decomposition in imaginary time

For the final of our three decompositions, we move to imaginary time, and write, $\tau-\tau'>0$,

$$\begin{aligned} \chi(\tau-\tau') &= \sum_{\lambda,\zeta} e^{-\beta(E_\lambda-F)}\left\{\left\langle\lambda\left|A(\tau)\right|\zeta\right\rangle\left\langle\zeta\left|A(\tau')\right|\lambda\right\rangle\right\} \\ &= \sum_{\lambda,\zeta} e^{-\beta(E_\lambda-F)}e^{-(E_\lambda-E_\zeta)(\tau-\tau')}\left|\left\langle\zeta\left|A\right|\lambda\right\rangle\right|^2. \end{aligned}$$

Now

$$\int_0^\beta d\tau\, e^{i\nu_n\tau}e^{-(E_\lambda-E_\zeta)\tau} = \frac{1}{(E_\zeta-E_\lambda-i\nu_n)}(1-e^{-(E_\lambda-E_\zeta)\beta}),$$

so

$$\begin{aligned} \chi(i\nu_n) &= \int_0^\beta d\tau\, e^{i\nu_n\tau}\chi(\tau) \\ &= \sum_{\lambda,\zeta} e^{-\beta(E_\lambda-F)}(1-e^{-\beta(E_\zeta-E_\lambda)})\left|\left\langle\zeta\left|A\right|\lambda\right\rangle\right|^2\frac{1}{(E_\zeta-E_\lambda-i\nu_n)}. \end{aligned}$$

Using (10.10), we can write this as

$$\chi(i\nu_n) = \int\frac{d\omega}{\pi}\frac{1}{\omega-i\nu_n}\chi''(\omega) \tag{10.14}$$

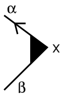
so that $\chi(i\nu_n)$ is the unique analytic extension of $\chi(\omega)$ into the complex plane. Our procedure to calculate response functions will be to write $\chi(i\nu_n)$ in the form 10.14, and to use this to read off $\chi''(\omega)$.

10.4 Calculation of response functions

Having made the link between the imaginary time, and real time response functions, we are ready to discuss how we can calculate response functions from Feynman diagrams. Our procedure is to compute the imaginary time response function, and then analytically continue to real frequencies. Suppose we are interested in the response function for A where,

$$A(x) = \psi^\dagger{}_\alpha(x)A_{\alpha\beta}\psi_\beta(x).$$

(See table 10.0). The corresponding operator generates the vertex



$$= A_{\alpha\beta} \tag{10.15}$$

Table. 10.0 Selected Operators and corresponding response function.

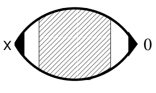
Quantity	Operator $\hat{A}$	$A(\mathbf{k})$	Response Function
Density	$\hat{\rho}(x)=\psi^\dagger(x)\psi(x)$	$\rho_{\alpha\beta}=\delta_{\alpha\beta}$	Charge susceptibility
Spin density	$\vec{S}(x)=\psi_\alpha{}^\dagger(x)\left(\frac{\vec{\sigma}}{2}\right)_{\alpha\beta}\psi_\beta(x)$	$\vec{M}_{\alpha\beta}=\mu_B\vec{\sigma}_{\alpha\beta}$	Spin susceptibility
Current density	$\frac{e}{m}\psi^\dagger(x)\left(-i\hbar\overleftrightarrow{\nabla}-e\vec{A}\right)\psi(x)$	$\vec{j}=e\vec{v}_{\mathbf{k}}=e\vec{\nabla}\epsilon_{\mathbf{k}}$	Conductivity
Thermal current	$\frac{\hbar^2}{2m}\psi^\dagger(x)\overleftrightarrow{\nabla}\overleftrightarrow{\partial}_t\,\psi(x)$	$\vec{j}_T=i\omega_n\vec{v}_{\mathbf{k}}=i\omega_n\vec{\nabla}\epsilon_{\mathbf{k}}$	Thermal conductivity

(Where $\overleftrightarrow{\nabla}\equiv\frac{1}{2}\left(\overrightarrow{\nabla}-\overleftarrow{\nabla}\right)$, $\overleftrightarrow{\partial}_t\equiv\frac{1}{2}\left(\overrightarrow{\partial}_t-\overleftarrow{\partial}_t\right)$)

where the spin variables $\alpha\beta$ are to be contracted with the internal spin variables of the Feynman diagram. This innevitably means that the variable $A_{\alpha\beta}$ becomes part of an internal trace over spin variables. If we expand the corresponding response function $\chi(x)=\langle A(x)A(0)\rangle$ using Feynman diagrams, then we obtain

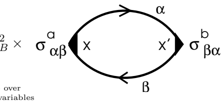
$$\chi(\tau)=\langle A(x)A(0)\rangle = \sum\text{closed linked two-vertex diagrams}$$

$$=$$



For example, in a non-interacting electron system, the imaginary time spin response function involves $A(x)=\mu_B\psi_\alpha{}^\dagger(x)\sigma_{\alpha\beta}\psi_\beta(x)$, so the corresponding response function is

$$\chi^{ab}(x-x') = \mu_B^2\times$$



$$\begin{aligned} &= -\overbrace{\text{Tr}}^{\substack{\text{Trace over}\\ \text{spin variables}}}\left[\sigma^a\mathcal{G}(x-x')\sigma^b\mathcal{G}(x'-x)\right] \\ &= -\delta^{ab}2\mu_B^2\mathcal{G}(x-x')\mathcal{G}(x'-x) \end{aligned} \tag{10.16}$$

Now to analytically continue to real frequencies, we need to transform to Fourier space, writing

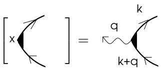
$$\chi(q) = \int d^4x e^{-iqx}\chi(x)$$

where the integral over time τ runs from 0 to β. This procedure converts the Feynman diagram from a real-space, to a momentum space Feynman diagram. At the measurement vertex at position x, the incoming and outgoing momenta of the fermion line give the following integral

$$\int d^4x e^{-iqx} e^{i(k_{in}-k_{out})x} = \beta V \delta^4(k_{out} - k_{in} + q).$$

As in the case of the Free energy, the βV term cancels with the $1/(\beta V)\sum_k$ terms associated with each propogator, leaving behind one factor of $1/(\beta V) = T/V$ per internal momentum loop. Schematically, the effect of the Fourier transform on the measurement vertex at position x, is then

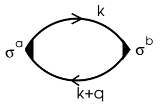
$$\int d^4x e^{-iqx}$$



(10.17)

For example, the momentum-dependent spin response function of the free electron gas is given by

$$\chi^{ab}(q) \;=\; \mu_B^2 \times$$



$$= -\frac{1}{\beta V}\sum_k \mathrm{Tr}\left[\sigma^a \mathcal{G}(k+q)\sigma^b\mathcal{G}(k)\right] = \delta^{ab}\chi(q) \qquad (10.18)$$

where

$$\chi(\mathbf{q}, i\nu_r) \;=\; -2\mu_B^2 \int_{\mathbf{k}} T\sum_{i\omega_n}\mathcal{G}(\mathbf{k}+\mathbf{q}, i\omega_n + i\nu_r)\mathcal{G}(\mathbf{k}, i\omega_n) \qquad (10.19)$$

When we carry out the Matsubara summation in the above expression by a contour integral, (see Chapter 9), we obtain

$$\begin{aligned} -T\sum_{i\omega_n}\mathcal{G}(\mathbf{k}+\mathbf{q}, i\omega_n + i\nu_r)\mathcal{G}(\mathbf{k}, i\omega_n) &= -\int_{C'}\frac{dz}{2\pi i}f(z)\mathcal{G}(\mathbf{k}+\mathbf{q}, z+i\nu_r)\mathcal{G}(\mathbf{k}, z) \\ &= \left(\frac{f_{\mathbf{k}} - f_{\mathbf{k}-\mathbf{q}}}{(\epsilon_{\mathbf{k}+\mathbf{q}} - \epsilon_{\mathbf{k}}) - i\nu_r}\right), \end{aligned} \qquad (10.20)$$

where C' encloses the poles of the Green functions. Inserting this into (10.19), we obtain $\chi(\mathbf{q}, i\nu_r) = \chi(\mathbf{q}, z)|_{z=i\nu_r}, where$

$$\chi(\mathbf{q}, z) = 2\mu_B^2 \int_{\mathbf{k}} \left(\frac{f_{\mathbf{k}} - f_{\mathbf{k}-\mathbf{q}}}{(\epsilon_{\mathbf{k}+\mathbf{q}} - \epsilon_{\mathbf{k}}) - i\nu_r}\right) \qquad (10.21)$$

From this we can also read off the power-spectrum of spin fluctuations

$$\chi''(\mathbf{q}, \omega) = \mathrm{Im}\chi(\mathbf{q}, \omega + i\delta) = 2\mu_B^2 \int_{\mathbf{q}} \pi\delta(\epsilon_{\mathbf{q}+\mathbf{k}} - \epsilon_{\mathbf{k}} - \omega)\left[f_{\mathbf{k}} - f_{\mathbf{k}+\mathbf{q}}\right] \qquad (10.22)$$

When we come to consider conductivities, which involve the response function of current operators, we need to know how to deal with an operator that involves spatial, or temporal derivatives. To do this, it is convenient to examine the Fourier transform of the operator $A(x)$,

$$\int d^4x e^{-iqx}\psi^\dagger(x)A\psi(x) = \sum_k \psi^\dagger(k - q/2)A\psi(k + q/2)$$

In current operators, A is a function of gradient terms such as $\overset{\leftrightarrow}{\nabla}$ and $\overset{\leftrightarrow}{\partial}_t$. In this case, the use of the symmetrized gradient terms ensures that when we Fourier transform, the derivative terms are replaced by the midpoint momentum and frequency of the incoming or outgoing electron.

$$\int d^4x e^{-iqx}\psi^\dagger(x)A[-i\overset{\leftrightarrow}{\nabla}, i\overset{\leftrightarrow}{\partial}_t]\psi(x) = \sum_k \psi^\dagger(k - q/2)A(\mathbf{k}, i\omega_n)\psi(k + q/2)$$

for example, the current operator $\vec{J}(x) = \frac{e\hbar}{m}\left(-i\overset{\leftrightarrow}{\nabla}\right)$ becomes

$$J(q) = \sum_k e\vec{v}_{\mathbf{k}}\psi^\dagger(k - q/2)\psi(k + q/2),$$

where $\vec{v}_{\mathbf{k}} = \frac{\hbar\vec{k}}{m}$ is the electron velocity. For the thermal current operator $\vec{J}_t(\vec{x}) = \frac{\hbar^2}{m}\left(\overset{\leftrightarrow}{\nabla}\overset{\leftrightarrow}{\partial}_t\right)$,

$$\vec{J}_t(q) = \sum_k i\omega_n\frac{\hbar^2\vec{k}}{m}\psi^\dagger(k - q/2)\psi(k + q/2).$$

Example: Calculate the imaginary part of the dynamic susceptibility for non-interacting electrons and show that at low energies $\omega << \epsilon_F$,

$$\frac{\chi''(\mathbf{q}, \omega)}{\omega} = \begin{cases} \mu_B^2 \frac{N(0)}{v_F q} & (q \le 2k_F) \\ 0 & (q > 2k_F) \end{cases}$$

where $v_F = \hbar k_F/m$ is the Fermi velocity.

Solution: Starting with (10.22) In the low energy limit, we can write

$$\begin{aligned} \lim_{\omega\to 0}\frac{\chi''(\mathbf{q}, \omega)}{\omega} &= 2\mu_B^2 \int_{\mathbf{q}} \delta(\epsilon_{\mathbf{q}+\mathbf{k}} - \epsilon_{\mathbf{k}})\frac{f_{\mathbf{k}+\mathbf{q}} - f_{\mathbf{k}}}{\epsilon_{\mathbf{k}} - \epsilon_{\mathbf{k}+\mathbf{q}}} \\ &= 2\mu_B^2 \int_{\mathbf{q}} \delta(\epsilon_{\mathbf{q}+\mathbf{k}} - \epsilon_{\mathbf{k}})\left(-\frac{df}{d\epsilon_{\mathbf{k}}}\right) \end{aligned} \qquad (10.23)$$

Replacing

$$\int_{\mathbf{q}} \to \int d\epsilon N(\epsilon)\int_{-1}^{1}\frac{d\cos\theta}{2}$$

we obtain

$$\begin{aligned} \lim_{\omega\to 0}\frac{\chi''(\mathbf{q}, \omega)}{\omega} &= 2\mu_B^2 N(0)\int_{-1}^{1}\frac{d\cos\theta}{2}\delta(\frac{q^2}{2m} + \frac{qk_F}{m}\cos\theta) \\ &= 2\mu_B^2 N(0)\frac{m}{2qk_F} = \mu_B^2\left(\frac{N(0)}{v_F q}\right) \qquad (q < 2k_F) \end{aligned} \qquad (10.24)$$

10.5 Electron, Spin and Charge Spectroscopies

10.5.1 The link between measurement and correlation functions

The spectroscopies of condensed matter provide the essential window on the underlying excitation spectrum, the collective modes and ultimately the ground-state correlations of the medium. Research in condensed matter depends critically on the creative new interpretations given to measurements. It is from these interpretations, that new models can be built, and new insights discovered, leading ultimately to quantitative theories of matter.

Table. 10.1 Selected Spectroscopies .

	NAME	SPECTRUM	$\hat{A}$	Questions and Issues
ELECTRON	STM $\frac{dI}{dV}$	$\frac{dI}{dV}(\mathbf{x}) \propto A(\mathbf{x}, \omega)\vert_{\omega=\mathbf{eV}}$	$\psi(x)$	Surface probe. $T \sim 0$ measurement. Is the surface different?
	ARPES	$I(\mathbf{k}, \omega) \propto f(-\omega)A(\mathbf{k}, -\omega)$	$c_{\mathbf{k}\sigma}(t)$	$p_\perp$ unresolved. Surface probe. No magnetic field
	Inverse PES	$I(\omega) \propto \sum_{\mathbf{k}}[1 - f(\omega)]A(\mathbf{k}, \omega)$	$c^\dagger{}_{\mathbf{k}\sigma}(t)$	**p** unresolved. Surface probe.
SPIN	χ_{DC} Uniform Susceptibility	$\chi_{DC} = \int \frac{d\omega}{\pi\omega}\chi''(\mathbf{q} = 0, \omega)$	M	$\chi \sim \frac{1}{T}$ local moments. $\chi \sim$ cons paramagnet
	Inelastic Neutron Scattering $\frac{d^2\sigma}{d\Omega d\omega}$	$S(\mathbf{q}, \omega) = \frac{1}{1 - e^{-\beta\omega}}\chi''(\mathbf{q}, \omega)$	$S(\mathbf{q}, t)$	What is the background? Quality of crystal?
	NMR Knight Shift	$K_{contact} \propto \chi_{\mathrm{local}}$	$S(\mathbf{x}, t)$	How is the orbital part subtracted?
	$\frac{1}{T_1}$	$T\int_q F(\mathbf{q})\frac{\chi''(\mathbf{q}, \omega)}{\omega}\Big\vert_{\omega=\omega_N}$		How does powdering affect sample?
CHARGE	Resistivity ρ	$\rho = \frac{1}{\sigma(0)}$	$\vec{j}(q = 0)$	What is the resistance ratio? (R_{300}/R_0)
	Optical Conductivity	$\sigma(\omega) = \frac{1}{-i\omega}\left[\langle j(\omega')j(-\omega')\rangle\right]_0^\omega$	$\vec{j}(\omega)$	Reflectivity: How was the Kramer's Krönig done? Spectral weight transfer?

Understanding the link between experiment and the microscopic world is essential for theorist and experimentalist. At the start of a career, the student is often flung into a seminar room, where it is often difficult to absorb the content of the talk, because the true meaning of the spectroscopy or measurements is obscure to all but the expert - so it is important to get a rough idea of how and what each measurement technique probes - to know some of the pitfalls of interpretation - and to have an idea about how one begin to calculate the corresponding quantities from simple theoretical models.

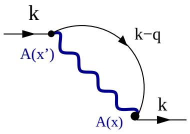
Fundamentally, each measurement is related to a given correlation function. This is seen most explicity in scattering experiments. Here, one is sending in one a beam of particles, and measuring the flux of outgoing particles at a given energy transfer E and momentum transfer $\mathbf{q}$. The ratio of outgoing to incoming particle flux determines the differential scattering cross-section

$$\frac{d^2\sigma}{d\Omega d\omega} = \frac{\text{Outward particle flux}}{\text{Inward particle flux}}$$

When the particles scatter, they couple to some microscopic variable $A(x)$ within the matter, such as the spin density in neutron scattering, or the particle field itself $A(x) = \psi(x)$ in photo-emission. The differential scattering cross-section this gives rise to is, in essence a measure of the autocorrelation function of $A(x)$ at the wavevector $\mathbf{q}$ and frequency $\omega = E/\hbar$ inside the material,

$$\frac{d^2\sigma}{d\Omega d\omega} \sim \int d^4x \langle A(\mathbf{x}, t)A(0)\rangle e^{-i(\mathbf{q}\cdot\mathbf{x}-\omega t)} = S(\mathbf{q}, \omega)$$

Remarkably scattering probes matter at two points in space! How can this be? To understand it, recall that the differential scattering rate is actually an (imaginary) part of the forward scattering amplitude of the incoming particle. The amplitude for the incoming particle to scatter in a forward direction, contains the Feynman process where it omits a fluctuation of the quantity A at position x', travelling for a brief period of time as a scattered particle, before reabsorbing the fluctuation at x. The amplitude for the intermediate process is nothing more than



$$\text{amplitude} \quad = \quad \overbrace{\langle A(x)A(x')\rangle}^{\textbf{amplitude for fluctuation}} \times \underbrace{e^{i[\mathbf{q}\cdot(\mathbf{x}-\mathbf{x}')-\omega(\mathbf{t}-\mathbf{t}')]}}_{\substack{\textbf{amplitude for particle to scatter at x',} \\ \textbf{and reabsorb fluctuation at } x\ .}} \tag{10.25}$$

(In practice, since the whole process is translationally invariant, we can replace x by $x - x'$ and set $x' = 0$.)

The relationship between the correlation function and scattering rate is really a natural consequence of Fermi's Golden rule, according to which

$$\frac{d^2\sigma}{d\Omega d\omega} \sim \Gamma_{i\to f} = \frac{2\pi}{\hbar}\sum_f p_i |\langle f|V|i\rangle|^2 \delta(E_f - E_i)$$

where p_i is the probability of being in the initial state $|i\rangle$. Typically, an incoming particle (photon, electron, neutron) with momentum $\mathbf{k}$ scatters into an outgoing particle state (photon, electron, neutron) with momentum $\mathbf{k}'$, and the system undergoes a transition from a state $|\lambda\rangle$ to a final state $|\lambda'\rangle$:

$$|i\rangle = |\lambda\rangle|\mathbf{k}\rangle, \qquad\qquad |f\rangle = |\lambda'\rangle|\mathbf{k}'\rangle$$

If the scattering Hamiltonian with $V \sim g\int_x \rho(x)A(x)$, where $\rho(x)$ is the density of the particle beam, then the scattering matrix element is

$$\langle f|\hat{V}|i\rangle = g\int_{\mathbf{x}'}\langle \mathbf{k}'|\mathbf{x}\rangle\langle\lambda'|A(\mathbf{x}')|\lambda\rangle\langle\mathbf{x}|\mathbf{k}\rangle = \frac{g}{V_o}\int_{\mathbf{x}'} e^{i\mathbf{q}\cdot\mathbf{x}'}\langle\lambda'|A(\mathbf{x})|\lambda\rangle \tag{10.26}$$

so the scattering rate is

$$\Gamma_{i\to f} = \frac{1}{V_0^2}\int_{\mathbf{x},\ \mathbf{x}'} p_\lambda\langle\lambda|A(x)|\lambda'\rangle\langle\lambda'|A(\mathbf{x}')|\lambda\rangle e^{-i\mathbf{q}\cdot(\mathbf{x}-\mathbf{x}')}2\pi\delta(E_{\lambda'} - E_\lambda - \omega) \tag{10.27}$$

where $p_\lambda = e^{-\beta(E_\lambda - F)}$ is the Boltzmann probability. Now if we repeat the spectral decomposition of the correlation function made in (10.9)

$$\int dte^{i\omega t}\langle A(\mathbf{x}, t)A(\mathbf{x}', 0)\rangle = 2\pi\sum_{\lambda,\lambda'} p_\lambda\langle\lambda|A(x)|\lambda'\rangle\langle\lambda'|A(\mathbf{x}')|\lambda\rangle\delta(E_{\lambda'} - E_\lambda - \omega),$$

we see that

$$\begin{aligned}\Gamma_{i\to f} \quad &\sim \quad \frac{g^2}{V_0^2}\int_{\mathbf{x},\mathbf{x}'} dte^{i\omega t)}\langle A(\mathbf{x}, t)A(\mathbf{x}', 0)\rangle \\ &= \quad \frac{g^2}{V_0}\int d^3xdte^{i\omega(t)}\langle A(\mathbf{x}, t)A(0)\rangle\end{aligned}$$

where the last simplification results from translational invariance. Finally, if we divide the transition rate by the incoming flux of particles $\sim 1/V_0$, we obtain the differential scattering cross-section.

For example, in an inelastic neutron scattering (INS) experiment, the neutrons couple to the electron spin density $A = S(x)$ of the material, so that

$$\frac{d^2\sigma}{d\Omega d\omega}(\mathbf{q}, \omega) \sim \int d^4x\langle S_-(\mathbf{x}, t)S_+(0)\rangle e^{-i(\mathbf{q}\cdot\mathbf{x}-\omega t)} \propto \frac{1}{1 - e^{-\beta\omega}}\chi''(\mathbf{q}, \omega)$$

where $\chi(\mathbf{q}, \omega)$ is the dynamic spin susceptibility which determines the magnetization $M(\mathbf{q}, \omega) = \chi(\mathbf{q}, \omega)B(\mathbf{q}, \omega)$ by a modulated magnetic field of wavevector $\mathbf{q}$, frequency ω. By contrast, in an angle resolved photo-emission (ARPES) experiment, incoming X-rays eject electrons from the material, leaving behind "holes", so that $A = \psi$ is the electron annihilation operator and the intensity of emitted electrons measures the correlation function

$$I(\mathbf{k}, \omega) \sim \int d^4x\langle\psi^\dagger(x)\psi(0)\rangle e^{-i(\mathbf{k}\cdot\mathbf{x}-\omega t)} = \overbrace{\frac{1}{1 + e^{\beta\omega}}}^{f(-\omega)} A(\mathbf{k}, -\omega)$$

where the Fermi function replaces the Bose function in the fluctuation dissipation theorem.

10.5.2 Electron Spectroscopies

Some formal properties of the electron Green function

The spectral decompositions carried out for a bosonic variable A can all be generalized to the fermionic variable $c_{\mathbf{k}\sigma}$. The basic electron "correlation" functions are

$$\begin{aligned}\langle c_{\mathbf{k}\sigma}(t)c^\dagger{}_{\mathbf{k}\sigma}(0)\rangle \quad &= \quad \int\frac{d\omega}{2\pi}G_>(\mathbf{k}, \omega)e^{-i\omega t} \\ \langle c^\dagger{}_{\mathbf{k}\sigma}(0)c_{\mathbf{k}\sigma}(t)\rangle \quad &= \quad \int\frac{d\omega}{2\pi}G_<(\mathbf{k}, \omega)e^{-i\omega t}\end{aligned} \tag{10.28}$$

called the "greater" and "lesser" Green functions. A spectral decomposition of these relations reveals that

$$\boxed{\begin{aligned}G_>(\mathbf{k}, \omega) \quad &= \quad \sum_{\lambda,\zeta} p_\lambda|\langle\zeta|c^\dagger{}_{\mathbf{k}\sigma}|\lambda\rangle|^2 2\pi\delta(E_\zeta - E_\lambda - \omega) \\ G_<(\mathbf{k}, \omega) \quad &= \quad \sum_{\lambda,\zeta} p_\lambda|\langle\zeta|c_{\mathbf{k}\sigma}|\lambda\rangle|^2 2\pi\delta(E_\zeta - E_\lambda + \omega)\end{aligned}}$$

describe the positive energy distribution functions for particles ($G_>$) and the negative energ distribution function for holes ($G_<$) respectively. By relabelling $\zeta \leftrightarrow \lambda$ in (10.29) it is straightforward to show that

$$G_<(\mathbf{k}, \omega) = e^{-\beta\omega}G_>(\mathbf{k}, \omega)$$

We also need to introduce the retarded electron Green function, given by

$$G_R(\mathbf{k}, t) = -i\langle\{c_{\mathbf{k}\sigma}(t), c^\dagger{}_{\mathbf{k}\sigma}(0)\}\rangle\theta(t) = \int\frac{d\omega}{2\pi}G_R(\mathbf{k}, \omega)e^{-i\omega t}$$

(note the appearance of an anticommutator for fermions and the minus sign pre-factor) which is the real-time analog of the imaginary time Green function

$$\mathcal{G}(\mathbf{k}, \tau) = -\langle Tc_{\mathbf{k}\sigma}(\tau)c^\dagger{}_{\mathbf{k}\sigma}(0)\rangle = T\sum_n \mathcal{G}(\mathbf{k}, i\omega_n)e^{-i\omega_n\tau}$$

A spectral decomposition of these two functions reveals that reveals that they share the same power-spectrum and Kramer's Krönig relation, and can both be related to the generalized Green function

$$\mathcal{G}(\mathbf{k}, z) \quad = \quad \int\frac{d\omega'}{\pi}\frac{1}{z - \omega}A(\mathbf{k}, \omega) \tag{10.29}$$

where

$$\begin{aligned}G_R(\mathbf{k}, \omega) \quad &= \quad \mathcal{G}(\mathbf{k}, \omega + i\delta) = \int\frac{d\omega'}{\pi}\frac{1}{\omega - \omega' + i\delta}A(\mathbf{k}, \omega) \\ \mathcal{G}(\mathbf{k}, i\omega_n) \quad &= \quad \mathcal{G}(\mathbf{k}, z)|_{z=i\omega_n} = \int\frac{d\omega}{\pi}\frac{1}{i\omega_n - \omega}A(\mathbf{k}, \omega),\end{aligned} \tag{10.30}$$

and the spectral function

$$\boxed{\begin{aligned}A(\mathbf{k}, \omega) \quad &= \quad (1 + e^{-\beta\omega})\sum_{\lambda,\zeta}|\langle\zeta|c^\dagger{}_{\mathbf{k}\sigma}|\lambda\rangle|^2\pi\delta(E_\zeta - E_\lambda - \omega) \\ &= \quad \frac{1}{2}\left[G_>(\mathbf{k}, \omega) + G_<(\mathbf{k}, \omega)\right] \qquad (10.31)\end{aligned}}$$

is the sum of the particle and hole energy distribution functions. From the second of (10.31) and (10.28), it follows that $A(\mathbf{k}, \omega)$ is the Fourier transform of the anticommutator

$$\langle\{c_{\mathbf{k}\sigma}(t),\ c^\dagger{}_{\mathbf{k}\sigma}(0)\}\rangle = \int\frac{d\omega}{\pi}A(\mathbf{k}, \omega)e^{-i\omega t} \tag{10.32}$$

At equal times, the commutator is equal to unity, $\{c_{\mathbf{k}\sigma},\ c^\dagger{}_{\mathbf{k}\sigma}\} = 1$, from which we deduce the normalization

$$\int\frac{d\omega}{\pi}A(\mathbf{k}, \omega) = 1.$$

For non-interacting fermions, the spectral function is a pure delta-function, but in Fermi liquids the delta-function is renormalized by a factor Z and the remainder of the spectral weight is transfered to an incoherent background.

$$\frac{A(\mathbf{k}, \omega)}{\pi} = Z_{\mathbf{k}}\delta(\omega - E_{\mathbf{k}}) + \text{background}$$

The relations

$$\begin{aligned}G_>(\mathbf{k}, \omega) \quad &= \quad \frac{2}{1 + e^{-\beta\omega}}A(\mathbf{k}, \omega) = 2(1 - f(\omega))A(\mathbf{k}, \omega) \qquad \text{(particles)} \\ G_<(\mathbf{k}, \omega) \quad &= \quad \frac{2}{1 + e^{\beta\omega}}A(\mathbf{k}, \omega) = 2f(\omega)A(\mathbf{k}, \omega) \qquad \text{(holes)}\end{aligned} \tag{10.33}$$

are the fermion analog of the fluctuation dissipation theorem.

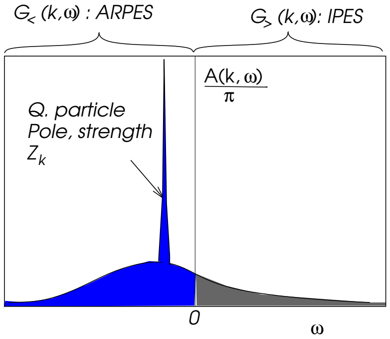


Figure 10.2: Showing the redistribution of the quasiparticle weight into an incoherent background in a Fermi liquid.

Tunneling spectroscopy

Tunneling spectroscopy is one of the most direct ways of probing the electron spectral function. The basic idea behind tunneling spectroscopy, is that a tunneling probe is close enough to the surface that electrons can tunnel through the forbidden region between the probe and surface material. Traditionally, tunneling was carried out using point contact spectroscopy, whereby a sharp probe is brought into contact with the surface, and tunneling takes place through the oxide layer separating probe and surface. With the invention of the Scanning Tunneling Microscope, by Gerd Binnig and Heinrich Rohrer in the 80's has revolutionized the field. In recent times, Seamus Davis has developed this tool into a method that permits the spectral function of electrons to be mapped out with Angstrom level precision across the surface of a conductor.

In the WKB approximation, the amplitude for an electron to tunnel between probe and surface is

$$t(x_1,x_2) \sim \exp\left[-\frac{1}{\hbar}\int_{x_1}^{x_2}\sqrt{2m[V(x)-E]}ds\right] \qquad (10.34)$$

where the integral is evaluated along the saddle-point path between probe and surface. The exponential dependence of this quantity on distance means that tunneling is dominated

by the extremal path from a single atom at the end of a scanning probe, giving rise to Angström - level spatial resolution.

The Hamiltonian governing the interaction between the probe and the sample can be written

$$\hat{V} = \sum_{\mathbf{k},\mathbf{k}'} t_{\mathbf{k},\mathbf{k}'}\left[c^\dagger{}_{\mathbf{k}\sigma}p_{\mathbf{k}'\sigma} + \text{H.c.}\right].$$

where $t_{\mathbf{k},\mathbf{k}'}$ is the tunnelling matrix element between the probe and substrate, $c^\dagger{}_{\mathbf{k}\sigma}$ and $p^\dagger{}_{\mathbf{k}\sigma}$ create electrons in the sample and the probe respectively. The tunneling current of electrons from probe to sample is given by

$$I_{P\to S} = 2\pi e \sum_{\mathbf{k},\mathbf{k}',\zeta,\zeta',\lambda,\lambda',\sigma} p_\lambda p_{\lambda'}\ |t_{\mathbf{k},\mathbf{k}'}|^2 |\langle\zeta,\zeta'|c^\dagger{}_{\mathbf{k}\sigma}p_{\mathbf{k}'\sigma}|\lambda,\lambda'\rangle|^2\delta(E_\zeta + E_{\zeta'} - E_\lambda - E_{\lambda'})$$

where $|\lambda,\lambda'\rangle \equiv |\lambda\rangle|\lambda'\rangle$ and $|\zeta,\zeta'\rangle \equiv |\zeta\rangle|\zeta'\rangle$ refer to the joint many body states of the sample (unprimed) and probe (primed), and we have dropped $\hbar$ from the equation. This term creates electrons in the sample, leaving behind holes in the probe. Now if we rewrite this expression in terms of the spectral functions of the probe and sample, after a little work, we obtain

$$I_{P\to S} = 4\pi e \sum_{\mathbf{k},\mathbf{k}'} |t_{\mathbf{k},\mathbf{k}'}|^2 \int d\omega \frac{A_S(\mathbf{k},\omega)}{\pi}\frac{A_P(\mathbf{k},\omega)}{\pi}(1-f(\omega))f_P(\omega).$$

where we have taken care to use the notation $f_P(\omega) = f(\omega + eV)$ for the energy distribution of the probe, and doubled the expression to account for spin. You can check the validity of these expressions by expanding the spectral functions using (10.31), but the expression is simply recognized as a product of matrix element, density of states and Fermi-Dirac electron and hole occupancy factors.

Similarly, the tunneling current of electrons from sample to probe is

$$\begin{aligned} I_{s\to p} &= 2\pi e \sum_{\mathbf{k},\mathbf{k}',\zeta,\zeta',\lambda,\lambda',\sigma} p_\lambda p_{\lambda'}\ |t_{\mathbf{k},\mathbf{k}'}|^2 |\langle\zeta,\zeta'|p^\dagger{}_{\mathbf{k}'\sigma}c_{\mathbf{k}\sigma}|\lambda,\lambda'\rangle|^2\delta(E_\zeta + E_{\zeta'} - E_\lambda - E_{\lambda'}) \\ &= 4\pi e \sum_{\mathbf{k},\mathbf{k}'} |t_{\mathbf{k},\mathbf{k}'}|^2 \int d\omega \frac{A_S(\mathbf{k},\omega)}{\pi}\frac{A_P(\mathbf{k},\omega)}{\pi}[1-f_P(\omega)]f(\omega). \end{aligned} \qquad (10.35)$$

Subtracting these two expressions, we obtain

$$I = 4\pi e \sum_{\mathbf{k},\mathbf{k}'} |t_{\mathbf{k},\mathbf{k}'}|^2 \int d\omega \frac{A_S(\mathbf{k},\omega)}{\pi}\frac{A_P(\mathbf{k},\omega)}{\pi}[f(\omega - eV) - f(\omega)]. \qquad (10.36)$$

We shall ignore the momentum dependence of the tunneling matrix elements, writing $|t|^2 = \overline{|t_{\mathbf{k},\mathbf{k}'}|^2}$, we obtain

$$I(V) = 2e\overbrace{2\pi|t|^2 N(0)}^{\Gamma}\int \frac{d\omega}{\pi}\frac{A_S(\omega)}{\pi}[f(\omega - eV) - f(\omega)]. \qquad (10.37)$$

where

$$\begin{aligned} A_S(\omega) &= \sum_{\mathbf{k}} A_S(\mathbf{k},\omega) \\ N(\omega) &= \sum_{\mathbf{k}} A_P(\mathbf{k},\omega) \sim N(0) \end{aligned} \qquad (10.38)$$

are now the *local* spectral functions for the sample and probe, respectively. Typically, the probe is a metal with a featureless density of states, and this justifies the replacement $N(\omega) \sim N(0)$ in the above expression. The quantity $2\pi t^2 N(0) = \Gamma$ is the characteristic resonance broadening width created by the tunnelling out of the probe. If we now differentiate the current with respect to the applied voltage, we see that the differential conductivity

$$G(V) = \frac{dI}{dV} = \left(\frac{2e^2}{\hbar}\right)\Gamma\int\frac{d\omega}{\pi}A(S)(\omega)\overbrace{\left(-\frac{df(\omega - eV)}{d\omega}\right)}^{\sim\delta(\omega - eV)}$$

At low temperatures, the derivative of the Fermi function gives a delta function in energy, so that

$$G(V) = \left(\frac{4e^2\Gamma}{h}\right) A_S(\omega)|_{\omega = eV}$$

Thus by mapping out the differential conductance as a function of position, it becomes possible to obtain a complete spatial map of the spectral function on the surface of the sample.

ARPES and inverse PES

ARPES (angle resolved photoemission) and inverse PES (invers photo-electron spectrosopy) are the two alternative ways of probing the hole and electron spectra in matter. The first - involves "photon in, electron out", the second "electron in, photon out". The coupling of radiation to light involves the dipole coupling term

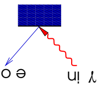
$$H_I = -\int d^3x \vec{j}(x)\cdot\vec{A}(x)$$

where $\vec{j}(x) = -i\frac{e\hbar}{2m}\psi_\sigma{}^\dagger(x)\vec{\nabla}\psi_\sigma(x)$ is the paramagnetic current operator. Unlike STM or neutron scattering, this is a strongly coupled interaction, and the assumption that we can use the Golden Rule to relate the absorption to a correlation function is on much shakier ground. ARPES spectroscopy involves the absorption of a photon, and the emission of a photo-electron from the material. The interpretation of ARPES spectra is based on the "sudden approximation", whereby it is assumed that the dipole matrix element between the intial and final states has a slow dependence on the incoming photon energy and momentum, so that the matrix element is i.e

$$\langle\zeta,\mathbf{k}+\mathbf{q}| - \vec{j}\cdot\vec{A}|\lambda,\mathbf{q}\rangle \sim \Lambda(\mathbf{q},\hat{e}_\lambda)\langle\zeta|c_{\mathbf{k}\sigma}|\lambda\rangle$$

On the assumption that Λ is weakly energy and momentum dependent, we are able to directly relate the absorption intensity to the spectral density beneath the Fermi energy,

$$I_{ARPES}(\mathbf{k},\omega) \propto f(-\omega)A(\mathbf{k},-\omega) \qquad (10.39)$$

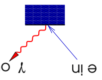


The appearance of the Fermi function masks states above the Fermi energy, and sometimes causes problems for the interpretation of ARPES spectra near the Fermi energy - particularly for the estimation of anisotropic, superconducting gaps. There is a large caveat to go with this equation: when photo-electrons escape from a surface, the component of their momentum perpendicular to the surface is modified by interactions with the surface. Consequently, ARPES spectroscopy can not resolve the momenta of the spectral function perpendicular to the surface. The other consideration about ARPES, is that it is essentially a surface probe - X-ray radiation has only the smallest ability to penetrate samples, so that the information obtained by these methods provides strictly a surface probe of the system.

In recent years, tremendous strides in the resolution of ARPES have taken place, in large part because of the interest in probing the electron spectrum of the quasi- two-dimensional cuprate superconductors. These methods have, for example, played an important role in exhibiting the anisotropic d-wave gap of these materials.

Inverse photo-electron spectroscopy probes the spectral function above the Fermi energy. At present, angle resolved IPES is not a as well developed, and most IPES work involves unresolved momenta, i.e

$$I_{IPES}(\omega) \propto \sum_{\mathbf{k}}[1-f(\omega)]A(\mathbf{k},\omega) \qquad (10.40)$$



In certain materials, both PES and IPES spectra are available. A classic example is in the spectroscopy of mixed valent cerium compounds. In these materials, the Ce atoms have a singly occupied f-level, in the $4f^1$ configuration. PES spectroscopy is able to resolve the energy for the hole excitation

$$4f_1 \to 4f^0 + e^-, \qquad \Delta E_I = -E_f$$

where E_f is the energy of a single occupied $4f$ level. By contrast, inverse PES reveals the energy to add an electron to the $4f^1$ state,

$$e^- + 4f_1 \to 4f^2, \qquad \Delta E_{II} = E_f + U$$

where U is the size of the Coulomb interaction between two electrons in an f-state. By comparing these two absorption energies, it is possible to determine the size of the Coulomb interaction energy

10.5.3 Spin Spectroscopy

D.C. magnetic susceptibility

If one measures the static D. C. magnetization of a medium, one is measuring the magnetic response at zero wavevector $\mathbf{q} = 0$ and zero frequency $\omega = 0$. By the Kramer's Krönig relation encountered in (10.12), we know that

$$\chi_{DC} = \int \frac{d\omega}{\pi} \frac{\chi''(\mathbf{q} = 0, \omega)}{\omega}$$

So the static magnetic susceptibility is an economy-class measurement of the magnetic fluctuation power spectrum at zero wavevector. Indeed, this link between the two measurements sometimes provides an important consistency check of neutron scattering experiments.

In static susceptibility measurements, there are two important limiting classes of behavior, Pauli paramagnetism, in which the susceptibility is derived from the polarization of a Fermi surface, and is weakly temperature dependent,

$$\chi \sim \frac{\mu_B^2}{\epsilon_F} \sim \text{constant.} \qquad\qquad \text{(Pauli paramagnetism)}$$

and Curie paramagnetism, produced by unpaired electrons localized inside atoms, commonly known as "local moments". where the magnetic susceptibilty is inversely proportional to the temperature, or more generally

$$\chi(T) \sim n_i \overbrace{\left(\frac{g^2\mu_B^2 j(j+1)}{3}\right)}^{M_{eff}^2} \times \frac{1}{T + T^*} \qquad\qquad \text{(local moment paramagnetism)}$$

where n_i is the concentration of local moments and M_{eff}^2 is the effective moment produced by a moment of total angular momentum j, with gyromagnetic ratio, g. T^* is a measure of the interaction between local moments. For Ferromagnets, $T^* = -T_c < 0$, and ferromagnetic magnetic order sets in at $T = T_c$, where the uniform magnetic susceptibility diverges. For antiferromagnetis, $T^* > 0$ gives a measure of the strength of interaction between the local moments.

Neutron scattering

Neutrons interact weakly with matter, so that unlike electrons or photons, they provide an ideal probe of the bulk properties of matter. Neutrons interact with atomic nucleii via an interaction of the form

$$\hat{H}_I = \alpha \int d^3x \psi^\dagger{}_N(x)\psi_N(x)\rho(x),$$

where $\rho(x)$ is the density of nucleii and $\psi_N(x)$ is the field of the neutrons. This interaction produces unpolarized scattering of the neutrons, with an inelastic scattering cross-section of the form (see example below),

$$\frac{d^2\tilde{\sigma}}{d\Omega dE} = \frac{k_f}{k_i}\left(\frac{\alpha m_N}{2\pi\hbar^2}\right)^2 \frac{S(\mathbf{q}, E)}{2\pi}$$

where $S(\mathbf{q}, E)$ is the autocorrelation function of nuclear density fluctuations in the medium. Where do these come from? They are of course produced by phonons in the crystal. The neutrons transfer energy to the nucleii by exciting phonons, and we expect that

$$S(\mathbf{q}, E) \sim (1 + n_B(E))\delta(E - \hbar\omega_{\mathbf{q}})$$

where $\omega_{\mathbf{q}\lambda}$ is the phonon dispersion spectrum inside the medium.

The second important interaction between neutrons and matter, is produced by the interaction between the nuclear moment and the magnetic fields inside the material. The magnetic moment of the neutron is given by

$$\vec{M} = \gamma\mu_N \frac{\vec{\sigma}}{2}$$

where $\gamma = -1.91$ is the gyromagnetic ratio of the neutron and $\mu_N = \frac{e\hbar}{2m_N}$ is the neutron Bohr magneton. The interaction with the fields inside the material is then given by

$$\hat{H}_I = \frac{\gamma\mu_N}{2}\int d^3x \psi^\dagger{}_N(x)\vec{\sigma}\psi_N(x) \cdot \vec{B}(x),$$

The magnetic field inside matter is produced by two sources- the dipole field generated by the electron spins, and the orbital field produced by the motion of electrons. We will only discuss the spin component here. The dipole magnetic field produced by spins is given by

$$B(\mathbf{x}) = \int d^3x' \underline{V}(\mathbf{x} - \mathbf{x}') \cdot \vec{\mathbf{M}}(\mathbf{x}')$$

where $\vec{M}(\mathbf{x}) = \mu_{\mathbf{B}}\psi^\dagger(\mathbf{x})\vec{\sigma}\psi(\mathbf{x})$ is the electron spin density and

$$\underline{V}(\mathbf{x}) = -\vec{\nabla} \times \vec{\nabla} \times \left(\frac{\mu_{\mathbf{0}}}{\mathbf{4}\pi|\mathbf{x}|}\right)$$

We can readily Fourier transform this expression, by making the replacements

$$\vec{\nabla} \to i\vec{q}, \qquad\qquad \frac{1}{(4\pi|x|)} \to \frac{1}{q^2} \tag{10.41}$$

so that in Fourier space,

$$[\underline{V}(\mathbf{q})]_{ab} \;=\; \mu_0\left[\vec{q} \times \vec{q} \times \left(\frac{1}{q^2}\right)\right]_{ab} = \mu_0\left[\hat{q} \times \hat{q} \times\right]_{ab}$$

$$= \mu_0 \overbrace{\left[\delta_{ab} - \hat{q}_a\hat{q}_b\right]}^{\mathcal{P}_{ab}(\hat{q})}. \tag{10.42}$$

The only effect of the complicated dipole interaction, is to remove the component of the spin parallel to the q-vector. The interaction between the neutron and electron spin density is simply written

$$H_I = g\int_{\mathbf{q}} \sigma_N(-\mathbf{q})\underline{\mathcal{P}}(\hat{\mathbf{q}}) \cdot \vec{S}_e(\mathbf{q}), \qquad\qquad g = \mu_0\gamma\mu_N\mu_B$$

Apart from the projector term, this is essentially, a "point interaction" between the neutron and electron spin density. Using this result, we can easily generalize our earlier expression for the nuclear differential scattering to the case of unpolarized neutron scattering by replacing $\alpha \to g$, and identifying

$$S_\perp(\mathbf{q}, E) = \mathcal{P}_{ab}(\hat{q})S^{ab}(\mathbf{q}, E)$$

as the projection of the spin-spin correlation function perpendicular to the q-vector. For unpolarized neutrons, the differential scattering cross-section is then

$$\frac{d^2\tilde{\sigma}}{d\Omega dE} = \frac{k_f}{k_i} r_o^2 S_\perp(\mathbf{q}, E)$$

where

$$\begin{aligned} r_0 &= \left(\frac{gm_N}{2\pi\hbar^2}\right) = \frac{\gamma}{2}\overbrace{\left(\frac{\mu_0}{4\pi}\right)}^{\frac{1}{4\pi\epsilon_0 c^2}}\frac{e^2}{m} \\ &= \left(\frac{\gamma}{2}\right)\frac{e_{cgs}^2}{mc^2} \end{aligned} \tag{10.43}$$

is, apart from the prefactor, the classical radius of the electron.

Example: Calculate, in the imaginary time formalism, the self-energy of a neutron interacting with matter and use this to compute the differential scattering cross-section. Assume the interaction between the neutron and matter is given by

$$\hat{H}_I = \alpha \int d^3x \psi^\dagger{}_N(x)\psi_N(x)\rho(x)$$

where $\psi_N(x)$ is the neutron field and $\rho(x)$ is the density of nuclear matter.

Solution:

We begin by noting that the the real-space self-energy of the neutron is given by

$$\Sigma(x - x') = \alpha^2\langle\delta\rho(x)\delta\rho(x')\rangle\mathcal{G}(x - x')$$

where $\langle\delta\rho(x)\delta\rho(x')\rangle = \chi(x - x')$ is the real-time density response function of the nuclear matter. (Note that the minus sign in $-\alpha^2$ associated with the vertices is absent because the propagator used here $\langle\delta\rho(x)\delta\rho(0)\rangle$ contains no minus sign pre-factor.) If we Fourier transform this expression, we obtain

$$\begin{aligned} \Sigma(k) &= \frac{\alpha^2}{\beta V}\sum_q \mathcal{G}(k - q)\chi(q) \\ &= \alpha^2 \int_{\mathbf{q}} T \sum_{i\nu_n} \mathcal{G}(k - q)\chi(q) \end{aligned} \tag{10.44}$$

Carrying out the Matsubara summation, we obtain

$$\Sigma(\mathbf{k}, z) = \alpha^2 \int_{\mathbf{q}} \frac{dE'}{\pi} \frac{1 + n(E') - f_{\mathbf{k}-\mathbf{q}}}{z - (E_{\mathbf{k}-\mathbf{q}} + E')}\chi''(\mathbf{q}, E')$$

where $E_{\mathbf{k}}$ is the kinetic energy of the neutron and the Fermi function $f_{\mathbf{k}}$ of the neutron can be ultimately set to zero (there is no Fermi sea of neutrons), $f_{\mathbf{k}} \to 0$, so that

$$\Sigma(\mathbf{k}, z) = \alpha^2 \int_{\mathbf{q}} \frac{dE'}{\pi} \frac{1}{z - (E_{\mathbf{k}-\mathbf{q}} + E')} \overbrace{(1 + n(E'))\chi''(\mathbf{q}, E')}^{S(\mathbf{q},E)}$$

From the imaginary part of the self-energy, we deduce that the lifetime τ of the neutron is given by

$$\frac{1}{\tau} = \frac{2}{\hbar} Im\Sigma(\mathbf{k}, E_{\mathbf{k}} - i\delta) = \frac{2\alpha^2}{\hbar}\int_{\mathbf{k}'} S(\mathbf{k} - \mathbf{k}', E_{\mathbf{k}} - E_{\mathbf{k}'})$$

where we have changed the momentum integration variable from $\mathbf{q}$ to $\mathbf{k}' = \mathbf{k} - \mathbf{q}$. Splitting the momentum integration up into an integral over solid angle and an integral over energy, we have

$$\int_{\mathbf{k}'} = \int \left(\frac{m_N k_f}{8\pi^2\hbar^2}\right) dE' d\Omega'$$

from which we deduce that the mean-free path l of the neutron is given by

$$\frac{1}{l} = \frac{1}{v_N\tau} = \frac{1}{v_N} 2Im\Sigma(\mathbf{k}, E_{\mathbf{k}} - i\delta) = \int d\Omega_{\mathbf{k}'} dE_{\mathbf{k}'} \times \left[\frac{k_f}{k_i}\left(\frac{\alpha m_N}{2\pi\hbar^2}\right)^2 S(\mathbf{q}, E)\right]$$

where $\mathbf{q} = \mathbf{k} - \mathbf{k}'$ and $E = E_{\mathbf{k}} - E_{\mathbf{k}'}$ and $v_N = \hbar k_i/m_N$ is the incoming neutron velocity.

Normally we write $l = 1/(n_i\sigma)$, where σ is the cross-section of each scatterer and n_i is the concentration of scattering centers. Suppose $\tilde{\sigma} = n_i\sigma$ is the scattering cross-section per unit volume, then $\tilde{\sigma} = 1/l$, so it follows that

$$\tilde{\sigma} = \frac{1}{v_N} 2Im\Sigma(\mathbf{k}, E_{\mathbf{k}} - i\delta) = \int d\Omega_{\mathbf{k}'} dE_{\mathbf{k}'} \times \left[\frac{k_f}{k_i}\left(\frac{\alpha m_N}{2\pi\hbar^2}\right)^2 S(\mathbf{q}, E)\right]$$

from which we may identify the differential scattering cross-section as

$$\frac{d^2\tilde{\sigma}}{d\Omega dE} = \frac{k_f}{k_i}\left(\frac{\alpha m_N}{2\pi\hbar^2}\right)^2 S(\mathbf{q},E)$$

NMR

Knight Shift K

Nuclear Magnetic resonance, or "Magnetic resonance imaging" (MRI), as it is more commonly referred to in medical usage, is the use of nuclear magnetic absorption lines to probe the local spin environment in a material. The basic idea, is that the Zeeman interaction of a nuclear spin in a magnetic field gives rise to a resonant absorption line in the microwave domain. The interaction of the nucleus with surrounding spins and orbital moments produces a "Knight shift" this line and it also broadens the line, giving it a width that is associated with the nuclear spin relaxation rate $1/T_1$.

The basic Hamiltonian describing a nuclear spin is

$$H = -\mu_n \vec{I}\cdot\vec{B} + H_{hf}$$

where $\vec{I}$ is the nuclear spin, μ_n is the nuclear magnetic moment. The term H_{hf} describes the "hyperfine" interaction between the nuclear spin and surrounding spin degrees of freedom. The hyperfine interaction between a nucleus at site i and the nearby spins can be written

$$\begin{aligned} H_{hf} &= -\vec{I}_i\cdot\vec{B}_{hf}(i) \\ \vec{B}_{hf}(i) &= \underline{A}_{\textbf{contact}}\cdot\vec{S}_i + \underline{A}_{\textbf{orbital}}\cdot\vec{L}_i + \sum_j \underline{A}_{\textbf{trans}}(i-j)\cdot S_j. \end{aligned} \tag{10.45}$$

where $B_{hf}(i)$ is an effective field induced by the hyperfine couplings. The three terms in this Hamiltonian are derived from a local contact interaction, with s-electrons at the same site, an orbital interaction, and lastly, a transfered hyperfine interaction with spins at neighboring sites. The various tensors $\underline{A}$ are not generally isotropic, but for pedagogical purposes, let us ignore the anisotropy.

The Knight shift - the shift in the magnetic resonance line, is basically the expectation value of the term that couples In a magnetic field, the electronic spins inside the material become polarized, with $\langle S_j\rangle \sim \chi B$, where χ is the magnetic susceptibility, so in the simplest situation, the Knight shift is simply a measure of the local magnetic susceptibility of the medium. in turn, a measure of the electron density of states $\langle N(\epsilon)\rangle$, thermally averaged around the Fermi energy, so

$$K \sim B_{hf} \sim \chi B \sim \langle N(\epsilon)\rangle B.$$

One of the classic indications of the development of a gap in the electron excitation spectrum of an an electronic system, is the sudden reduction in the Knight shift. In more complex systems, where there are different spin sites, the dependence of the Knight shift can depart from the global spin susceptibility.

Another application of the Knight shift, is as a method to detect magnetic, or antiferromagnetic order. If the electrons inside a metal develop magnetic order, then this produces a large, field-independent Knight shift that can be directly related to the size of the ordered magnetic moment

$$K \sim \langle S_{\text{local}}\rangle$$

Unlike neutron scattering, NMR is able to distinguish between homogenious and inhomogenious magnetic order.

Relaxation rate $1/T_1$

The second aspect to NMR, is the broadening of the nuclear resonance. If we ignore all but the contact interaction, then the spin-flip decay rate of the local spin is determined by the Golden Rule,

$$\frac{1}{T_1} = \frac{2\pi}{\hbar} I^2 A^2_{contact} S_{+-}(\omega)\Big|_{\omega=\omega_N}$$

where ω_N is the nuclear resonance frequency and

$$\begin{aligned} S_{+-}(\omega) &= \int_{\mathbf{q}} [1+n_B(\omega)]\,\chi''_{+-}(\mathbf{q},\omega) \\ &\sim T\int \frac{d^3q}{(2\pi)^3}\frac{1}{\omega}\chi''_{+-}(\mathbf{q},\omega) \end{aligned} \tag{10.46}$$

at frequencies $\omega \sim \omega_N$, so for a contact interaction, The net nuclear relaxation rate is then

$$\frac{1}{T_1} = \frac{2\pi}{\hbar} I^2 A^2_{contact} \times T\int \frac{d^3q}{(2\pi)^3}\frac{1}{\omega}\chi''_{+-}(\mathbf{q},\omega)\Big|_{\omega=\omega_N}$$

In a classical metal, $\chi''(\omega)/\omega \sim N(0)^2$ is determined by the square of the density of states. This leads to an NMR relaxation rate

$$\frac{1}{T_1} \propto TN(0)^2 \sim \frac{k_BT}{\epsilon_F^2} \qquad \text{Korringa relaxation}$$

This linear dependence of the nuclear relaxation rate on temperature is name a "Korringa relaxation" law, after the Japanese theorist who first discovered it. Korringa relaxation occurs because the Pauli principle allows only a fraction fraction $TN(0) \sim T/\epsilon_F$ of the electrons to relax the nuclear moment. In a more generally, Fermi system, the NMR relaxation rate is determined by the thermally averaged square density of states.

$$\frac{1}{T_1} \sim T\int\left(-\frac{df(\omega)}{d\omega}\right)N(\omega)^2 \sim T\times[N(\omega\sim k_BT)]^2$$

In a wide class of anisotropic superconductors with lines of nodes along the Fermi surface, the density of states is a linear function of energy. One of the classic signatures of these line nodes across the Fermi surface is then a cubic dependence of $1/T_1$ on the temperature

$$\text{line nodes in gap} \Rightarrow N(\epsilon)\propto\epsilon, \qquad \Rightarrow \frac{1}{T_1}\propto T^3$$

In cases where the transferred hyperfine couplings are important, the non-locality introduces a momentum dependence into $A(\mathbf{k}) = \sum_{\vec{R}} A(\vec{R}_j)e^{-i\mathbf{k}\cdot\vec{R}_j}$these couplings. In this case,

$$\frac{1}{T_1} = \frac{2\pi}{\hbar} I^2 \times T\int \frac{d^3q}{(2\pi)^3}A(\mathbf{q})^2\frac{1}{\omega}\chi''_{+-}(\mathbf{q},\omega)\Big|_{\omega=\omega_N}$$

These momentum dependences can lead to radically different temperature dependences in the relaxation rate at different sites. One of the classic examples of this behavior occurs in the normal state of the high temperature superconductors. The active physics of these materials takes place in quasi-two dimensional layers of copper oxide, and the NMR relaxation rate can be measured at both the oxygen (O^{17}) and copper sites.

$$\left(\frac{1}{T_1}\right)_{Cu} \sim \text{constant}, \qquad \left(\frac{1}{T_1}\right)_O \sim \text{T},$$

The appearance of two qualitatively different relaxation rates is surprising, because the physics of the copper-oxide layers is thought to be described by a single-band model, with a single Fermi surface that can be seen in ARPES measurements. Why then are there two relaxation rates?

One explanation for this behavior has been advanced by Mila and Rice, who argue that there is indeed a single spin fluid, located at the copper sites. They noticed that whereas the copper relaxation involves spins at the same site, so that

$$A_{Cu}(\mathbf{q}) \sim \text{constant},$$

the spin relaxation rate on the oxygen sites involves a transfered hyperfine coupling between the oxygen p_x or p_y orbitals and the neigboring copper spins. The odd-parity of a p_x or p_y orbital means that the corresponding form factors have the form

$$A_{p_x}(\mathbf{q}) \sim \sin(q_x a/2).$$

Now high temperature superconductors are doped insulators. In the insulating state, cuprate superconductors are "Mott insulators", in which the spins on the Copper sites are antiferromagnetically ordered. In the doped metallic state, the spin fluctuations on the copper sites still contain strong antiferromagnetic correlations, and they are strongly peaked around $\vec{Q}_0 \sim (\pi/a,\pi/a)$, where a is the unit cell size. But this is precisely the point in momentum space where the transfered hyperfine couplings for the Oxygen sites vanish. The absence of the Korringa relaxation at the cupper sites is then taken as a sign that the copper relaxation rate is driven by strong antiferromagnetic spin fluctuations which do not couple to oxygen nucleii.

10.6 Electron Transport spectroscopy

10.6.1 Resistivity and the transport relaxation rate

One of the remarkable things about electron transport, is that one of the simplest possible measurements - the measurement of electrical resistivity, requires quite a sophisticated

understanding of the interaction between matter and radiation for its microscopic understanding. We shall cover this relationship in more detail in the next chapter, however, at basic level, DC electrical resistivity can be interpreted in terms of the basic Drude formula

$$\sigma = \frac{ne^2}{m}\tau_{tr}$$

where $1/\tau_{tr}$ is the transport relaxation rate. In Drude theory, the electron scattering rate τ_{tr} is related to the electron mean-free path l via the relation

$$l = v_F\tau$$

where v_F is the Fermi velocity. We need to sharpen this understanding, for $1/\tau_{tr}$ is not the actual electron scattering rate, it is the rate at which currents decay in the material. For example, if we consider impurity scattering of electrons with a scattering amplitude $u(\theta)$ which depends on the scattering angle θ, the electron scattering rate is

$$\frac{1}{\tau} = 2\pi n_i N(0)\overline{|u(\theta)|^2}$$

where

$$\overline{|u(\theta)|^2} = \int_{-1}^{1}\frac{d\cos\theta}{2}|u(\theta)|^2.$$

denotes the angular average of the scattering rate. However, as we shall see shortly, the transport scattering rate which governs the decay of electrical current is contains an extra weighting factor:

$$\begin{aligned} \frac{1}{\tau_{tr}} &= 2\pi n_i N(0)\overline{|u(\theta)|^2(1-\cos\theta)} \\ \overline{|u(\theta)|^2(1-\cos\theta)} &= \int_{-1}^{1}\frac{d\cos\theta}{2}|u(\theta)|^2(1-\cos\theta). \end{aligned} \tag{10.47}$$

The angular weighting factor $(1-\cos\theta)$ derives from the fact that the change in the current carried by an electron upon scattering through an angle θe is $ev_F(1-\cos\theta)$. In other words, only large angle scattering causes current decay. For impurity scattering, this distinction is not very important but in systems where the scattering is concentrated near $q=0$, such as scattering off ferromagnetic spin fluctuations, the $(1-\cos\theta)$ term substantially reduces the effectiveness of scattering as a source of resistance.

At zero temperature, the electron scattering is purely elastic, and the zero temperature resistance R_0 is then a measure of the elastic scattering rate off impurities. At finite temperatures, electrons also experience inelastic scattering, which can be strongly temperature dependent. One of the most important diagnostic quantities to characterize the quality of a metal is the resistance ratio - the ratio of resistance at room temperature to the resistance at absolute zero

$$RR = \text{Resistance Ratio} = \frac{R(300\text{K})}{R(0)}$$

The higher this ratio, the lower the amount of impurities and the higher the quality of sample. Hardware quality copper piping already has a resistance ratio of order a thousand! A high resistance ratio is vital for the observation of properties which depend on the coherent balistic motion of Bloch waves, such as de-Haas van Alphen oscillations or the development of anisotropic superconductivity, which is ultra-sensitive to impurity scattering.

With small caveat of distinction between transport and scattering relaxation rates, the temperature dependent resistivity is an excellent diagnostic tool for understanding the inelastic scattering rates of electrons:

$$\rho(T) = \frac{m}{ne^2} \times \left(\frac{1}{\tau_{tr}(T)} \right)$$

There are three classic dependences that you should be familiar with:

- **Electron phonon scattering above the Debye temperature**

$$\frac{1}{\tau_{tr}} = 2\pi\lambda k_B T$$

Linear resistivity is produced by electron-phonon scattering at temperatures above the Debye temperature, where the coefficient λ is the electron-phonon coupling constant defined in the previous chapter. In practice, this type of scattering always tends to saturate once the electron mean-free path starts to become comparable with the electron wavelength. It is this type of scattering that is responsible for the weak linear temperature dependence of resistivity in many metals. A note of caution - for linear resistivity does not necessarily imply electron phonon scattering! The most well-known example of linear resitivity occurs in the normal state of the cuprate superconductors, but here the resistance does not saturate at high temperatures, and the scattering mechanism is almost certainly a consequence of electron-electron scattering.

Electron-electron or Baber scattering

$$\frac{1}{\tau_{tr}} = \frac{\pi}{\hbar} \overline{|UN(0)|^2} N(0)(\pi k_B T)^2$$

where

$$\overline{|UN(0)|^2} = N(0)^2 \int \frac{d\Omega_{\hat{k}'}}{4\pi} |U(\mathbf{k}-\mathbf{k}')|^2 (1 - \cos(\theta_{\mathbf{k},\mathbf{k}'}))$$

is the weighted average of the electron-electron interaction $U(\mathbf{q})$. This quadratic temperature dependence of the inelastic scattering rate can be derived from the Golden rule scattering rate

$$\frac{1}{\tau_{tr}} = \frac{4\pi}{\hbar} \sum_{\mathbf{k}',\mathbf{k}''} |U(\mathbf{k}-\mathbf{k}')|^2 (1 - \cos\theta_{\mathbf{k},\mathbf{k}'})(1 - f_{\mathbf{k}'})(1 - f_{\mathbf{k}''}) f_{\mathbf{k}'+\mathbf{k}''-\mathbf{k}} \delta(\epsilon_{\mathbf{k}'} + \epsilon_{\mathbf{k}''} - \epsilon_{\mathbf{k}'''})$$

where the $4\pi = 2 \times 2\pi$ prefactor is derived from the sum over internal spin indices If we neglect the momentum dependence of the scattering amplitude, then this quantity is determined entirely by the three-particle phase space

$$\begin{aligned} \frac{1}{\tau_{tr}} &\propto \int d\epsilon' d\epsilon'' (1 - f(\epsilon'))(1 - f(\epsilon''))f(-\epsilon' - \epsilon'') \\ &= T^2 \int dx dy \left(\frac{1}{1-e^{-x}}\right)\left(\frac{1}{1-e^{-y}}\right)\left(\frac{1}{1-e^{-(x+y)}}\right) = \frac{\pi^2}{4}T^2 \qquad (10.48) \end{aligned}$$

In practice, this type of resistivity is only easily observed in strongly interacting electron materials, where it is generally seen to develop at low temperatures when a Landau Fermi liquid develops. The T^2 resistivity is a classic hallmark of Fermi liquid behavior.

Kondo spin-flip scattering

In metals containing a dilute concentration of magnetic impurities, the spin-flip scattering generated by the impurities gives rise to a temperature dependent scattering rate of the form

$$\frac{1}{\tau_{tr}} \sim n_i \frac{1}{\ln^2\left(\frac{T}{T_K}\right)}$$

where T_K is the "Kondo temperature", which characterizes the characteristic spin fluctuation rate of magnetic impurity. This scattering is unusual, because it becomes stronger at lower temperatures, giving rise to a " resistance minimum" in the resistivity.

In heavy electron materials, the Kondo spin-flip scattering is seen at high temperatures, but once a coherent Fermi liquid is formed, the resistivity drops down again at low temperatures, ultimately following a T^2 behavior.

10.6.2 Optical conductivity

Probing the electrical properties of matter at finite frequencies requires the use of optical spectroscopy. In principle, optical spectroscopy provides a direct probe of the frequency dependent conductivity inside a conductor. The frequency dependent conductivity is defined by the relation

$$\vec{j}(\omega) = \sigma(\omega)\vec{E}(\omega)$$

Modern optical conductivity measurements can be made from frequencies in the infra -red of order $\omega \sim 10cm^{-1} \sim 1meV$ up to frequencies in the optical, of order $50,000cm^{-1} \sim 5eV$. The most direct way of obtaining the optical conductivity is from the reflectivity, which is given by

$$r(\omega) = \frac{1 - n(\omega)}{1 + n(\omega)} = \frac{1 - \sqrt{\epsilon(\omega)}}{1 + \sqrt{\epsilon(\omega)}},$$

where $n(\omega) = \sqrt{\epsilon(\omega)}$ is the diffractive index and $\epsilon(\omega)$ is the frequency dependent dielectric constant. Now $\epsilon(\omega) = 1 + \chi(\omega)$ where $\chi(\omega)$ is the frequency dependent dielectric susceptibility. Now since the polarization $P(\omega) = \chi(\omega)E(\omega)$, and since the current is given by $j = \partial_t P$, it follows that $j(\omega) = -i\omega P(\omega) = -i\omega\chi(\omega)E(\omega)$, so that $\chi(\omega) = \sigma(\omega)/(-i\omega)$ and hence

$$\epsilon(\omega) = 1 + \frac{\sigma(\omega)}{-i\omega}.$$

Thus in principle, knowledge of the complex reflectivity determines the opical conductivity.

In the simplest measurements, it is only possible to measure the intensity of reflected radiation, giving $|r(\omega)|^2$. More sophisticated " elipsometry" techniques which measure the reflectivity as a function of angle and polarization, are able to provide both the amplitude and phase of the reflectivity, but here we shall discuss the simplest case where only the amplitude $|r(\omega)|$ is available. In this situation, experimentalists use the "Kramers' Kronig" relationship which determines the imaginary part imaginary part $\sigma_2(\omega)$ of the optical conductivity in terms of the real part, $\sigma_1(\omega)$, (Appendix A)

$$\sigma_2(\omega) = \omega \int_0^\infty \frac{d\omega'}{\pi} \frac{\sigma_1(\omega')}{\omega^2 - \omega'^2}$$

This is a very general relationship that relies on the retarded nature of the optical response. In principle, this uniquely determines the dielectric function and reflectivity. However, since the range of measurement is limited below about $5eV$, an assumption has to be made about the high frequency behavior of the optical conductivity where normally, a Lorentzian form is assumed.

With these provisos, it becomes possible to invert the frequency dependent reflectivity in terms of the frequency dependent conductivity. We shall return in the next chapter for a consideration of the detailed relationship between the optical conductivity and the microscopic correlation functions. We will see shortly that the interaction of an electromagnetic field with matter involves the transverse vector potential, which couples to the currents in the material without changing the charge density. The optical conductivity can be related to the following response function

$$\sigma(\omega) = \frac{1}{-i\omega}\left[\frac{ne^2}{m} - \langle j(\omega)j(-\omega)\rangle\right]$$

This expression contains two parts - a leading diamagnetic part, which describes the high frequency, short-time response of the medium to the vector potential, and a second, "paramagnetic" part, which describes the slow recovery of the current towards zero. We have used the shorthand

$$\langle j(\omega)j(-\omega)\rangle = i\int_0^\infty dt d^3x \langle [j(x,t), j(0)]\rangle e^{i\omega t}$$

to denote the retarded response function for the "paramagnetic" part of the electron current density $j(x) = -i\frac{\hbar}{m}\psi^\dagger\vec{\nabla}\psi(x)$.

10.6.3 Optical conductivity and the f-sum rule.

One of the most valuable relations for the analysis of optical conductivity data, is the so-called "f-sum rule", according to which the total integrated weight under the conductivity spectrum is constrained to equal the plasma frequency of the medium,

$$\int_0^\infty \frac{d\omega}{\pi}\sigma(\omega) = \frac{ne^2}{m} = \omega_P^2\epsilon_0$$

where n is the density of electronic charge and ω_P is the Plasma frequency. To understand this relation, suppose we apply a sudden pulse of electric field to a conductor

$$E(t) = E_0\delta(t),$$

then immediately after the pulse, the net drift velocity of the electrons is changed to $v = eE_0/m$, so the instantaneous current after the field pulse is

$$j(0^+) = nev = \frac{ne^2}{m}E_0,$$

where n is the density of carriers. After the current pulse, the electric current will decay. For example, in the Drude theory, there is a single current relaxation time rate τ_{tr}, so that

$$j(t) = \frac{ne^2}{m}e^{-t/\tau_{tr}}E_0$$

and thus

$$\sigma(t - t') = \frac{ne^2}{m}e^{-(t-t')/\tau_{tr}}\theta(t - t')$$

and by Fourier transforming we deduce that

$$\sigma(\omega) = \int_0^\infty dt e^{i\omega t}\sigma(t) = \frac{ne^2}{m}\frac{1}{\tau_{tr}^{-1} - i\omega}$$

Actually, the f-sum rule does not depend on the detailed form of the curent relaxation. All we need to use, is Newton's law, according to which

$$J(t = 0^+) = E_o\sigma(t = 0^+) = E_o\int_{-\infty}^\infty \frac{d\omega}{2\pi}e^{-i0^+}\sigma(\omega) = \frac{ne^2}{m}E_0$$

is a consequence of Newton's law. It follows that (independently of how the current subsequently decays),

$$\int_0^\infty \frac{d\omega}{\pi}\sigma(\omega) = \frac{ne^2}{m} = \epsilon_0\omega_p^2$$

where we have identified $\epsilon_0\omega_p^2 = \frac{ne^2}{m}$ with the plasma frequency ω_p of the gas. This relationship is called the f-sum rule, and it is important because it holds, independently of the details of how the current decays.

The important point about the f-sum rule, is that in principle, the total weight under the optical spectrum, is a constant, providing one integrates up to a high-enough energy. When the temperature changes however, it is possible for the spectral weight to redistribute. In a simple metal, the optical conductivity forms a simple "Drude peak" - Lorentzian of width $1/\tau_{tr}$ around zero frequency. In a semi-conductor, the weight inside this peak decays as $e^{-\Delta/T}$, where Δ is the semi-conducting gap. In a simple insulator, the balance of spectral weight must then reappear at energies above the direct gap energy Δ_g. By contrast, in a superonductor, the formation of a superconducting condensate causes the spectral weight in the optical conductivity to collapse into a delta-function peak.

Appendix A: Kramer's Krönig relation

The Kramer's Krönig relation applies to any retarded linear response function, but we shall derive it here in special reference to the conductivity. In time, the current and electric field are related by the retarded response function

$$j(t) = \int_{-\infty}^{t} dt'\sigma(t-t')E(t') \tag{10.49}$$

which becomes $j(\omega) = \sigma(\omega)E(\omega)$ in Fourier space, where $\sigma(\omega)$ is the Fourier transform of the real-time response function $\sigma(t-t')$

$$\sigma(\omega) = \int_0^\infty dte^{i\omega t}\sigma(t).$$

This function can be analytically extended into the upper-half complex plain ,

$$\sigma(z) = \sigma(x+iy) = \int_0^\infty dte^{izt}\sigma(t) = .\int_0^\infty dte^{ixt-yt}\sigma(t).$$

So long as z lies above the real axis, the real part $-yt$ of the exponent is negative, guaranteeing that the integral is and $\sigma(z)$ is an analytic function. Provided $Imz_0 > 0$, then the conductivity can be written down using Cauchy's theorem

$$\sigma(z_0) = \int_{C'} \frac{dz}{2\pi i}\frac{\sigma(z)}{z - z_o}$$

where C' runs anti-clockwise around the point z_0. By distorting the contour onto the real axis, and neglecting the contour at infinity, it follows that

$$\sigma(z_0) = \int_{-\infty}^{\infty} \frac{d\omega'}{2\pi i}\frac{\sigma(\omega')}{\omega' - z_0}$$

Taking $z_0 = \omega + i\delta$, and writing $\sigma(\omega + i\delta) = \sigma_1(\omega) + i\sigma_2(\omega)$ on the real axis, we arrive at the "Kramer's Krönig" relations

$$\begin{aligned}\sigma_2(\omega) &= -\int_{-\infty}^{\infty}\frac{d\omega'}{2\pi}\frac{\sigma_1(\omega')}{\omega'-\omega} = \omega\int_0^\infty \frac{d\omega'}{\pi}\frac{\sigma_1(\omega')}{\omega^2-\omega'^2}\\ \sigma_1(\omega) &= \int_{-\infty}^{\infty}\frac{d\omega'}{2\pi}\frac{\sigma_2(\omega')}{\omega'-\omega} = \int_0^\infty \frac{d\omega'}{\pi}\frac{\omega'\sigma_2(\omega')}{\omega^2-\omega'^2}\end{aligned} \tag{10.50}$$

10.7 Exercises for chapter 10

1. Spectral decomposition. The dynamic spin susceptibility of a magnetic system, is defined as

$$\chi(\mathbf{q},t) = i\langle[S^-(\mathbf{q},t_1), S^+(-\mathbf{q},t_2)] > \theta(t_1 - t_2) \tag{10.51}$$

where $S^\pm(\mathbf{q}) = S_x(\mathbf{q}) \pm iS_y(\mathbf{q})$ are the spin raising and lowering operators at wavevector $\mathbf{q}$, i.e

$$S^\pm(\mathbf{q}) = \int d^3e^{-i\mathbf{q}\cdot\mathbf{x}}S^\pm(\mathbf{x}) \tag{10.52}$$

so that $S^-(\mathbf{q}) = [S^+(-\mathbf{q})]^\dagger$. The dynamic spin susceptibility determines the response of the magnetization at wavevector $\mathbf{q}$ in response to an applied magnetic field at this wavevector

$$M(\mathbf{q},t) = \frac{\mu_B}{2}\int dt'\chi(\mathbf{q},t-t')B(t'). \tag{10.53}$$

(i)Make a spectral decomposition, and show that

$$\chi(\mathbf{q},t) = i\theta(t)\int\frac{d\omega}{\pi}\chi''(\mathbf{q},\omega)e^{i\omega t} \tag{10.54}$$

where $\chi''(\mathbf{q},\omega)$ (often called the "power-spectrum" of spin fluctuations) is given by

$$\chi''(\mathbf{q},\omega) = (1 - e^{-\beta\omega})\sum_{\lambda,\zeta} e^{-\beta(E_\lambda - F)}|\langle\zeta|S^+(-\mathbf{q})|\lambda\rangle|^2\pi\delta[\omega - (E_\zeta - E_\lambda)] \tag{10.55}$$

and F is the Free energy.

(ii)Fourier transform the above result to obtain a simple integral transform which relates $\chi(\mathbf{q},\omega)$ and $\chi''(\mathbf{q},\omega)$. The correct result is called a "Kramers Kronig" transformation.

(iii)In neutron scattering experiments, the inelastic scattering cross-section is directly proportional to a spectral function called $S(\mathbf{q},\omega)$,

$$\frac{d^2\sigma}{d\Omega d\omega} \propto S(\mathbf{q},\omega) \tag{10.56}$$

where $S(\mathbf{q},\omega)$ is the Fourier transform of a correlation function:

$$S(\mathbf{q},\omega) = \int_{-\infty}^{\infty} dte^{i\omega t}\langle S^-(\mathbf{q},t)S^+(-\mathbf{q},0)\rangle \tag{10.57}$$

By carrying out a spectral decomposition, show that

$$S(\mathbf{q},\omega) = (1 + n(\omega))\chi''(\mathbf{q},\omega) \tag{10.58}$$

This relationship, plus the one you derived in part (i) can be used to completely the dynamical spin susceptibility via inelastic neutron scattering.

Chapter 11

Electron transport Theory

11.1 Introduction

Resistivity is one of the most basic properties of conductors. Surprisingly, Ohm's law

$$V = IR$$

requires quite a sophisticated understanding of the quantum many body physics for its understanding. In the classical electron gas, the electron current density

$$\vec{j}(x) = ne\vec{v}(x)$$

is a simple c-number related to the average drift velocity $\vec{v}(x)$ of the electron fluid. This is the basis of the Drude model of electricity, which Paul Drude introduced shortly after the discovery of the electron. Fortunately, many of the key concepts evolved in the Drude model extend to the a quantum description of electrons, where $\vec{j}(x)$ is an operator. To derive the current operator, we may appeal to the continuity equation, or alternatively, we can take the derivative of the Hamiltonian with respect to the vector potential,

$$\vec{j}(x) = -\frac{\delta H}{\delta\vec{A}(x)}$$

where

$$H = \int d^3x\left[\frac{1}{2m}\psi^\dagger(x)\left(-i\hbar\vec{\nabla} - e\vec{A}(x)\right)^2\psi(x) - e\phi(x)\psi^\dagger(x)\psi(x)\right] + V_{INT}$$

Now only the Kinetic term depends on $\vec{A}$, so that

$$\vec{j}(x) = \frac{-i\hbar}{2m}\psi^\dagger(x)\overleftrightarrow{\nabla}\psi(x) - \left(\frac{e^2}{m}\right)\vec{A}(x)\rho(x). \tag{11.1}$$

The discussion we shall follow dates back to pioneering work by Fritz London. London noticed in connection with his research on superconductivity, that the current operator splits

up into components, which he identified with the paramagnetic and diamagnetic response of the electron fluid:

$$\vec{j}(x) = \vec{j}_P(x) + \vec{j}_D(x)$$

where

$$\vec{j}_P(x) = \frac{-i\hbar}{2m}\psi^\dagger(x)\overleftrightarrow{\nabla}\psi(x)$$

and

$$\vec{j}_D(x) = -\left(\frac{e^2}{m}\right)\vec{A}(x)\rho(x).$$

Although the complete expression for the current density *is* invariant under gauge transformations $\psi(x) \to e^{i\phi(x)}\psi(x)$, $\vec{A}(x) \to \vec{A} + \frac{\hbar}{e}\vec{\nabla}\phi(x)$ the separate parts are not. However, in a *specific* gauge, such as the London or Coulomb gauge, where $\vec{\nabla}\cdot A = 0$, they do have physical meaning. We shall identify this last term as the term responsible for the diamagnetic response of a conductor, and the first term, the "paramagnetic current", is responsible for the decay of the current a metal.

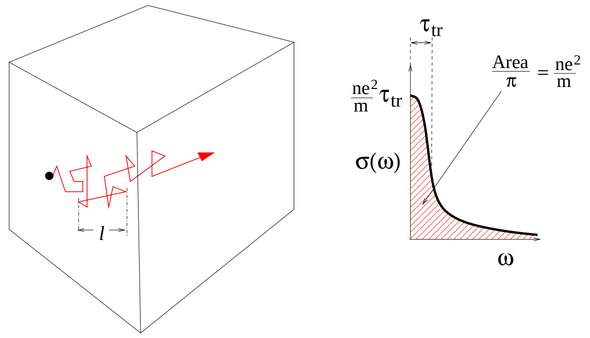


Figure 11.1: (a) Illustrating the diffusion of electrons on length-scales large compared with the mean-free path l, (b) The Drude frequency dependent conductivity. The short-time behavior of the current is determined by Newton's law, which constrains the area under the curve to equal $\int d\omega\sigma(\omega) = \pi\frac{ne^2}{m}$, a relation known as the f-sum rule.

In a non-interacting system, the current operator commutes with the Kinetic energy operator H_0 and is formally a constant of the motion. In a periodic crystal, electron momentum is replaced by the lattice momentum **k**, which is, in the absence of lattice vibrations, a constant of the motion, with the result that the electron current still does not decay. What is the origin of electrical resistance?

There are then two basic sources of current decay inside a conductor:

- Disorder - which destroys the translational invariance of the crystal,
- Interactions - between the electrons and phonons, and between the electrons themselves, which cause the electron momenta and currents to decay.

The key response function which determines electron current is the conductivity, relating the Fourier component of current density at frequency ω, to the corresponding frequency dependent electric field,

$$\vec{j}(\omega) = \sigma(\omega)\vec{E}(\omega)$$

We should like to understand how to calculate this response function in terms of microscopic correlation functions.

The classical picture of electron conductivity was developed by Paul Drude, shortly after the discovery of the electron. Although his model was introduced before the advent of quantum mechanics, many of the basic concepts he introduced carry over to the quantum theory of conductivity. Drude introduced the the concept of the electron mean-free path l - the mean distance between scattering events. The characteristic timescale between scattering events is called the transport scattering time τ_{tr}. (We use the "tr" subscript to delineate this quantity from the quasiparticle scattering time τ, because not all scattering events decay the electric current.) In a Fermi gas, the characteristic velocity of electrons is the Fermi velocity and the mean-free path and transport scattering time are related by the simple relation

$$l = v_F\tau_{tr}$$

The ratio of the mean-free path to the electron wavelength is the same order of magnitude as the ratio of the scattering time to the characteristic timescale associated with the Fermi energy $\hbar/\epsilon_F$ is determined by the product of the Fermi wavevector and the mean-free path

$$\frac{l}{\lambda_F} = \frac{k_F l}{2\pi} \sim \frac{\tau_{tr}}{\hbar/\epsilon_F} = \frac{\epsilon\tau_{tr}}{\hbar}$$

In very pure metals , the mean-free path of Bloch wave electrons l can be tens, even hundreds of microns, $l \sim 10^{-6}m$, so that this ratio can become as large as 10^4 or even 10^6. From this perspective, the rate at which current decays in a good metal is very slow on atomic time-scales.

There are two important aspects to the Drude model:

- the diffusive nature of density fluctuations,

- the Lorentzian line-shape of the optical conductivity

$$\sigma(\omega) = \frac{ne^2}{m}\frac{1}{\tau_{tr}^{-1} - i\omega}$$

Drude recognized that on length scales much larger than the mean-free path multiple scattering events induce diffusion into the electron motion. On large length scales, the current and density will be related by he diffusion equation,

$$\vec{j}(x) = -D\vec{\nabla}\rho(x),$$

where $D = \frac{1}{3}\frac{l^2}{\tau_{tr}} = \frac{1}{3}v_F^2\tau_{tr}$, which together with the continuity equation

$$\vec{\nabla}\cdot\vec{j} = -\frac{\partial\rho}{\partial t}$$

gives rise to the diffusion equation

$$\left[-\frac{\partial}{\partial t} + D\nabla^2\right]\rho = 0.$$

The response function $\chi(q,\nu)$ of the density to small changes in potential must be the Green's function for this equation, so that in Fourier space

$$[i\nu - Dq^2]\chi(q,\nu) = 1$$

from which we expect the response function and density-density correlation functions to contain a diffusive pole

$$\langle\delta\rho(q,\nu)\delta\rho(-q,-\nu)\rangle \sim \frac{1}{i\nu - Dq^2}$$

The second aspect of the Drude theory concerns the slow decay of current on the typical time-scale τ_{tr}, so that in response to an electric field pulse $E = E_0\delta(t)$, the current decays as

$$j(t) = e^{-\frac{t}{\tau_{tr}}}$$

In the last chapter, we discussed how, from a quantum perspective, this current is made up of two components, a diamagnetic component

$$j_{DIA} = -\frac{ne^2}{m}A = \frac{ne^2}{m}E_0, \qquad (t > 0)$$

and a paramagnetic part associated with the relax9ation of the electron wavefunction, which grows to cancel this component,

$$j_{PARA} = \frac{ne^2}{m}E_0(e^{-t/\tau_{tr}} - 1), \qquad (t > 0)$$

We should now like to see how each of these heuristic features emerges from a microscopic treatment of the conductivity and charge response functions. To do this, we need to relate the conductivity to a response fucntion - and this brings us to the Kubo formula.

11.2 The Kubo Formula

Lets now look again at the form of the current density operator. According to (11.1), it can divided into two parts

$$\vec{j}(x) = \vec{j}_P + \vec{j}_D \tag{11.2}$$

where

$$\begin{aligned} \vec{j}_P &= -\frac{i\hbar}{m}\psi^\dagger(x)\overleftrightarrow{\nabla}\psi(x) && \text{paramagnetic current} \\ \vec{j}_D &= -\frac{e^2}{m}\int d^3x\,\rho(x)\vec{A}(x) && \text{diamagnetic current} \end{aligned} \tag{11.3}$$

are the "paramagnetic" and " diamagnetic" parts of the current. The total current operator is invariant under gauge transformations $\psi(x) \rightarrow e^{i\phi(x)}\psi(x)$, $\vec{A}(x) \rightarrow \vec{A} + \frac{\hbar}{e}\vec{\nabla}\phi(x)$ and speaking, the two terms in this expression for the current can't be separated in a gauge invariant fashion. However, in a specific gauge. We shall work in the London gauge

$$\vec{\nabla}\cdot\vec{A} = 0 \qquad \text{"London Gauge"} .$$

In this gauge, the vector potential is completely transverse, $\vec{q}\cdot\vec{A}(\vec{q}) = 0$. The equations of the electromagnetic field in the London Gauge are

$$\begin{aligned} \left(\frac{1}{c^2}\partial_t^2 - \nabla^2\right)\vec{A}(x) &= \mu_0\vec{j}(x) \\ -\nabla^2\phi(x) &= \frac{\rho(x)}{\epsilon_0} \end{aligned} \tag{11.4}$$

so that the potential field $\rho(x)$ is entirely determined by the distribution of charges inside the material, and the only independent external dynamic field coupling to the material is the vector potential. We shall then regard the vector potential as the only external field coupling to the material.

We shall now follow Fritz London's argument for the interpretation of these two terms. Let us carry out a thought experiment, in which we imagine a toroidal piece of metal, as in Fig. 11.2 in which a magnetic flux is turned on at $t = 0$, passing up through the conducting ring, creating a vector potential around the ring given by $A = A_0\theta(t) = \frac{\phi_0}{2\pi r}\theta(t)$, where r is the radius of the ring. The Electric field is related to the external vector potential via the relation

$$\vec{E} = -\frac{\partial\vec{A}}{\partial t} = -A_0\delta(t)$$

so $\vec{E} = -\vec{A}_o\delta(t)$ is a sudden inductively induced electrical pulse.

Suppose the system is described in the Schrödinger representation by the wavefunction $|\psi(t)\rangle$, then the current flowing after time t is given by

$$\langle\vec{j}(t)\rangle = \langle\psi(t)|\vec{j}_P|\psi(t)\rangle - \frac{ne^2}{m}A_o\theta(t) \tag{11.5}$$

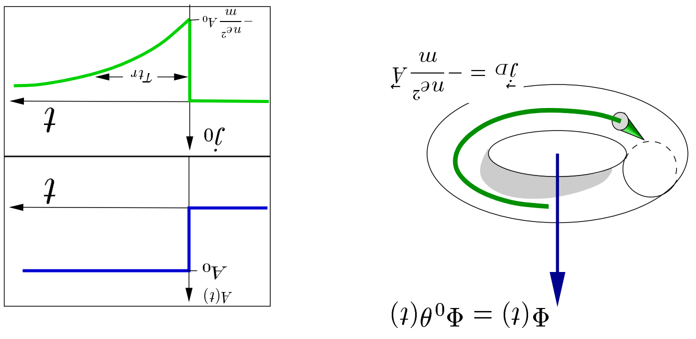


Figure 11.2: Schematic diagram to illustrate diamagnetic current pulse produced by a sudden change of flux through the conducting loop.

where we have assumed that $\langle\rho(x)\rangle = n$ is the equilibrium density of electrons in the material. We see that the second "diamagnetic" term switches on immediately after the pulse. This is nothing more than the diamagnetic response - the effect of the field induced by Faraday's effect. What is so interesting, is that this component of the current remains *indefinitely*, after the initial step in the flux through the toroid. But the current must decay! How?

The answer is that the initial "paramagnetic" contribution to the current starts to develop after the flux is turned on. Once the vector potential is present, the wavefunction $|\psi(t)\rangle$ starts to evolve, producing a paramagnetic current that rises and in a regular conductor, ultimately *exactly cancels* the time-independent diamagnetic current. From this point of view, the only difference between an insulator and a metal, is the timescale required for the paramagnetic current to cancel the diamagnetic component. In an insulator, this time-scale is of order the inverse (direct) gap Δ_g, $\tau \sim \hbar/\Delta_g$, whereas in a metal, it is the transport relaxation time $\tau \sim \tau_{tr}$.

These arguments were first advanced by Fritz London. He noticed that if, for some unknown reason the wavefunction of the material could become "rigid", so that it would not respond to the applied vector potential. In this special case, the paramagnetic current would never build up, and one would then have a perfect diamagnet - a superconductor. Lets now look at this in more detail. We need to compute

$$\vec{j}(\vec{x},t)=\langle \vec{j}_P(x,t)\rangle-\frac{ne^2}{m}\vec{A}(x,t)$$

Now if we are to compute the response of the current to the applied field, we need to compute the build up of the paramagnetic part of the current. Here we can use linear response theory. The coupling of the vector potential to the paramagnetic current is simply $-\int d^3x\vec{j}(x)\cdot\vec{A}(x)$, so the response of this current is given by

$$\langle j_P^\alpha(t)\rangle=\int_{t'<t}d^3x'dt'i\langle[j_P^\alpha(x),j_P^\beta(x')]\rangle A^\beta(x') \tag{11.6}$$

In other words, we may write

$$\boxed{\begin{aligned}\vec{j}(1)&=-\int d2\underline{Q}(1-2)\vec{A}(2)\\ Q^{\alpha\beta}(1-2)&=\frac{ne^2}{m}\delta^{\alpha\beta}\delta(1-2)-i\langle[j_P^\alpha(1),j_P^\beta(2)]\rangle\theta(t_1-t_2).\end{aligned}} \tag{11.7}$$

The quantity $\underline{Q}(1-2)$ is the "London response" Kernel. In the most general case, this response is non-local in both space and time. In a metal, this response is non-local over a distance given by the electron mean-free path $l=v_F\tau_{tr}$. In a superconductor the response to the vector potential is non-local over the "Pippard coherence length", $\xi=v_F/\Delta$, where Δ is the superconducting gap. We can write the above result in Fourier space as

$$\vec{j}(q)=-\underline{Q}(q)\vec{A}(q)$$

where

$$Q^{\alpha\beta}(q)=\frac{ne^2}{m}\delta^{\alpha\beta}-i\langle[j^\alpha(q),\ j^\beta(-q)]\rangle$$

and we have used the cavalier notation,

$$\langle[j^\alpha(q),\ j^\beta(-q)]\rangle=\int d^3x\int_0^\infty dt\langle[j^\alpha(x,t),\ j^\beta(0)]\rangle e^{-i(\vec{q}\cdot\vec{x}-\nu t)}.$$

Finally, if we write $\vec{E}=-\frac{\partial A}{\partial t}$, or $A(q)=\frac{1}{i\nu}E(q)$, we deduce that

Kubo formula

$$\boxed{\begin{aligned}\vec{j}(q)&=\underline{\sigma}(q)\vec{E}(q)\\ \sigma^{\alpha\beta}(q)&=-\frac{1}{i\nu}Q^{\alpha\beta}(q)=\frac{1}{-i\nu}\left\{\frac{ne^2}{m}\delta^{\alpha\beta}-i\langle[j^\alpha(q),\ j^\beta(-q)]\rangle\right\}\end{aligned}} \tag{11.8}$$

Now in practice, the high velocity of light means that $q=\nu/c<<k_F$ is much shorter than an electronic wavevector, so that in electronic condensed matter physics, we may consider the limit $\vec{q}=0$, writing $\sigma(\nu)=\sigma(\vec{q}=0,\nu)$. This is the quantity that is measured in optical conductivity measurements. The D.C. conductivity is given by the zero-frequency limit of the uniform conductivity, i.e. $\sigma_{DC}=Lt_{\nu\to 0}\sigma(\nu)$.

In a regular conductor, σ_{DC} is finite, which implies that $Q(\nu=0)=0$, so that in a conductor

$$i\langle[j^\alpha(q),\ j^\beta(-q)]\rangle|_{q=0}=\frac{ne^2}{m}\delta^{\alpha\beta}$$

We shall see that this identity breaks down in a system with broken gauge invariance - and this is the origin of superconductivity. In a normal fluid however, we can use this identity to rewrite the expression for the conductivity as

$$\sigma^{\alpha\beta}(\nu)=\frac{1}{-i\nu}\Big[-i\langle[j^\alpha(\nu'),\ j^\beta(-\nu')]\rangle\Big]_{\nu'=0}^{\nu'=\nu} \tag{11.9}$$

A practical calculation of conductivity depends on our ability to extract this quantity from the imaginary time response function. We can quickly generalize expression (11.7) to imaginary time, by replacing $i\langle[A(1),B(2)]\rangle\to\langle TA(1)B(2)\rangle$, so that in imaginary time,

$$\begin{aligned}\vec{j}(1)&=-\int d2\underline{Q}(1-2)\vec{A}(2),\qquad(1\equiv(\vec{x}_1,\tau_1))\\ Q^{\alpha\beta}(1-2)&=\frac{ne^2}{m}\delta^{\alpha\beta}\delta(1-2)-\langle Tj_P^\alpha(1)j_P^\beta(2)\rangle\end{aligned} \tag{11.10}$$

so that in Fourier space, our expression for the optical conductivity is given by

$$\sigma^{\alpha\beta}(i\nu_n)=-\frac{1}{\nu_n}\Big[\ \langle Tj^\alpha(\nu')j^\beta(-\nu')\rangle\Big]_{\nu'=0}^{\nu'=i\nu_n} \tag{11.11}$$

where we have used the short-hand notation

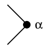
$$\langle Tj^\alpha(i\nu_n)j^\beta(-i\nu_n)\rangle=\int_0^\beta d\tau e^{i\nu_n\tau}\langle Tj^\alpha(\tau)j^\beta(0)\rangle$$

11.3 Drude conductivity: diagramatic derivation

In the last section we showed how the fluctuations of the electrical current can be related to the optical conductivity. Let us now see how these fluctuations can be computed using Feynman diagrams in a disordered electron gas with dispersion $\epsilon_{\mathbf{k}}=\frac{k^2}{2m}$. First, let us review the Feynman rules. We shall assume that we have taken the leading order effects of disorder into account in the electron propagator, denoted by

$$\longrightarrow=G(k)=\frac{1}{i\omega_n-\epsilon_{\mathbf{k}}+i\mathrm{sgn}\omega_n\frac{1}{2\tau}}$$

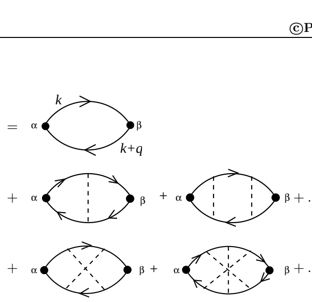
The current operator is $j^\alpha(q)=\sum e\frac{k^\alpha}{m}\psi^\dagger{}_{k-q/2\sigma}\psi_{k+q/2\sigma}$, which we denote by the vertex



$$\alpha\equiv e\frac{k^\alpha}{m}$$

The set of diagrams that represent the current fluctuations can then be written

$$\langle j^\alpha(q)j^\beta(-q)\rangle\ =$$

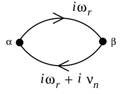


(11.12)

In the above expansion, we have identified three classes of diagrams. The first diagram, denotes the simplest contribution to the current fluctuation: we shall see shortly that this is already sufficient to capture the Drude conductivity. The second set of diagrams represent the leading impurity corrections to the current vertex: these terms take account of the fact that low-angle scattering does not affect the electric current, and it is these terms that are responsible for the replacement of the electron scattering rate τ by the transport relaxation rate τ_{tr}. We shall see that these terms vanish for isotropicaly scattering impurities, and justifying our neglect of these contributions in our warm-up calculation of the conductivity.

The last set of diagrams involve crossed impurity scattering lines - we have already encountered these types of diagrams in passing, and the momentum restrictions associated with crossed diagrams lead to a reduction factor of order $O(\frac{1}{k_Fl})\sim\frac{\lambda}{l}$, or the ratio of the electron wavelength to the mean-free path. These are the "quantum corrections" to the conductivity. These importance of these terms was not appreciated during the early years of research into electron transport - it was not until the late 1970's that they became associated with the physics of electron localization - more on this later.

Using the Feynman rules, the first contribution to the current fluctuations is given by



$$\begin{aligned}&=\langle j^\alpha(i\nu_n)j^\beta(-i\nu_n)\rangle\\ &=-2e^2T\sum_{\mathbf{k},i\omega_r}\frac{k^\alpha k^\beta}{m^2}G(\mathbf{k},i\omega_r+i\nu_n)G(\mathbf{k},i\omega_r)\end{aligned} \tag{11.13}$$

where the minus sign derives from the fermion loop and the factor of two derives from the sum over spin components. The difference between the fluctuations at finite and zero frequencies is then

$$\left[\langle j^\alpha(\nu)j^\beta(-\nu)\rangle\right]_0^{i\nu_n} = -2e^2T\sum_{\mathbf{k},i\omega_r}\frac{k^\alpha k^\beta}{m^2}\left[G(\mathbf{k},i\omega_r+i\nu_n)G(\mathbf{k},i\omega_r)-\{i\nu_n\to 0\}\right] \quad (11.14)$$

Now the amplitude at current fluctuations at any one frequency involves electron states far from the Fermi surface. However, the *difference* between the current fluctuations at two low frequencies cancels out most of these contributions, and the only important remaining contributions involve electrons with near the Fermi surface. This observation means that we can replace the momentum summation in (11.14) by an energy integral in which the density of states is approximated by a constant, and the limits are extended to infinity, as follows

$$\begin{aligned}\sum_{\mathbf{k}}\frac{k^\alpha k^\beta}{m^2}\Big[\ldots\Big] &\to \int\frac{4\pi k^2dk}{(2\pi)^3}\int\frac{d\Omega_{\hat{\mathbf{k}}}}{4\pi}\frac{k^\alpha k^\beta}{m^2}\Big[\ldots\Big]\\ &\to \delta^{\alpha\beta}\frac{v_F^2N(0)}{3}\int_{-\infty}^{\infty}d\epsilon\Big[\ldots\Big] \qquad (11.15)\end{aligned}$$

The London Kernel then becomes

$$\begin{aligned}Q^{\alpha\beta}(i\nu_n) &= 2\delta^{\alpha\beta}\frac{e^2v_F^2N(0)}{3}T\sum_{\omega_r}\times\\ & 2\int_{-\infty}^{\infty}d\epsilon\left\{\overbrace{\left(\frac{1}{i\omega_r^+-\epsilon+i\mathrm{sgn}\omega_r^+/2\tau}\right)\left(\frac{1}{i\omega_r-\epsilon+i\mathrm{sgn}\omega_r/2\tau}\right)}^{\text{Poles on opposite side if }\omega_r^+>\omega_r}-\overbrace{\Big(\quad i\nu_n\to 0\Big)}^{\text{Poles on same side}}\right\}\end{aligned}$$

We can now carry out the energy integral by contour methods. We shall assume that $\nu_n > 0$. Now, provided that $i\omega_r^+ > 0$ and $i\omega_r < 0$, the first term inside this summation has poles on opposite sides of the real axis, at $\epsilon = i\omega_r + i/2\tau$ and $\epsilon = i\omega_r - 1/2\tau$, whereas the second term has poles on the same side of the real axis. Thus, when we complete the energy integral we only pick up contributions from the first term. (It doesn't matter which side of the real axis we complete the contour, but if we choose the contour to lie on the side where there are no poles in the second term, we are able to immediately see that this term gives no contribution.) The result of the integrals is then

$$\begin{aligned}Q^{\alpha\beta}(i\nu_n) &= \delta^{\alpha\beta}\overbrace{\frac{2e^2v_F^2N(0)}{3}}^{\frac{ne^2}{m}}T\sum_{0>\omega_r>-\nu_n,}\frac{2\pi i}{i\nu_n+i\tau^{-1}}\\ &= \delta^{\alpha\beta}\frac{ne^2}{m}\frac{\nu_n}{\tau^{-1}+\nu_n} \qquad (11.16)\end{aligned}$$

Converting the London Kernel into the optical conductivity,

$$\sigma^{\alpha\beta}(i\nu_n) = \frac{1}{\nu_n}Q^{\alpha\beta}(i\nu_n) = \delta^{\alpha\beta}\frac{ne^2}{m}\frac{1}{\tau^{-1}-i(i\nu_n)}$$

Finally, analytically continuing onto the real axis, we obtain

$$\boxed{\sigma^{\alpha\beta}(\nu+i\delta) = \frac{ne^2}{m}\frac{1}{\tau^{-1}-i\nu} \qquad \text{Transverse conductivity}}$$

There are a number of important points to make about this result

- Our result ignores the effects of anisotropic scattering. To obtain these we need to include the "ladder" vertex corrections, which we will shortly see, replace

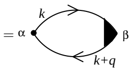
$$\frac{1}{\tau}\to\frac{1}{\tau_{tr}} = 2\pi n_iN(0)\overline{(1-\cos\theta)|u(\theta)|^2}, \qquad (11.17)$$

  where the $(1-\cos\theta)$ term takes into account that small angle scattering does not relax the electrical current.

- Our result ignores localization effects that become important when $\frac{1}{k_Fl}\sim 1$. In one or two dimensions, the effects of these scattering events accumulates at long distances, ultimately localizing electrons, no matter *how* weak the impurity scattering.

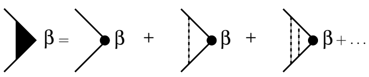
- Transverse current fluctuations are not diffusive - this is not surprising, since transverse current fluctuations do not involve any fluctuation in the charge density.

To improve our calculation, let us now examine the vertex corrections that we have so far neglected. Let us now re-introduce the "ladder" vertex corrections shown in (11.12). We shall write the current-current correlator as

$\langle j^\alpha(q)j^\beta(-q)\rangle =$ 

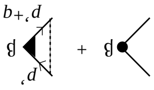
(11.18)

where the vertex correction is approximated by a sum of ladder diagrams, as follows



$+\ldots = \Lambda e v_F^\beta$ (11.19)

We shall re-write the vertex part as a self-consistent Dyson equation, as follows:

$\Lambda e v_F^\beta =$ 

(11.20)

where $q = (0, i\nu_n)$ and $p' = (\vec{p}\,', i\omega_r)$. The equation for the vertex part is then

$$ev_F^\beta\Lambda(\omega_r,\nu_n) = ev_F^\beta + n_i\sum_{\vec{p}\,'}|u(\vec{p}-\vec{p}\,')|^2G(\vec{p}\,',i\omega_r^+)G(\vec{p}\,',i\omega_r)\Lambda(\omega_r,\nu_n)ev_F'^\beta. \qquad (11.21)$$

Assuming that the vertex part only depends on frequencies, and has no momentum dependence, we may then write

$$\Lambda = 1+\Lambda n_i\int\frac{d\cos\theta}{2}|u(\theta)|^2\cos\theta\int\frac{d^3p'}{(2\pi)^3}G(\vec{p}\,',i\omega_r^+)G(\vec{p}\,',i\omega_r)$$

We can now carry out the integral over $\vec{p}\,'$ as an energy integral, writing

$$N(0)\int d\epsilon G(\epsilon,i\omega_r^+)G(\epsilon,i\omega_r) = N(0)\int d\epsilon\frac{1}{i\tilde{\omega}_n^+-\epsilon}\frac{1}{i\tilde{\omega}_n-\epsilon}$$

where

$$\tilde{\omega}_n = \omega_n + \mathrm{sign}\omega_n(\frac{1}{2\tau})$$

Carrying out this integral, we obtain

$$N(0)\int d\epsilon G(\epsilon,i\omega_r^+)G(\epsilon,i\omega_r) = \begin{cases}\pi N(0)\frac{1}{\nu_n+\tau^{-1}} & -\nu_n<\omega_r<0\\ 0 & \text{otherwise}\end{cases}$$

so that

$$\Lambda = 1+\left(\frac{\tilde{\tau}^{-1}}{\nu_n+\tau^{-1}}\right)\Lambda\theta_{\nu_n,\omega_r}$$

where $\tilde{\tau}^{-1} = 2\pi n_iN(0)\overline{\cos\theta|u(\theta)|^2}$ and $\theta_{\nu_n,\omega_r} = 1$ if $-\nu_n < \omega_r < 0$ and zero otherwise, so that

$$\Lambda = \begin{cases}\frac{\nu_n+\tau^{-1}}{\nu_n+\tau_{tr}^{-1}} & -\nu_n<\omega_r<0\\ 1 & \text{otherwise}\end{cases} \qquad (11.22)$$

where

$$\tau_{tr}^{-1} = \tau^{-1}-\tilde{\tau}^{-1} = 2\pi n_iN(0)\overline{(1-\cos\theta)|u(\theta)|^2}.$$

when we now repeat the calculation, we obtain

$$Q^{\alpha\beta}(i\omega_n) = \frac{ne^2}{m}\delta^{\alpha\beta}T\sum_{i\omega_r}\int_{-\infty}^{\infty}d\epsilon\left[G(\epsilon,i\omega_r^+)G(\epsilon,i\omega_r)-(i\nu_n\to 0)\right]\Lambda(i\omega_r,i\nu_n)$$

$$\begin{aligned}&= \frac{ne^2}{m}\delta^{\alpha\beta}T\sum_{i\omega_r}\frac{2\pi i}{i\nu_n+i\tau^{-1}}\frac{\nu_n+\tau^{-1}}{\nu_n+\tau_{tr}^{-1}}\\ &= \frac{ne^2}{m}\left(\frac{\nu_n}{\nu_n+\tau_{tr}^{-1}}\right)\delta^{\alpha\beta} \qquad (11.23)\end{aligned}$$

So making the analytic continuation to real frequencies, we obtain

$$\sigma(\nu+i\delta) = \frac{ne^2}{m}\frac{1}{\tau_{tr}^{-1}-i\nu}$$

Note that

- We see that transverse current fluctuations decay at a rate $\tau_{tr}^{-1} < \tau$. By renormalizing $\tau \to \tau_{tr}$, we take into account the fact that only backwards scattering relaxes the current. τ_{tr} and τ_{tr} are only identical in the special case of isotropic scattering. This distinction between scattering rates becomes particularly marked when the scattering is dominated by low angle scattering, which contributes to τ^{-1}, but does not contribute to the decay of current fluctuations.

- There is no diffusive pole in the transverse current fluctuations. This is not surprising, since transverse current fluctuations do not change the charge density.

11.4 Electron Diffusion

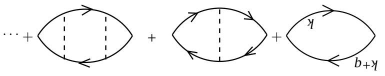
To display the presence of diffusion, we need to examine the density response function. Remember that a change in density is given by

$$\langle\delta\rho(q)\rangle = i\langle[\rho(q),\rho(-q)]\rangle\overbrace{\delta\mu(q)}^{-eV(q)}$$

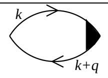
where V is the change in the electrical potential and

$$i\langle[\rho(q),\rho(-q)]\rangle = \int d^3xdti\langle[\rho(x,t),\rho(0)]\rangle e^{-i\vec{q}\cdot\vec{x}+i\omega t}$$

We shall calculate this using the same set of ladder diagrams, but now using the charge vertex. Working with Matsubara frequencies, we have

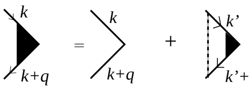
$\langle\rho(q,i\nu_n)\rho(-q,-i\nu_n)\rangle =$ 

$$= $$



(11.24)

where the current vertex



$$= \Lambda_c(k,q). \qquad (11.25)$$

Let us now rewrite (11.24) and (11.25) as equations. From (11.24) the density-density response function is given by

$$\langle\rho(q,i\nu_n)\rho(-q,-i\nu_n)\rangle = -2T\sum_k G(k+q)G(k)\Lambda_c(k,q).$$

From (11.25), the Dyson equation for the vertex is

$$\Lambda_c(k,q) = 1 + n_i\sum_{p'}|u(\mathbf{k}-\mathbf{k}')|^2 G(k'+q)G(k')\Lambda_c(k',q) \qquad (11.26)$$

For convenience, we will assume point scattering, so that $u = u_0$ is momentum independent so that $\Lambda_c(k,q)$ only depends on the frequency component part of $k = (i\omega_r, \mathbf{k})$, so

$$\begin{aligned}\Lambda_c(i\omega_r,q) &= 1 + n_i u_0^2\sum_{p'} G(k'+q)G(k')\Lambda_c(i\omega_r,q)\\ &= 1 + \Pi(i\omega_r,q)\Lambda_c(i\omega_r,q) \qquad (11.27)\end{aligned}$$

or

$$\Lambda_c(i\omega_r,q) = \frac{1}{1-\Pi(i\omega_r,q)}$$

where the polarization bubble

$$\begin{aligned}\Pi(i\omega_r,q) &= n_i u_0^2\sum_{p'} G(k'+q)G(k')\\ &= n_i u_0^2 N(0)\int\frac{d\Omega}{4\pi}\int d\epsilon\frac{1}{i\tilde{\omega}_r^+ - (\epsilon+\vec{q}\cdot\vec{v}_F)}\frac{1}{i\tilde{\omega}_r-\epsilon} \qquad (11.28)\end{aligned}$$

Now if $i\nu_n > 0$, then the energy integral in $\pi(i\omega_r,q)$ will only give a finite result if $-\nu_n < \omega_r < 0$. Outside this frequency range, $\pi(i\omega_r,q) = 0$ and $\Lambda_c = 1$. Inside this frequency range, $\Pi(i\omega_r,q) = \Pi(q)$ is frequency independent, and given by

$$\Pi(q) = \overbrace{n_i u_0^2 N(0)}^{\tau^{-1}/(2\pi)}\int\frac{d\Omega}{4\pi}\frac{2\pi i}{i\nu_n + i\tau^{-1} + \vec{q}\cdot\vec{v}_F}$$

$$= \int\frac{d\Omega}{4\pi}\frac{1}{1+\nu_n\tau - i\vec{q}\cdot\vec{v}_F\tau} \qquad (11.29)$$

Now we would like to examine the slow, very long wavelength charge flucations, which means we are interested in q small compared with the inverse mean-free path, $q << l^{-1} = 1/(v_F\tau)$, and in frequencies that are much smaller than the inverse scattering length $\nu_n\tau << 1$. This permits us to expand Π in powers of $\vec{q}$. We shall take the first non-zero contribution, which comes in at order q^2. With these considerations in mind, we may expand Π as follows

$$\begin{aligned}\Pi(q) &= \int\frac{d\Omega}{4\pi}\left(1-\nu_n\tau + i\vec{q}\cdot\vec{v}_F\tau + i^2(v_F\cdot\mathbf{q})^2\tau^2+\dots\right)\\ &= \left(1-\nu_n\tau - \frac{v_F^2\tau}{3}q^2\tau + \dots\right) \qquad (11.30)\end{aligned}$$

where we neglect terms of order $O(q^2\nu_n)$. We may identify the combination $v_f^2\tau/3 = D$ in the second term with the diffusion constant D. Note that had we done this integral in d dimensions, the "3" in the denominator of the second term above would be replaced by d, but the general form for the diffusion constant in d dimensions is $D = v_f^2\tau/d$, so that in any dimension, we obtain

$$\Pi(q) = \left(1-\nu_n\tau - Dq^2\tau + \dots\right) \qquad (11.31)$$

We then obtain

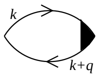
$$\Lambda_c(q) = \frac{1}{1-\Pi(q)} = \frac{\tau^{-1}}{\nu_n + Dq^2}, \qquad (-\nu_n < \omega_r < 0). \qquad (11.32)$$

Summarizing then, the long-wavelength, low frequency charge vertex has the form

$$\Lambda_c(i\omega_r,q) = \begin{cases}\frac{i\tau^{-1}}{\nu_n+Dq^2}, & (-|\nu_n| < \mathrm{sgn}(\nu_n)\omega_r < 0)\\ 1 & \text{otherwise}\end{cases}$$

and thus the dynamic charge correlation function is given by

$$\langle\rho(q)\rho(-q)\rangle = $$



$$= -2N(0)T\sum_{i\omega_r}\int d\epsilon G(\epsilon,i\omega_r^+)G(\epsilon,i\omega_r)\Lambda_c(\omega_r,\nu_n) \qquad (11.33)$$

Now if we evaluate this quantity at zero frequency, $\nu_n = 0$, where $\Lambda_c = 1$, we obtain the static susceptibility

$$\chi_0 = -2T\sum_{r,k}\frac{!}{(i\tilde{\omega}_r-\epsilon_k)^2}$$

$$\begin{aligned}&= 2\int d\epsilon N(\epsilon)\int\frac{d\omega}{2\pi i}f(\omega)\left\{\frac{1}{(\omega+i/(2\tau)-\epsilon)^2} - \frac{1}{(\omega-i/(2\tau)-\epsilon)^2}\right\}\\ &= 2\int d\epsilon N(\epsilon)\int\frac{d\omega}{2\pi i}\frac{df(\omega)}{d\omega}\overbrace{\left\{\frac{1}{(\omega+i/(2\tau)-\epsilon)} - \frac{1}{(\omega)-i/(2\tau)-\epsilon)}\right\}}^{-2iA(\epsilon,\omega)}\\ &= 2\int d\omega\left(-\frac{df(\omega)}{d\omega}\right)\overbrace{\int d\epsilon\frac{N(\epsilon)}{\pi}A(\epsilon,\omega)}^{=N(\omega)} = 2N(0) \qquad \text{unrenormalized} \quad (11.34)\end{aligned}$$

so that the static charge susceptibility is unaffected by the disorder. This enables us to write

$$\langle\rho(q)\rho(-q)\rangle = \chi_0 - 2T\sum_{i\omega_r}\int N(\epsilon)d\epsilon\left[G(\epsilon,i\omega_r^+)G(\epsilon,i\omega_r)\Lambda_c(\omega_r,\nu_n) - \{\nu_n\to 0\}\right]$$

Since this intgeral is dominated by contributions near the Fermi energy, we can extend the energy integral over the whole real axis, replacing

$$\int N(\epsilon)d\epsilon \to N(0)\int_{-\infty}^{\infty}d\epsilon$$

enabling the energy integral to be carried out by contour methods, whereupon,

$$\begin{aligned}\langle\rho(q)\rho(-q)\rangle &= \chi_0 - 2TN(0)\sum_{i\omega_r}\int_{-\infty}^{\infty}d\epsilon\left[G(\epsilon,i\omega_r^+)G(\epsilon,i\omega_r)\Lambda_c(\omega_r,\nu_n) - \{\nu_n\to 0\}\right]\\ &= \chi_0 - \chi_0\overbrace{\left(\frac{\nu_n}{\nu_n+\tau^{-1}}\right)}^{\to\nu_n\tau}\left[\frac{\tau^{-1}}{\nu_n+Dq^2}\right]\end{aligned}$$

where, again, in the last step we have assumed $|\nu_n|\tau << 1$. The Matsubara form for the charge susceptibility is then

$$\chi_o(\vec{q},i\nu_n) = \chi_0\frac{Dq^2}{|\nu_n| + Dq^2}$$

Analytically continuing this result, we finally obtain

$$\boxed{\chi(\vec{q},\nu+i\delta) = \chi_0\left(\frac{Dq^2}{Dq^2-i\nu}\right)} \qquad (11.35)$$

. Note that:

- Density fluctuations are diffusive. Indeed, we could have anticipated the above form on heuristic grounds. The solution of the diffusion equation $D\nabla^2\rho = \frac{\partial\rho}{\partial t}$ is, in Fourier space,

$$\rho(\vec{q},\nu) = \frac{1}{Dq^2-i\nu}\rho(q)$$

where $\rho(q)$ is the Fourier transform of the initial charge distribution. If we require $\rho(\vec{q},\nu=0) = \chi_0 U(\vec{q})$, where $U(\vec{q})$ is the Fourier transform of the applied potential, then this implies (11.35)

- The order of limits is important, for whereas

$$\lim_{q\to 0}\lim_{\nu\to 0}\chi(q,\nu) = \chi_0$$

which is the response to a static potential of large, but finite wavelength,

$$\lim_{\nu\to 0}\lim_{q\to 0}\chi(q,\nu) = 0$$

which states that the response to a uniform potential of vanishingly small frequency is zero. The difference in these two response functions is due to the conservation of charge - if one wants to change the charge density in one place, it can only be done by redistributing the charge. If one applies a static uniform potential, the charge density does not change.

- We can use these results to deduce the longitudinal conductivity - the current response to a longitudinal electric field for which $\vec{q}\cdot\vec{E}\neq 0$. Let $\phi(q)$ be the electric potential, then $\delta\rho(q) = -\chi(q)e\phi(q)$, so that

$$\begin{aligned}\delta\rho(q) = -\chi_0\frac{Dq^2}{Dq^2-i\nu}e\phi(q) &= \chi_0\frac{Di\vec{q}\cdot\overbrace{(i\vec{q}\phi(q))}^{\vec{\nabla}\phi=-\vec{E}(q)}}{Dq^2-i\nu}\\ &= -\chi_0\left(\frac{Di\vec{q}}{Dq^2-i\nu}\right)\cdot\vec{E}(q) \qquad (11.36)\end{aligned}$$

Now since $\frac{\partial\rho}{\partial t}\equiv -i\nu\rho(q)$, it follows that

$$\dot{\rho}(q) = -e\chi_0\left(\frac{D\nu\vec{q}}{Dq^2-i\nu}\right)\cdot\vec{E}(q). \qquad (11.37)$$

Now by continuity, $e\frac{\partial\rho}{\partial t} = -\vec{\nabla}\cdot\vec{j}(q) = -\vec{\nabla}\vec{j}(q) == -i\vec{q}\cdot\vec{j}(q)$, where $\vec{j}$ is the charge current, so by comparing with (11.36) we deduce that the longitudinal current is

$$j_L(q) = e^2\chi_0 D\left(\frac{i\nu}{i\nu-Dq^2}\right)\vec{E}(q),$$

so the longitudinal conductivity contains a diffusive pole

$$\sigma_{LONG}(q) = \chi_0 D\left(\frac{i\nu}{i\nu-Dq^2}\right).$$

Note also that at $q=0$, $\sigma = e^2\chi_0 D$, which can be written as the Einstein relation

$$\sigma = e^2\chi_0 D = \frac{ne^2}{m}\tau \qquad \text{Einstein Relation}$$

11.5 Weak Localization

We should like to finish our brief introduction to electron transport by touching on the concept of electron localization. The disorder that has been considered in this chapter is weak and the electron states we have considered are delocalized. We have remarked on a few occasions that disorder is like a kind of "attractive" but infinitely retarded interaction, and like other attractive interactions, it has the capacity to induce new kinds of collective behavior amongst the electrons. Infact, disorder actually gives rise to collective interference effects within the electron gas, which ultimately lead to the localization of the electron wavefunction. This idea was first proposed by Anderson in the late 1950's, but it took two decades for the idea to gain acceptance in the physics community. Our modern understanding of electron localization dates back to a conceptual break-through on this problem that was made by the so called "Gang of Four", Abrahams, Anderson Licciardello and Ramakrishnan, in the late seventies. These three authors proposed that electron localization results from the coherent interference between electron waves, and may be regarded as a kind of phase transition. Like phase transitions, localization is very sensitive to the dimensionality of the conductor. Whereas in three dimensions, electron localization requires that the disorder exceed a critical value, in two and one dimension, an arbitrarily small amount of disorder is sufficient to localize electrons, and the leading order effects of localization can already be seen in weakly disordered materials.

To develop a rudimentary understanding of electron localization, we shall follow a heuristic argument by Altshuler, Aronov, Larkin and Khmelnitskii[??], who pointed out that weak localization results from the constructive interference between electrons passing along time-reversed paths. Consider the amplitude for an electron to return to its starting point. In general, it can do this by pass around a a sequence of scattering sites labelled 1 through n, as shown in Fig. 11.3, where we identify $n \equiv 1$ as the same scattering site. The amplitude for scattering around this loop is

$$A_P = G_R(n, n-1)G_R(n-1, n-2)\dots G_R(2,1)$$

where

$$G_R(\vec{x}_1, \vec{x}_2) = \int \frac{d^dk}{(2\pi)^d}\frac{1}{\omega - \epsilon_{\mathbf{k}} + i\delta}e^{i\vec{k}\cdot(\vec{x}_1 - \vec{x}_2)}$$

is the retarded propagator describing the amplitude for an electron of frequency ω to propagate between two sites. Now for each path P, there is a corresponding time-reversed path $\tilde{P}$. The amplitude for the same electron to follow $\tilde{P}$ starting at $1 \equiv n$, is

$$A_{\tilde{P}} = G_R(1,2)G_R(2,3)\dots G_R(n-1,n)$$

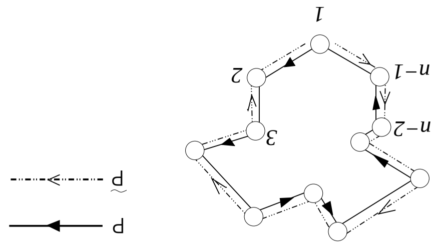


Figure 11.3: Scattering of an electron around two time-reversed paths

The total propability associated with passage along both paths is given by

$$P = |A_P + A_{\tilde{P}}|^2 = |A_P|^2 + |A_{\tilde{P}}|^2 + 2\mathrm{Re}[A^*_{\tilde{P}}A_P]$$

Now if $A_P = \sqrt{p_1}e^{i\phi_1}$ and $A_{\tilde{P}} = \sqrt{p_2}e^{i\phi_2}$ then total probability to scatter back to the starting point via the two paths,

$$p_{TOT} = p_1 + p_2 + 2\sqrt{p_1p_2}\cos(\phi_2 - \phi_1).$$

contains an interference term $2\sqrt{p_1p_2}\cos(\phi_2 - \phi_1)$. If the two paths were unrelated, then the impurity average of interference term would be zero, and we would expect $\overline{P} = p_1 + p_2$. However! The two paths *are* related by time-reversalk, so that $A_{\tilde{P}} = A_P$, with precisely the same magnitude and phase, and so the two processes always *constructively interfere*,

$$p_{TOT} = 4p_1$$

Had we ignored the interference, we would have gotten $p_{TOT} = 2p_1$, so we see that constructive interference between time-reversed paths doubles the chance that an electron will return to its starting point.

This means that an electron that enters into a random medium has an quantum-mechanically *enhanced* probability of returning to its starting point - quantum electrons "bounce back" twice as often as classical electrons in a a random medium! The same phenomenon causes the light from a car's headlamps to reflect backwards in a Fog. These effects tend to localize waves - causing light localization in the case of fog - and electron localization in disordered conductors. We shall see that the return probability is enhanced in lower dimensions, and in one, or two dimensions, these effects innevitably lead to the localization of electrons, for arbitrarily small amounts of disorder.

Let us now make a diagramatic identification of these interference terms. The complex conjugate of the retarded propagator is the advanced propagator

$$G_R(2-1,\omega)^* = G(2-1,\omega+i\delta)^* = G(2-1,\omega-i\delta) == G_A(2-1,\omega)$$

so the interference term

$$A^*_{\tilde{P}}A_P = \prod_{j=1}^{n-1} G_R(j+1,j;\omega)G_A(j,j+1;\omega)$$

But this is nothing more than a "ladder diagram" for repeated scattering of electron pairs. The sum of all such diagrams is called a "Cooperon", because of the close similarity to

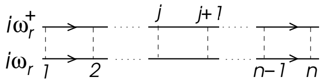


Figure 11.4: n-th order contribution to the "Cooperon"

electron pairs in superconductivity. Notice that the lower electron line involves the advanced propagator G_A, whereas the upper involves the retarded propagator G_R. In the Matsubara approach the distinction between these two propagators is enforced by running a frequency $i\omega_r^+ \equiv i\omega_r + i\nu_n$ along the top line, and a frequency $i\omega_r$ along the bottom. When ν_n is analytically continued and ultimately set to zero, this enforces the distinction betwen the two propagators. Now if we twist the Cooperon around, we see that it is equivalent to a maximally crossed, or "Langer-Neal" diagram

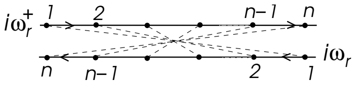
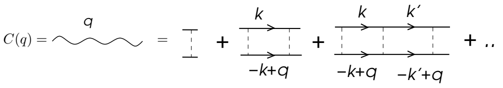


Figure 11.5: A twisted cooper diagram forms a maximally crossed diagram.

Let us now compute the amplitudes associated with these localization corrections to the conductivity. We begin by denoting the Cooperon by a sum of ladder diagrams



$$= \frac{n_iu_0^2}{1-\tilde{\Pi}(q)} \tag{11.38}$$

where

$$\tilde{\Pi}(q) = n_iu_0^2\sum_{\mathbf{k}} G_R(k)G_A(-k+q)$$

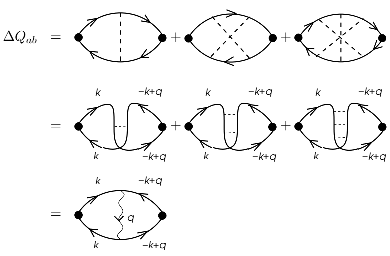
where we have denoted $G_R(k) \equiv G(\mathbf{k}, i\omega_r^+)$ and $G_A(k) \equiv G(\mathbf{k}, i\omega_r)$, implicitly assuming that ω_r^+ and ω_r are of opposite sign. Now if we look carefully at $\tilde{P}i$, we see that it is identical to the particle hole bubble Π that we encountered when computing diffusive charge fluctuations in (11.28), excepting that in going from hole, to particle, has been reversed, replacing $\mathbf{k}+\mathbf{q} \to -\mathbf{k}+\mathbf{q}$. However, provided that time-reversal symmetry holds, this this does not change the value of the polarization bubble, so we may immediately conclude that

$$\tilde{\Pi}(q) = \Big(1 - \nu_n\tau - Dq^2\tau + \dots\Big)$$

and thus

$$C(q) = n_iu_0^2\frac{\tau^{-1}}{Dq^2+|\nu_n|} = \frac{1}{2\pi N(0)\tau^2}\frac{1}{Dq^2+|\nu_n|}$$

We shall redraw the maximally crossed contributions to the conductivity in the following form



(11.39)

Written out explicitly, this gives

$$\begin{aligned}\Delta\sigma^{ab}(i\nu_n) &= \frac{\Delta Q^{ab}}{\nu_n}\\ &= \frac{2e^2T}{\nu_n}\sum_{\mathbf{k},\mathbf{q},i\omega_r} v^a_{\mathbf{k}}v^b_{-\mathbf{k}+\mathbf{q}}\left[C(q)G^+(k)G^-(k)G^+(-k+q)G^-(-k+q) - \{i\nu_n \to 0\}\right]\end{aligned}$$

Now in principal, we need to take account of the q dependence of the electron propagators in this diagram. However, if we are interested in the most singular, long-distance effects of localization, we can ignore the q dependence of the conduction electron lines, decoupling the localization correction to the conductivity into a product of two terms, as follows

$$\begin{aligned}\Delta\sigma^{ab}(i\nu_n) &= \frac{2e^2T}{\nu_n}\sum_{\mathbf q} C(q) \overbrace{\sum_k v^a_{\mathbf k} v^b_{-\mathbf k}}^{-\frac{\nu_n}{2\pi T}\frac{ne^2}{m}\delta^{ab}\int d\epsilon} \left[(G^+(k))^2(G^-(k))^2 - \{i\nu_n \to 0\}\right] \\ &= -\frac{ne^2}{m}\delta^{ab}\frac{1}{2\pi N(0)\tau^2}\int\frac{d^dq}{(2\pi)^d}\frac{1}{Dq^2+|\nu_n|}\int\frac{d\epsilon}{2\pi}G^2_R(\epsilon)G^2_A(\epsilon) \qquad (11.40)\end{aligned}$$

The energy integral in the second term yields

$$\int\frac{d\epsilon}{2\pi}G^2_R(\epsilon)G^2_A(\epsilon) = 2\tau^3.$$

We need to consider the upper and lower bounds to the momentum integral. The upper bound is set by the condition that $Dq^2 = \tau^{-1}$, the elastic scattering rate. The lower bound is set either by the size of the system L, in which case $q = L^{-1}$, or by the *inelastic* scattering rate τ_i^{-1}. We may define

$$\tau_0^{-1} = \max(\frac{D}{L^2}, \tau_i^{-1})$$

as the inverse time-scale associated with the lower cutoff. The quantity

$$E_{th} = \hbar\frac{D}{L^2}$$

is called the "Thouless" energy, and corresponds to the energy scale associated with the phase-coherent diffusion of electrons from one side of the sample, to the other. In an ultra-pure, or small system, it is this scale that provides the infra-red cut-off to localization effects. We may then write

$$\Delta\sigma^{ab}(\nu) = -\delta^{ab}\left(\frac{ne^2\tau}{m}\right)\frac{1}{2\pi N(0)}\int_{(D\tau_o)^{-1/2}}^{(D\tau)^{-1/2}}\frac{d^dq}{(2\pi)^d}\frac{1}{Dq^2 - i\nu} \qquad (11.41)$$

If we apply a sudden pulse of electric field $E = E_0\delta(t)$, giving rise to a white noise field spectrum, $E(\nu) = E_0$, the current induced by localization effects has a frequency spectrum

$$j(\nu) = \Delta\sigma(\nu)E(\nu) = \Delta\sigma(\nu)E_0 \propto \int_{(D\tau_0)^{-1/2}}^{(D\tau)^{-1/2}}\frac{d^dq}{(2\pi)^d}\frac{1}{Dq^2 - i\nu}$$

In highly phase-coherent systems, the characteristic time scale of the localization backscattering response in the current pulse is given by $t \sim D/L^2$ which we recongnize as the time for electrons to diffuse across the entire sample. This is a kind of backscattering "echo" produced by the phase-coherent diffusion of electrons along time-reversed paths that cross the entire sample. The momentum integral in $\Delta\sigma$ is strongly dependent on dimensionality. in three and higher dimensions, this term is finite, so that the weak-localization effects are a perturbation to the Drude conductivity. However, if the dimension $d \leq 2$, this integral becomes divergent, and in a non-interacting system, it is cut off only by the frequency, or the finite size L of the system. In two dimensions,

$$\int_{(D\tau_o)^{-1/2}}^{(D\tau)^{-1/2}}\frac{d^dq}{(2\pi)^d}\frac{1}{Dq^2 - i\nu} = \frac{1}{4\pi D}\ln(\frac{\tau}{\tau_0})$$

giving rise to a localization correction to the static conductivity that is

$$\Delta\sigma = -\left(\frac{ne^2\tau}{m}\right)\frac{1}{8\pi^2N(0)D}\ln(\frac{\tau_0}{\tau}) \qquad (11.42)$$

Replacing $2\pi N(0)D = \epsilon_F\tau = \frac{1}{2}k_Fl$, the total conductivity can be written

$$\begin{aligned}\sigma &= \sigma_0\left[1 - \frac{1}{4\pi\epsilon_F\tau}\ln(\frac{\tau_0}{\tau})\right] \qquad (11.43)\\ \sigma &= \sigma_0\left[1 - \frac{1}{2\pi k_Fl}\ln(\frac{\tau_0}{\tau})\right] \qquad (11.44)\end{aligned}$$

Replacing $n\tau/m \to 2N(0)D$, we obtain

$$\Delta\sigma = -\left(\frac{e^2}{2\pi^2}\right)\ln(\frac{\tau}{\tau_0}) \to -\frac{1}{2\pi^2}\left(\frac{e^2}{\hbar}\right)\ln(\frac{\tau_0}{\tau}) \qquad (11.45)$$

where we have restored $\hbar$ into the expression. The quantity $g_0 = \frac{e^2}{\hbar} \sim \frac{1}{10}(k\Omega)^{-1}$ is known as the universal conductance.

There are a number of interesting consequences of these results

- We see that the quantum-interference correction to the conductivity is indeed of order $O(1/(k_Fl))$.
- If we consider the case where inelastic scattering is negligible, the localization correction to the conductivity in two dimensions is

  $$\begin{aligned}\sigma &= \sigma_0\left[1 - \frac{1}{2\pi k_Fl}\ln(\frac{1}{E_{Th}\tau})\right]\\ &\sim \sigma_0\left[1 - \frac{1}{\pi k_Fl}\ln(\frac{L}{l})\right] \qquad (11.46)\end{aligned}$$

  so that the conductivity drops gradually to zero as the size of the sample increases. The conductivity becomes of order g_0 at the localization length

  $$L \sim le^{k_Fl}$$

  independently of the strength of the interaction. At longer length-scales, the material evolves into insulator.

- The weak localization corrections are not divergent for dimensions greater than 2, but become much stronger in dimensions below $d = 2$. It was this observation that led the the "Gang of Four", Abrahams, Anderson, Licciardello and Ramakrishnan, to propose the scaling theory for localization, in which $d_c = 2$ is the critical dimensionality.

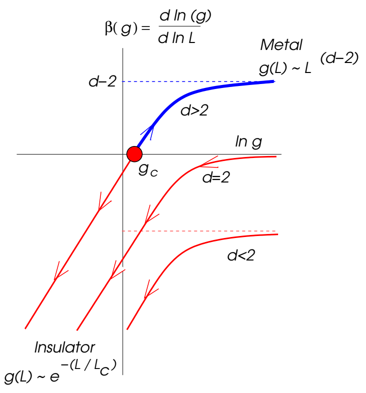


Figure 11.6: The scaling function $\beta(g)$ deduced by Abrahams et al. for a non-interacting metal. For $d > 2$ there is critical conductance g_c which gives rise to a disorder-driven metal-insulator transition. In $d \leq 2$, disorder always gives rise to localization and the formation of an insulator.

We shall end this section by making a brief remark about the scaling theory of localization. Stimulated by the results in two dimensions, and earlier work on one dimensional wires, by Thouless, Abrahams et al. were led to propose that in any dimension, conductance, or inverse resistance, $G = 1/R$ could always be normalized to form a dimensionless parameter

$$g(L) = \frac{1/R(L)}{\frac{e^2}{\hbar}}$$

whose behavior as a function of scale satisfies a one-parameter scaling equation

$$\frac{d\ln g(L)}{d\ln L} = \beta(g)$$

When this quantity is large, we may use the Drude model, so that $g(L) = \frac{ne^2\tau}{m}L^{d-2}$, and

$$\beta(g) = (d-2), \qquad (g \to \infty)$$

is independent of g. When the conductance was small $g \to 0$, they argued that $g(L) \sim e^{-L/L_c}$, where L_c is the localization length, so that in this limit,

$$\beta(g) \sim \ln g, \qquad (g \to 0)$$

By connecting up these two asymptotic limits, Abrahams et al were able to reason that the beta function for conductance would take the form shown in Fig. 11.6. In dimensions $d \leq 2$, the beta function is always negative, and the conductance always scales to zero. However in dimensions $d > 2$, there is a disorder-driven metal-insulator transition at the critical conductance $g = g_c$. As the amount of disorder is increased, when the short-distance conductance g passes below g_c, the material becomes an insulator in the thermodynamic limit. These heuristic arguments stimulated the development of a whole new field of research into the collective effects of disorder on conductors, and the basic results of the scaling theory of localization are well-established in metals where the effects of interactions between electrons are negligible. Interest in this field continues actively today, with the surprise discovery in the late 1990s that two dimensional electron gases formed within heterojunctions appear to exhibit a metal insulator transition - a result that confounds the one-parameter scaling theory, and is thought in some circles to result from electron-electron interaction effects.

11.6 Exercises for chapter 11

1. (Alternative derivation of the electrical conductivity.)

   In our treatment of the electrical transport, we derived the following expression for the conductivity.

   $$\sigma^{ab}(i\omega_n) = e^2\frac{T}{\nu_n}\sum_{\mathbf k, i\omega_r} v^a_{\mathbf k}v^b_{\mathbf k}\left[G(\mathbf k, i\omega_r + i\nu_n)G(\mathbf k, i\omega_r) - G(\mathbf k, i\omega_r)^2\right]$$

   This integral was carried out by first integrating over momentum, then integrating over frequency. This techique is hard to generalize and it is often more convenient to integrate the expression in the opposite order. This is the topic of this question.

   Consider the case where

   $$G(\mathbf k, i\omega_r) = \frac{1}{i\omega_r - \epsilon_{\mathbf k} - \Sigma(i\omega_r)}$$

   (a) By rewriting the momentum integral as an integral over kinetic energy ϵ and, angle show that the conductivity can be rewritten as $\sigma^{ab}(i\nu_n) = \delta^{ab}\sigma(i\nu_n)$, where

   $$\sigma(i\omega_n) = \frac{ne^2}{m}\frac{1}{\nu_n}\int_{-\infty}^{\infty}d\epsilon\, T\sum_{i\omega_r}\left[G(\epsilon, i\omega_r + i\nu_n)G(\epsilon, i\omega_r) - G(\epsilon, i\omega_r)^2\right].$$

   and

   $$G(\epsilon, z) \equiv \frac{1}{z - \epsilon - \Sigma(z)}$$

(b) Carry out the Matsubara sum in the above expression to obtain

$$\sigma(i\omega_n) = \frac{ne^2}{m}\frac{1}{\nu_n}\int_{-\infty}^{\infty}\frac{d\omega}{\pi}\int_{-\infty}^{\infty} d\epsilon f(\omega)\left[G(\epsilon,\omega+i\nu_n)+G(\epsilon,\omega-i\nu_n)\right]A(\epsilon,\omega),$$

where $A(\epsilon,\omega) = ImG(\epsilon,\omega-i\delta)$. (*Hint - replace* $T\sum_n \rightarrow -\int\frac{dz}{2\pi i}f(z)$, *and notice that while* $G(\epsilon,z)$ *has a branch cut along* $z=\omega$ *with discontinuity given by* $G(\epsilon,\omega-i\delta)-G(\epsilon,\omega+i\delta) = 2iA(\epsilon,\omega)$, *while while* $G(\epsilon,z+i\nu_n)$ *has a similar branch cut along* $z=\omega-i\nu_n$. *Wrap the contour around these branch cuts and evaluate the result*).

(c) Carry out the energy integral in the above expression to obtain

$$\begin{aligned}\sigma(i\omega_n) &= \frac{ne^2}{m}\frac{1}{\nu_n}\int_{-\infty}^{\infty}\frac{d\omega}{\pi}f(\omega)\\ &\times\left[\frac{1}{i\nu_n-(\Sigma(\omega+i\nu_n)-\Sigma(\omega-i\delta))}-\frac{1}{i\nu_n-(\Sigma(\omega+i\delta)-\Sigma(\omega-i\nu_n))}\right]\end{aligned} \qquad (11.47)$$

(d) Carry out the analytic continuation in the above expression to finally obtain

$$\begin{aligned}\sigma(\nu+i\delta) &= \frac{ne^2}{m}\int_{-\infty}^{\infty}d\omega\left[\frac{f(\omega-\nu/2)-f(\omega+\nu/2)}{\nu}\right]\times\\ &\frac{1}{-i\nu+i(\Sigma(\omega+\nu/2+i\delta)-\Sigma(\omega-\nu/2-i\delta))}.\end{aligned} \qquad (11.48)$$

(e) Show that your expression for the optical conductivity can be rewritten in the form

$$\sigma(\nu+i\delta) = \frac{ne^2}{m}\int_{-\infty}^{\infty}d\omega\left[\frac{f(\omega-\nu/2)-f(\omega+\nu/2)}{\nu}\right]\frac{1}{\tau^{-1}(\omega,\nu)-i\nu Z(\omega,\nu)}. \qquad (11.49)$$

where

$$\tau^{-1}(\omega,\nu) = \mathrm{Im}\left[\Sigma(\omega-nu/2-i\delta)+\Sigma(\omega+\nu/2-i\delta)\right] \qquad (11.50)$$

is the average of the scattering rate at frequencies $\omega \pm \nu/2$ and

$$Z^{-1}(\omega,\nu)-1 = -\frac{1}{\nu}\mathrm{Re}\left[\Sigma(\omega-\nu/2)-\Sigma(\omega+\nu/2)\right]$$

is a kind of "wavefunction renormalization".

(f) Show that if the ω dependence of Z and τ^{-1} can be neglected, one arrives at the phenomenological form

$$\sigma(\nu) = \frac{ne^2}{m}\left[\frac{1}{\tau^{-1}(\nu)-i\nu Z^{-1}(\nu)}\right]$$

This form is often used to analyze optical spectra.

(g) Show that the zero temperature conductivity is given by the thermal average

$$\sigma(\nu+i\delta) = \frac{ne^2\tau}{m} \qquad (11.51)$$

where $\tau^{-1} = 2Im\Sigma(0-i\delta)$.

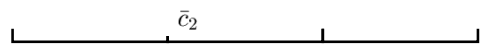
2. (a) Suppose $H = \epsilon c^\dagger c$ represents a single fermion state. Consider the approximation to the partition function obtained by dividing up the period $\tau \in [0,\beta]$ into N equal time-slices,

$$Z_N = \mathrm{Tr}[(e^{-\Delta\tau H})^N] \qquad (11.52)$$

where $\Delta\tau = \beta/N$. By using coherent states $|c\rangle = e^{\hat{c}^\dagger c}|0\rangle$, and approximating the matrix element from time τ_j to time τ_{j+1}, where $\tau_j = j\Delta\tau$ by

$$\langle\bar{c}_{j+1}|e^{-\Delta\tau H}|c_j\rangle = e^{\alpha\bar{c}_{j+1}c_j}+O(\Delta\tau^2) \qquad (11.53)$$

where $\alpha = (1-\Delta\tau\epsilon)$, (Fig. 1.)



(11.54)

show that Z_3 can be written as a "toy functional integral",

$$Z_3 = \int d\bar{c}_3 dc_3 d\bar{c}_2 dc_2 d\bar{c}_1 dc_1 \exp\left\{-(\bar{c}_3,\bar{c}_2,\bar{c}_1)\begin{bmatrix}1 & -\alpha & 0\\ 0 & 1 & -\alpha\\ \alpha & 0 & 1\end{bmatrix}\begin{pmatrix}c_3\\ c_2\\ c_1\end{pmatrix}\right\} \qquad (11.55)$$

(b) Evaluate Z_3.

(c) Generalize the result to N time slices and obtain an expression for Z_N. What is the limiting value of your result as $N \rightarrow \infty$?

3. Derive the completeness and trace formulae for a set of bosonic coherent states,

$$|\alpha\rangle = e^{b^\dagger\alpha}| \qquad (11.56)$$

You may assume the basic result

$$\delta_{nm} = \int\frac{d\bar{b}db}{2\pi i}e^{-\bar{b}b}b^n\bar{b}^m$$

In particular

(a) Show that the completeness relation is given by

$$\begin{aligned}\sum_{|b\rangle,\ |\bar{b}\rangle}|b\rangle\langle\bar{b}| &= 1\\ \sum_{|b\rangle,\ |\bar{b}\rangle} &= \int\frac{d\bar{b}db}{2\pi i}e^{-\bar{b}b}\end{aligned} \qquad (11.57)$$

(b) Show that the trace formula is given by

$$Tr[\hat{A}] = \sum_{|b\rangle,\ |\bar{b}\rangle}\langle\bar{b}|\hat{A}|b\rangle$$

(c) What is the key difference between the derivation of the Bosonic and the Fermionic path integrals?

Chapter 12

Path Integrals and Phase transitions

12.1 Introduction: Broken symmetry, coherent states and the path integral approach

In this chapter, we begin our effort to understand the concept of "Broken Symmetry". This concept represents one of the monumental achievements of the 20th century. In 1937, Landau[**?**] formulated the concept of broken symmetry- proposing that phase transitions take place via the process of symmetry reduction, which he described in terms of his order parameter concept. Landau introduced the idea of a an order parameter ψ, in terms of which the Free energy can be written

$$F[\psi] = -a(T_c - T)|\psi|^2 + b|\psi|^4$$

When the temperature T drops below $T = T_c$, the quadratic term in this function becomes negative, and the minimum of the Free energy moves from $\psi = 0$ to $\psi = \pm\sqrt{\rho}$, where $\rho = \psi|^2 = \frac{a}{2b}(T_c - T)$, thereby forming a state that breaks the $\psi \rightarrow -\psi$ invariance symmetry of F.

One can not understate the huge impact that order parameter and symmetry reduction concept, epitomized by Landau's almost trivial polynomial Free energy function, has had on physics today. The Landau Ginzburg generalization of this function, which includes gradient terms, provides the foundation to our understanding of phase transitions, superconductivity, the Meissner effect, and through it the so-called "Anderson Higg's" mechanism by which a gauge boson can acquire a mass as a result of symmetry breaking. This one concept explains at a stroke, the exclusion of magnetic fields from superconductors, and the weak force of radioactive β decay. Furthermore, the Landau concept provides the foundation for our understanding of criticality, and the concept of the renormalization group. It is only today, at the dawn of the 21st century that we are beginning to understand the important ways in which the Landau Ginzburg approach may break down.

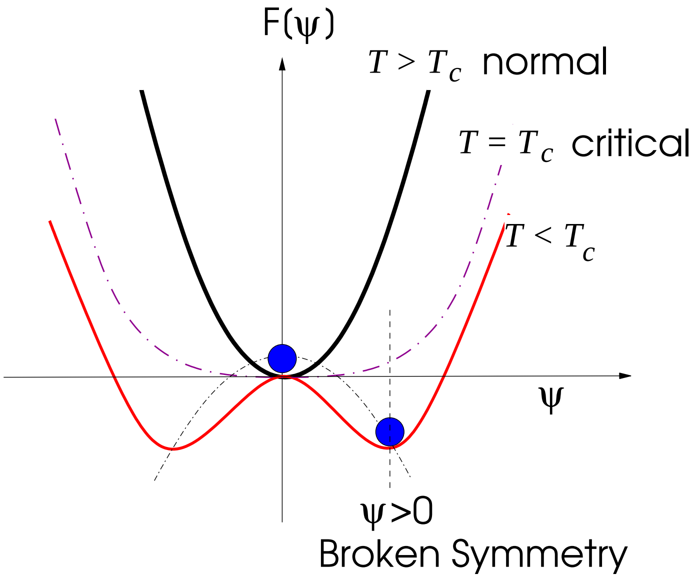


Figure 12.1: Illustrating the Landau free energy functional $F[\psi]$.

In this chapter, we should like to relate the order parameter concept to many body quantum physics. One of the key ideas that we will need here, is the concept of "off-diagonal long range order". This extension of Landau's broken symmetry idea was first developed by Onsager and Penrose in the early 1950's. They were interested in the microscopic nature of the order parameter in superfluid, which is really a Bose Einstein condensate in an interacting bosonic fluid. Penrose and Onsager proposed that a superfluid could be understood as a state of matter in which the two-particle density matrix

$$\rho(x,x') = \langle \psi^\dagger(x')\psi(x)\rangle$$

could be factorized as

$$\rho(x,x') = \psi^*(x')\psi(x) + \text{small terms}$$

where

$$\psi(x) = \sqrt{\rho)_s}e^{i\phi} = \langle N-1|\hat{\psi}(x)|N\rangle$$

is the order parameter of the superfluid. ρ_s is the superfluid density and ϕ the phase of the condensate. In this way, Onsager and Penrose were able to link Landau's phenomenological order parameter with a microscopic matrix element of the particle field. This concept of "off-diagonal long-range order" (ODLRO) was subsequently generalized to Fermi systems as part of the BCS theory of superconductivity, where the off-diagonal order parameter

$$F(x-x') = \langle N-2|\hat{\psi}_\downarrow(x)\hat{\psi}_\uparrow(x')|N\rangle$$

defines the wavefunction of the Cooper pair.

One of the remarkable spin-offs of superconductivity, was that it led to an understanding of how a gauge boson can acquire a mass as a result of symmetry breaking. This idea was first discussed by Anderson in 1959[14], and in more detail in 1964[**?**, **?**], but the concept evolved further and spread from Bell Laboratories to the particle physics community, ultimately re-appearing as the Higg's mechanism for spontaneous symmetry breaking in a Yang Mills theory. The Anderson-Higgs mechanism is a beautiful example of how the study of cryogenics led to a fundamentally new way of viewing the universe, providing a mechanism for the symmetry breaking between the electrical and weak forces in nature.

Another consequence of broken symmetry concept is the notion of "generalized rigidity"[**?**], a concept which has its origins in London's early model of superconductivity and the two-fluid models of superfluidity proposed independently by Tisza , according to which, if the phase of a boson or Cooper pair develops a rigidity, then it costs a phase bending energy

$$U(x) \sim \frac{1}{2}\rho_s(\nabla\phi(x))^2, \tag{12.1}$$

from which we derive that the "superflow" of particles is directly proportional to the amount of phase bending, or the gradient of the phase

$$j_{\rm S} = \rho_s \nabla\phi. \tag{12.2}$$

Anderson noted that we can generalize this concept to a wide variety of broken symmetries, each with their own type of superflow (see table 1). Thus broken translation symmetry leads to the superflow of momentum, or sheer stress, broken spin symmetry leads to the superflow of spin or spin superflow. There are undoubtedly new classes of broken symmetry yet to be discovered.

Table. 1. Order parameters, broken symmetry and rigidity.

Name	Broken Symmetry	Rigidity/Supercurrent
Crystal	Translation Symmetry	Momentum superflow (Sheer stress)
Superfluid	Gauge symmetry	Matter superflow
Superconductivity	E.M. Gauge symmetry	Charge superflow
Antiferromagnetism	Spin rotation symmetry	Spin superflow (x-y magnets only)
?	Time Translation Symmetry	Energy superflow ?

But to relate these various threads, we shall need some new tools. In particular, we shall need to introduce the concept of the "coherent state". Coherent states are simply eigenstates of the field operators. For example, the coherent state for a single boson is given by

$$|\alpha\rangle = e^{\hat{b}^\dagger \alpha}|0\rangle$$

We recall that since $[b, b^\dagger] = 1$, $[b, (b^\dagger)^n] = n(b^\dagger)^{n-1}$ and $[b, e^{\alpha b^\dagger}] = \alpha b e^{\alpha b^\dagger}$, it follows that

$$b|\alpha\rangle = \overbrace{e^{\alpha\hat{b}^\dagger} b|0\rangle}^{0} + \overbrace{[b, e^{\alpha\hat{b}^\dagger}]}^{\alpha e^{\alpha b^\dagger}}|0\rangle = \alpha|\alpha\rangle$$

is an eigenstate of the field operator. By taking $\alpha = \sqrt{N}e^{i\theta}$, where $N >> 1$ is the total number of particles in the condenstate, one arrives at the coherence state wavefunction for a "Bose-Einstein" or superfluid condensate in which

$$\langle b\rangle = \sqrt{N}e^{i\theta}$$

and N is the number of particles in the condensate. In a bosonic superfluid or Bose Einstein condensate,

$$b \equiv \frac{1}{\sqrt{V}}\int d^3x\psi(x)$$

is actually the zero momentum component of the field operator.

When we come to consider broken symmetry states involving fermions, the corresponding boson $\hat{b}$ is made up out of bilinears of fermions, for example the ground-sate of a Bardeen-Cooper-Schrieffer (BCS) wavefunction for a superconductor, for a Cooper pair, and

$$\hat{b}^\dagger \rightarrow \sum_{\mathbf{k}} \alpha_k c^\dagger{}_{k\uparrow} c^\dagger{}_{-k\downarrow}$$

becomes the creation operator for a Cooper pair, and the corresponding coherent state is written

$$|\alpha\rangle \quad = \quad e^{\sum_k \alpha_k c^\dagger{}_{k\uparrow} c^\dagger{}_{-k\downarrow}}|0\rangle. \tag{12.3}$$

We can expand this product

$$|\alpha\rangle = \prod_k \overbrace{e^{\alpha_k c^\dagger{}_{k\uparrow} c^\dagger{}_{-k\downarrow}}}^{(1+\alpha_k c^\dagger{}_{k\uparrow} c^\dagger{}_{-k\downarrow})}|0\rangle = \prod_k (1 + \alpha_k c^\dagger{}_{k\uparrow} c^\dagger{}_{-k\downarrow})|0\rangle \tag{12.4}$$

where the last step is made possible by Taylor expanding the exponential and noting that $(c^\dagger{}_{k\uparrow} c^\dagger{}_{-k\downarrow})^n = 0$ for $n > 1$. This last form for a coherent state is the famous BCS wavefunction, whose discovery led to a revolution in many body physics. To develop an understanding of these remarkable states of matter, we need to take a step back and develop the quantum physics of coherent states. This leads us naturally to the path integral formulation of many body physics.

There are two key ideas behind the path integration technique: (i) the Feynman concept of summing over quantum histories,

$$Z = \sum_{\text{path}} \exp\left[-S_{\text{path}}\right] \tag{12.5}$$

where S_{path} is the "action" associated with the particular configuration of fields and (ii) the concept of "coherent states", whereby one works with eigenstates of the microscopic quantum fields. We define

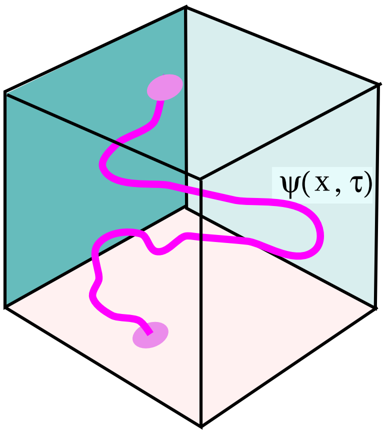
$$|\psi(x)\rangle = \exp\left[-\int d^3x \psi(x)\hat{\psi}^\dagger(x)\right]|0\rangle \tag{12.6}$$

to be the coherent state of the field ψ. This state is the eigenvector of the microscopic quantum field, in that

$$\hat{\psi}(x)|\psi\rangle = \psi(x)|\psi\rangle \tag{12.7}$$

where $\psi(x)$ is a "c-number", not an operator. We shall be able to do this for both bosons and fermions, by generalizing our concept of "c-numbers" to include anticommuting grassman numbers. Coherent states have several marvelous properties. In particular, we can immediately write down the matrix elements of the Hamiltonian in this basis, simply by replacing the field operators by their expectation values. More importantly, each set of functions $\psi(x,t)$ now defines a "history", or path over which the system evolves at each point in space. The action associated with each path is given simply by

$$S_{PATH} = \int_0^\beta d\tau \mathcal{L}[\bar{\psi}, \psi] \tag{12.8}$$



where

$$\mathcal{L}[\bar{\psi}, \psi] = \int d^3x[\bar{\psi}(x,\tau)\partial_\tau\psi(x,\tau)] + H[\bar{\psi}, \psi] \tag{12.9}$$

is the Lagrangian density, and H is the Hamiltonian, with field operators replaced by the c-numbers ψ, and their conjugates $\bar{\psi}$. It turns out that we can do the corresponding path integral for all non-interacting problems. This is already a major achievement. It is made still more powerful, by the fact that many broken symmetry problems can be transformed, by the method of "Hubbard Stratonovich", into a problem of "free" particles moving in a fluctuating effective field. This provides the formal back-bone for the study of broken symmetry phase transitions.

$$Z_{\text{interacting}} \longrightarrow \sum_{\{\Delta\}} \Big[\text{path integral of fermions moving in field } \Delta \Big] \tag{12.10}$$

where $\{\Delta\}$ denotes a given configuration of the symmetry breaking field Δ. In these notes I will show you how this works for the case of fermions. Fermions are more problematic than bosons, because the numbers $\psi(x)$ appearing in the coherent states must *anticommute* with each-other. They are thus a new kind of number, which requires some new algebraic tricks.

12.2 Coherent states and Grassman mathematics

To illustrate the basic approach, we shall consider the simpler problem, of a single fermionic field $\hat{c}^\dagger$. The coherent state for this field is

$$|c\rangle = e^{\hat{c}^\dagger c}|0\rangle$$

and its conjugate is given by

$$\langle \bar{c}| = \langle 0|e^{\bar{c}\hat{c}}$$

We use $\bar{c}$, rather than a dagger, because we shall need to consider c and $\bar{c}$ to be independent variables. Fermionic coherent states are a little tricky. On the one hand, the quantities c and $\bar{c}$ must behave as "c-numbers", in so far as they *commute* with all observables $\hat{O}$

$$c\hat{O} = \hat{O}c$$

On the other hand, in order that the numbers c and $\bar{c}$ correctly represent the anticommuting algebra of the original Fermi fields, they must anticommute amongst themselves, and with other Fermi operators, so that

$$\begin{aligned} c\bar{c} + \bar{c}c &= 0, && (12.11) \\ c\hat{\psi} + \hat{\psi}c &= 0, && (12.12) \end{aligned}$$

But c must also anticommute with itself, which means that

$$c^2 = \bar{c}^2 = 0,$$

But how can we possibly deal with numbers which when squared, give zero? At first sight this task might seem doomed to failure or triviality. Actually, this proves not to be the case, and the concept of anticommuting or "Grassman" numbers can be developed into a fully consistent calculus. Indeed, the leap to this new type of number is no worst than the jump from real, to complex numbers.

Table. 1. Grassman Calculus .

Algebra	$c_1c_2 = -c_2c_1$	anticommute with Fermions and other Grassman numbers
	$c\hat{b} = \hat{b}c, \quad c\hat{\psi} = -\hat{\psi}c$	commute with bosons, anticommute with Fermi operators.
Functions	$f[\bar{c}, c] = f_o + \bar{c}f_1 + \tilde{f}_1 c + f_{12}\bar{c}c$	Since $c^2 = 0$, truncate at linear order in each variable.
Calculus	$\partial f = -\tilde{f}_1 - f_{12}\bar{c}$	Differentiation
	$\bar{\partial} f = f_1 + f_{12}c$	
	$\int dc \equiv \partial_c$	$\int dc1 = \partial_c 1 = 0$
		$\int dcc = \partial_c c = 1$
Completeness	$\langle c\|c\rangle = e^{\bar{c}c}$	Over-complete basis.
	$\int d\bar{c}dce^{-\bar{c}c}\|c\rangle\langle\bar{c}\| = \underline{1}$	Completeness relation.
	$\mathrm{Tr}[\hat{A}] = -\int d\bar{c}dce^{\bar{c}c}\langle\bar{c}\|\hat{A}\|c\rangle$	Trace Formula.
Change of variable	$J\left(\frac{c_1 \ldots c_r}{\xi_1 \ldots \xi_r}\right) = \left\|\frac{\partial c_1 \ldots c_r}{\partial \xi_1 \ldots \xi_r}\right\|^{-1}$	Jacobian - inverse of Bosonic Jacobian.
Gaussian Integrals	$\int \prod_j d\bar{c}_j dc_j e^{-\left[\bar{c}\cdot A\cdot\bar{c} - \bar{j}\cdot c - \bar{c}\cdot j\right]} = \mathrm{detA} \times e^{\left[\bar{j}\cdot A^{-1}\cdot j\right]}$	

The main effect of the anticommuting properties of Grassmans is to drastically reduce the set of possible functions and the set of possible linear operations one can carry out on such functions. For example, the Taylor series expansion of Grassman functions has to truncate at first order in any particular variable. Thus a function of two variables, $f(\bar{c}, c)$

$$f[\bar{c}, c] = f_o + \bar{c}f_1 + \tilde{f}_1 c + f_{12}\bar{c}c$$

only has four terms! The coherent state (12.2) also truncates, so that

$$|c\rangle \;=\; |0\rangle + \hat{c}^\dagger c|0\rangle$$

$$= \quad |0\rangle + |1\rangle c \tag{12.13}$$

so that the overlap between the "n" fermion state ($n = 0, 1$) and the coherent state is given by

$$\langle n|c\rangle = c^n, \qquad (n = 0, 1)$$

To develop a path integral representation for fermions one needs to know how to carry out Grassman calculus. The key properties of Grassman algebra are summarized in table 1. A more detailed discussion of these properties is given in the appendix at the end of these notes.

12.2.1 Completeness and matrix elements

Coherent states are over-complete: you can see that

$$\langle\bar{c}|c\rangle = \langle 0|(1 + \bar{c}\hat{c})(1 + \hat{c}^\dagger c)|0\rangle = 1 + \bar{c}c = e^{\bar{c}c} \tag{12.14}$$

and we need to cancel out this term in the measure for summing over coherent states. If we start with the identity

$$\int d\bar{c}dc e^{-\bar{c}c} c^n \bar{c}^m = \delta_{nm}, \qquad (n, m = 0, 1)$$

we see that the overlap between the eigenstates $|n\rangle$ of definite particle number is given by

$$\begin{aligned} \langle n|m\rangle &= \int d\bar{c}dc e^{-\bar{c}c} \overbrace{c^n}^{\langle n|c\rangle} \overbrace{\bar{c}^m}^{\langle\bar{c}|m\rangle} \\ \delta_{nm} &= \int d\bar{c}dc e^{-\bar{c}c} \langle n|c\rangle\langle\bar{c}|m\rangle \end{aligned} \tag{12.15}$$

and since the basis $\{|n\rangle\} = \{|0\rangle, |1\rangle\}$ is complete, the only way this can hold true for all state $|n\rangle$, $|m\rangle$

$$\int d\bar{c}dc|c\rangle\langle\bar{c}|e^{-\bar{c}c} = |0\rangle\langle 0| + |1\rangle\langle 1| \equiv \underline{1} \tag{12.16}$$

is the identity. This is the completeness relation for coherent states. $|1\rangle = \hat{c}^\dagger|0\rangle$ is the state with one particle in it. The exponential may be loosely regarded as a normalizing factor which takes account of the over-completeness:

$$e^{-\bar{c}c}|c\rangle\langle\bar{c}| \sim \frac{|c\rangle\langle\bar{c}|}{\langle\bar{c}|c\rangle}.$$

We can regard the combination

$$\sum_{\bar{c},\ c} \equiv \int d\bar{c}dc|c\rangle\langle\bar{c}|e^{-\bar{c}c} \tag{12.17}$$

as the measure for fermionic coherent states, With this understanding, the completeness relation can be written simply as

$$\sum_{\bar{c},c} |c\rangle\langle\bar{c}| = \underline{1}$$

Matrix elements between coherent states are easy to evaluate. If an operator $A[\hat{c}^\dagger, \hat{c}]$ is *normal ordered*, then since the coherent states are eigenvectors of the quantum fields, it follows that

$$\langle\bar{c}|\hat{A}|c\rangle = \langle\bar{c}|c\rangle A[\bar{c}, c] = e^{\bar{c}c} A[\bar{c}, c], \tag{12.18}$$

i.e

$$\langle\bar{c}|\hat{A}|c\rangle = e^{\bar{c}c} \times \text{ c-number formed by replacing } (\hat{c}, \hat{c}^\dagger) \rightarrow (c, \bar{c}).$$

It is this wonderful feature that makes coherent states so very special, for at a swoop, we can convert normal-ordered operators into C-numbers.

The last result we need is the trace of A. We might guess that the appropriate expression is

$$Tr[\hat{A}] = \sum_{\bar{c},c} \langle\bar{c}|\hat{A}|c\rangle$$

actually - this is almost right, but infact, it turns out that the anticommuting properties of the Grassmann's force us to introduce a minus sign into this expression

$$Tr[\hat{A}] = \sum_{\bar{c},c} \langle-\bar{c}|\hat{A}|c\rangle = \int d\bar{c}dc e^{-\bar{c}c} \langle-\bar{c}|\hat{A}|c\rangle \tag{12.19}$$

which we shall shortly see, gives rise to the antisymmetric boundary conditions of fermionic fields. To prove the above result, write A in the basis of definite occupation,

$$\hat{A} = \sum_{n,m=0,1} |n\rangle A_{nm} \langle m|$$

and insert it into the above expression. This gives

$$\begin{aligned}
\int d\bar{c}dc e^{-\bar{c}c} \langle-\bar{c}|\hat{A}|c\rangle &= \sum_{n,m} \int d\bar{c}dc e^{-\bar{c}c} \langle-\bar{c}|n\rangle A_{nm} \langle m|c\rangle \\
&= \sum_{n,m} A_{nm} \int d\bar{c}dc e^{-\bar{c}c} (-\bar{c})^n c^m \\
&= \sum_{n,m} A_{nm} \overbrace{\int d\bar{c}dc e^{-\bar{c}c} c^m (\bar{c})^n}^{\delta_{mn}} \\
&= \sum_{n=0,1} A_{nn} = \text{Tr}[\hat{A}]
\end{aligned} \tag{12.20}$$

where the all-important minus sign is absorbed after the second line, when we anticommute c^m and $\bar{c}^n$. We shall make extensive use of the completeness and trace formulae (12.16) and (12.19) in developing the path integral. Both expressions are simply generalized to many fields c_j by making the appropriate change in the measure and by replacing $\bar{c}c$ in the exponent, by the dot product,

$$\begin{aligned} d\bar{c}dc &\equiv \prod_j d\bar{c}_j dc_j, \\ \bar{c}c &= \sum_j \bar{c}_j c_j. \end{aligned} \tag{12.21}$$

12.3 Path integral for the partition function

To begin with, we consider a single fermion, with Hamiltonian

$$H = \epsilon \hat{c}^\dagger \hat{c} \tag{12.22}$$

Using the trace formula (12.19), the partition function

$$Z = \mathrm{Tr} e^{-\beta H}$$

can be re-written in terms of coherent states as

$$Z = -\int d\bar{c}_N dc_1 e^{\bar{c}_N c_1} \langle \bar{c}_N | e^{-\beta H} | c_1 \rangle, \tag{12.23}$$

where the labeling anticipates the next step. Now we expand the exponential into a sequence of time-slices

$$e^{-\beta H} = \left(e^{-\Delta\tau H} \right)^N, \qquad \Delta\tau = \beta/N.$$

Between each time slice we introduce the completeness relation

$$\int d\bar{c}_j dc_{j+1} |c_{j+1}\rangle \langle \bar{c}_j | e^{-\bar{c}_j c_{j+1}} = 1$$

so that

$$Z = -\int d\bar{c}_N dc_1 e^{\bar{c}_N c_1} \prod_{j=1}^{N-1} d\bar{c}_j dc_{j+1} e^{-\bar{c}_j c_{j+1}} \prod_{j=1}^{N} \langle \bar{c}_j | e^{-H\Delta\tau} | c_j \rangle \tag{12.24}$$

where the first integral is associated with the trace and the subsequent integrals with the $N-1$ completeness relations. Now if we define

$$c_{N+1} = -c_1, \qquad \bar{c}_0 = -c_N \tag{12.25}$$

we are able to identify the $N+1$ st time slice with the 1st time slice and the 0 th time slice with the N the time-slice. In this way, the integral associated with the trace

$$\begin{aligned} -\int d\bar{c}_N dc_1 e^{\bar{c}_N c_1} \langle \bar{c}_N | \dots | c_1 \rangle &= \int d\bar{c}_N dc_{N+1} e^{-\bar{c}_N c_{N+1}} \langle \bar{c}_N | \dots | c_1 \rangle \\ &= \int d\bar{c}_0 dc_1 e^{-\bar{c}_0 c_1} \langle \bar{c}_N | \dots | c_1 \rangle \end{aligned} \tag{12.26}$$

can be absorbed into the other $N-1$ integrals, and furthermore, we notice that the fields entering into the discrete path integral are *antiperiodic*.

With this observation,

$$Z = -\int \prod_{j=1}^{N} d\bar{c}_j dc_{j+1} e^{-\bar{c}_j c_{j+1}} \prod_{j=1}^{N} \langle \bar{c}_j | e^{-H\Delta\tau} | c_j \rangle \tag{12.27}$$

Provided each time-slice is of sufficiently brief duration, we can replace $e^{-\Delta\tau H}$ by its normal ordered form, so that

$$\langle \bar{c}_j | e^{-H\Delta\tau} | c_j \rangle = e^{\bar{c}_j \bar{c}_j} e^{-H[\bar{c}_j c_j]\Delta\tau} + O(\Delta\tau^2),$$

where $H[\bar{c}, c] = \epsilon \bar{c} c$ is the normal-ordered Hamiltonian, with Grassman numbers replacing operators.

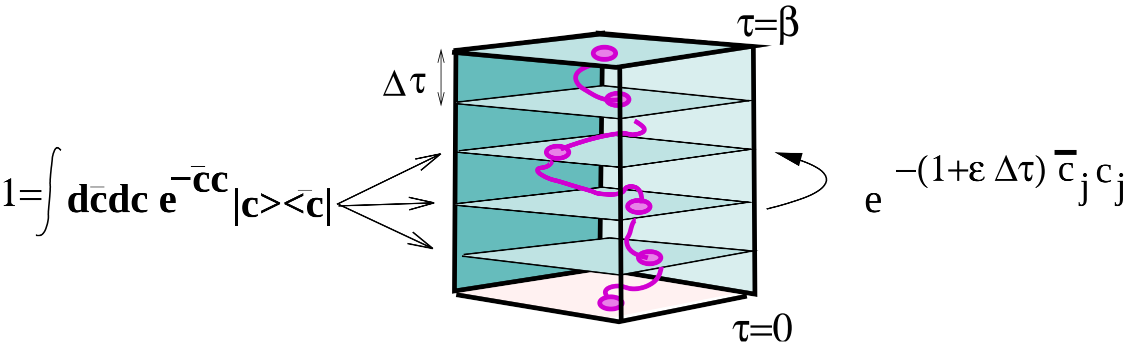


Fig. 2 Division of time evolution into "time-slices".

Combining (12.23) and (12.24) we can write

$$\begin{aligned} Z &= \mathrm{Lt}_{N\to\infty} Z_N \\ Z_N &= \int \prod_{j=1}^{N} d\bar{c}_j dc_j \exp\Big[-S\Big] \\ S &= \sum_{j=1}^{N} \Big[\bar{c}_j (c_{j+1} - c_j)/\Delta\tau + \epsilon \bar{c}_j, c_j\Big]\Delta\tau, \end{aligned} \tag{12.28}$$

Let us pause to reflect on what this means. This path integral represents a sum over all possible values "histories" of the fields:

$$c(\tau_j) \equiv \{c_1, c_2 \ldots c_N\}, \tag{12.29}$$

$$\bar{c}(\tau_j) \equiv \{\bar{c}_1, \bar{c}_2 \ldots \bar{c}_N\} \tag{12.30}$$

as illustrated in Fig. 2. This kind of integral is also called a "functional integral", because it involves integrating over all possible values of the functions $c(\tau)$ and $\bar{c}(\tau)$. When we take the thickness of the time slices to zero, the discrete functions $c(\tau)$ and $\bar{c}(\tau)$ become functions of continuous time. The boundary condition (12.25) implies that the set of complete functions which we sum over must satisfy anti-periodic boundary conditions

$$c(\tau+\beta) = -c(\tau), \qquad \bar{c}(\tau+\beta) = -\bar{c}(\tau)$$

In the continuum limit, $N \to \infty$, we now replace

$$\begin{aligned} \bar{c}_j(c_j - c_{j-1})/\Delta\tau &\rightarrow \bar{c}\partial_\tau c, \\ \sum_j \Delta\tau &\rightarrow \int_0^\beta d\tau. \end{aligned} \tag{12.31}$$

These cavalier replacements require some thought, for we are certainly not dealing with smooth functions - if such a notion is even valid for Grassman functions! The sense in which c_j becomes "close" to c_{j+1} needs to be carefully understood. Suppose we rewrite the antiperiodic c_j in terms of their frequency components as

$$c_j = \frac{1}{\sqrt{\beta}} \sum_{|n|\le N/2} c(i\omega_n) e^{-i\omega_n \tau_j},$$

then in this new basis,

$$\sum_j \bar{c}_j(c_{j+1} - c_j) = \sum_{|n|\le N/2} \bar{c}(i\omega_n) \left[\frac{e^{-i\omega_n \Delta\tau} - 1}{\Delta\tau}\right] c(i\omega_n)$$

In practice, the path-integral is dominated by functions c_j with a maximum characteristic temporal frequency $max(|\omega_n|) \sim \epsilon$, so that as $\Delta\tau \to 0$, we can replace

$$\left[\frac{e^{-i\omega_n \Delta\tau} - 1}{\Delta\tau}\right] \to -i\omega_n$$

which is the Fourier transform of ∂_τ.

With these provisos, the continuum limit of the action and path integral are then

$$\begin{aligned} S &= \int_0^\infty d\tau \Big[\bar{c}(\partial_\tau + \epsilon)c\Big], \\ Z &= \int \mathcal{D}[\bar{c}, c] \exp\Big[-S\Big] \end{aligned} \tag{12.32}$$

where we use the notation

$$\mathcal{D}[\bar{c}, c] = \prod_{\tau_l} d\bar{c}(\tau_l) dc(\tau_l)$$

At first sight, it might seem a horrendous task to carry out the integral over all possible functions $c(\tau)$. How can we possibly do this in a controlled fashion? The clue to this problem lies in the observation that the set of functions $c(\tau)$ (and its conjugate, $\bar{c}(\tau)$) are spanned by a *discrete* but complete set of anti-periodic functions, as follows

$$c(\tau) = \frac{1}{\sqrt{\beta}} \sum_n c_n e^{-i\omega_n \tau},$$

We can integrate over all possible functions $c(\tau)$ by integrating over all possible values of the coefficients c_n and since the transformation which links these two bases is unitary, the Jacobian which links the two bases is unity, i.e.

$$\mathcal{D}[\bar{c}, c] \equiv \prod_n d\bar{c}_n dc_n$$

It is much easier to visualize and work with a discrete basis. We can transform to this basis, by replacing $\partial_\tau \rightarrow -i\omega_n$ in the action, rewriting it as

$$S = \sum_n \bar{c}_n(-i\omega_n + \epsilon)c_n$$

Now the path integral is just a discrete Gaussian integral

$$Z = \int \prod_n d\bar{c}_n dc_n \exp\left[\sum_n \bar{c}_n(-i\omega_n + \epsilon)c_n\right] = \prod_n (-i\omega_n + \epsilon)$$

so that the Free energy is given by

$$F = -T\ln Z = -T \sum_n \ln(\epsilon - i\omega_n)e^{i\omega_n 0^+}$$

Here we have added a small convergence factor $e^{i\omega_n 0^+}$ because the time-evolution from $\tau = 0$ to $\tau = \beta$ is equivalent to time evolution from $\tau = 0$ to $\tau = 0^-$.

We can show that this reverts to the standard expression for one-particle free energy by replacing the Matsubara sum with a contour integral:

$$F = T \oint \frac{dz}{2\pi i} f(z) \ln[\epsilon_\lambda - z] e^{z0^+} \tag{12.33}$$

where the contour integral passes counter-clockwise around the poles of the Fermi function at $z = i\omega_n$, and the choice of $f(z)$ is dictated by the convergence factor. We take the logarithm to have a branch cut which extends from $z = \epsilon_\lambda$ to infinity. By deforming the integral around this branch cut we obtain

$$\begin{aligned} F &= -\int_\epsilon^\infty \frac{d\omega}{2\pi i} f(\omega) \Big[\ln(\epsilon - \omega - i\delta) - (\text{c.c.})\Big] \\ &= \int_\epsilon^\infty d\omega f(\omega) \\ &= -T\ln[1 + e^{-\beta\epsilon}] \end{aligned} \tag{12.34}$$

which is the well-known Free energy of a single fermion.

Of course, here we have used a sledge-hammer to crack a walnut, but the virtue of the method is the ease with which it can be generalized to much more complex problems. Three important points need to be made about this result:

- This result can easily be generalized to an arbitrary number of Fermi-fields. In this case,

$$S = \int_0^\infty d\tau \Big[\sum_\lambda \bar{c}_\lambda \partial_\tau c_\lambda + H[\bar{c}, c] \Big],$$

  and the measure for the path integral becomes

$$\mathcal{D}[\bar{c}, c] = \prod_{\tau_l, r} d\bar{c}_\lambda(\tau_l) dc_\lambda(\tau_l)$$

- The derivation did not depend on any details of H, and can thus be simply generalized to interacting Hamiltonians. In both cases, the conversion of the normal-order Hamiltonian occurs by simply replacing operators with the appropriate Grassman variables.

$$: H[c^\dagger, c] : \rightarrow H[\bar{c}, c]$$

- Because the Jacobian for a unitary transformation is unity, we can change basis inside the path integral. For example, if we start with the action for a gas of fermions

$$S = \int_0^\beta d\tau \sum_{\mathbf{k}} \bar{c}_{\mathbf{k}} (\partial_\tau + \epsilon_{\mathbf{k}}) c_{\mathbf{k}},$$

  where $\epsilon_{\mathbf{k}} = (k^2/2m) - \mu$, we can transform to a completely discrete basis by Fourier transforming in time,

$$\begin{aligned} c_{\mathbf{k}} &= \frac{1}{\sqrt{\beta}} \sum_n c_{\mathbf{k}n} e^{i\omega_n \tau}, \\ \partial_\tau &\rightarrow -i\omega_n \\ \mathcal{D}[\bar{c}, c] &\rightarrow \prod_{\mathbf{k}, n} d\bar{c}_{\mathbf{k}n} dc_{\mathbf{k}n}. \end{aligned} \tag{12.35}$$

  In the this discrete basis, the action becomes

$$S = \sum_{\mathbf{k}, n} (\epsilon_{\mathbf{k}} - i\omega_n) \bar{c}_{\mathbf{k}n} c_{\mathbf{k}n}$$

  This basis usually proves very useful for practical calculations. We can also transform to a continuum real-space basis, as follows

$$\begin{aligned} c_{\mathbf{k}} &= \frac{1}{\sqrt{V}} \int d^3x \psi(\mathbf{x}) e^{-i\mathbf{k}\cdot\mathbf{x}}, \\ \epsilon_{\mathbf{k}} &\rightarrow -\frac{\nabla^2}{2m} - \mu \\ \mathcal{D}[\bar{c}, c] &\rightarrow \mathcal{D}[\bar{\psi}, \psi]. \end{aligned} \tag{12.36}$$

In the new basis, the the action becomes

$$S = \int_0^\beta d\tau \int d^3x \bar{\psi}(\mathbf{x}) \Big[\partial_\tau - \frac{\nabla^2}{2m} - \mu\Big]\psi(\mathbf{x}).$$

As in the case of a single field, the discrete and continuous measures, (12.35) and (12.36) are equivalent

$$\prod_{\mathbf{k},n} d\bar{c}_{\mathbf{k}n} dc_{\mathbf{k}n} \equiv \mathcal{D}[\bar{\psi}, \psi].$$

because the space of continuous functions $\psi(x)$ is spanned by a complete, but discrete set of basis functions.

$$\psi(\mathbf{x}, \tau) = \frac{1}{\sqrt{\beta V}} \sum_{\mathbf{k},n} c_{\mathbf{k}n} e^{i(\mathbf{k}\cdot\mathbf{x} - \omega_n \tau)},$$

We can integrate over all possible functions $\psi(\mathbf{x}, \tau)$ by integrating over all values of the discrete vector $c_{\mathbf{k}n}$.

12.4 General evaluation of Path Integral for non-interacting Fermions

For non-interacting fermions the action only involves bilinears of the Fermi fields, so the path integral is of Gaussian form and can always be evaluated. To discuss the most general case, we shall include "source terms" in the original Hamiltonian, writing

$$H(\tau) = \sum_\lambda [\epsilon_\lambda c^\dagger{}_\lambda c_\lambda - \bar{j}_\lambda(\tau) c_\lambda - c^\dagger{}_\lambda j_\lambda(\tau)]$$

where $c^\dagger{}_\lambda$ creates a fermion in the eigenstate with energy ϵ_λ. With source terms, the partition function becomes a "generating functional"

$$Z[\bar{j}, j] = \mathrm{Tr}\Big[\mathrm{T}\exp\{-\int_0^\beta d\tau H(\tau)\}\Big].$$

Derivatives of the generating functional generate the irreducible Green's functions of the fermions, for instance,

$$\frac{\delta \ln Z[\bar{j}, j]}{\delta \bar{j}(1)} = \langle c(1) \rangle \quad (12.37)$$

$$\frac{\delta^2 \ln Z[\bar{j}, j]}{\delta \bar{j}(2) \delta j(1)} = \langle T[c(1) c^\dagger(2)] \rangle - \langle c(2) \rangle \langle c^\dagger(1) \rangle \quad (12.38)$$

where

$$\langle \ldots \rangle = \frac{1}{Z[\bar{j}, j]} \mathrm{Tr}\Big[\mathrm{T}\exp\{-\int_0^\beta d\tau H(\tau)\} \ldots\Big]$$

Transforming to a path integral representation, now

$$\begin{aligned} Z[\bar{j},j] &= \int \mathcal{D}[\bar{c},c]e^{-S} & (12.39)\\ S &= \int d\tau\Big[\bar{c}(\tau)(\partial_\tau+\underline{h})c(\tau)-\bar{j}(\tau)c(\tau)-\bar{c}(\tau)j(\tau)\Big] & (12.40)\end{aligned}$$

where $\underline{h}_{\alpha\beta}=\epsilon_\alpha\delta_{\alpha\beta}$ is the one-particle Hamiltonian. One can carry out functional derivatives on this integral without actually evaluating it. For example, we find that

$$\begin{aligned} \langle c(1)\rangle &= \frac{1}{Z[\bar{j},j]}\int \mathcal{D}[\bar{c},c]c(1)e^{-S} & (12.41)\\ \langle T[c(1)c^\dagger(2)]\rangle &= \frac{1}{Z[\bar{j},j]}\int \mathcal{D}[\bar{c},c]c(1)\bar{c}(2)e^{-S} & (12.42)\end{aligned}$$

Notice how the path integral automatically furnishes us with time-ordered expectation values.

Fortunately, the action has the Gaussian form derived above, with $A=\partial_\tau+\underline{h}$, so we can do the integral. Formally,

$$Z[\bar{j},j]=\det[\partial_\tau+\underline{h}]\exp\Big[-\int d\tau d\tau'\bar{j}(\tau)\underline{G}[\tau-\tau']j(\tau')\Big]$$

where

$$-(\partial_\tau+\underline{h})^{-1}=\underline{G}[\tau-\tau']$$

This result can be used as a basis for proving Wick's theorem. The Free energy is then given by

$$F=-T\ln Z=-T\ln\det[\partial_\tau+\underline{h}]=-T\mathrm{Tr}\ln[\partial_\tau+\underline{h}]=T\mathrm{Tr}\ln[-G^{-1}]$$

where we have used the result $\ln\det[A]=\mathrm{Tr}\ln[\partial_\tau+\underline{h}]$.

To explicitly compute the Free energy it is useful to transform to Fourier components,

$$\begin{aligned} c_\lambda(\tau) &= \frac{1}{\sqrt{\beta}}\sum_n c_{\lambda n}e^{-i\omega_n\tau},\\ j_\lambda(\tau) &= \frac{1}{\sqrt{\beta}}\sum_n j_{\lambda n}e^{-i\omega_n\tau}, & (12.43)\end{aligned}$$

In this basis,

$$\begin{aligned} (\partial_\tau+\epsilon_\lambda) &\longrightarrow (-i\omega_n+\epsilon_\lambda)\\ \underline{G}=-(\partial_\tau+\epsilon_\lambda)^{-1} &\longrightarrow (i\omega_n-\epsilon_\lambda)^{-1} & (12.44)\end{aligned}$$

so that

$$S=\sum_{\lambda,n}\Big[[-i\omega_n+\epsilon_\lambda]\bar{c}_{\lambda n}c_{\lambda n}-\bar{j}_{\lambda n}c_{\lambda n}-\bar{c}_{\lambda n}j_{\lambda n}\Big] \qquad (12.45)$$

whereupon,

$$\begin{aligned}\det[\partial_\tau + \underline{h}] = &= \prod_{\lambda,n}(-i\omega_n + \epsilon_\lambda)\\ Z[\bar{j}, j] &= \prod_{\lambda,n}(-i\omega_n + \epsilon_\lambda)\exp\Bigl[\sum_{\lambda,n}(-i\omega_n + \epsilon_\lambda)^{-1}\bar{j}_{\lambda n} j_{\lambda n}\Bigr] \qquad (12.46)\end{aligned}$$

If we set $j = 0$ in Z we obtain the Free energy in terms of the Fermionic Green function.

$$F = -T\sum_{\lambda,n}\ln[-i\omega_n + \epsilon_\lambda]$$

As in the case of a single field, by replacing the Matsubara sum with a contour integral we obtain

$$\begin{aligned}F &= T\sum_\lambda \oint \frac{dz}{2\pi i} f(z)\ln[\epsilon_\lambda - z] \qquad (12.47)\\ &= -T\sum_\lambda \ln[1 + e^{-\beta\epsilon_\lambda}] \qquad (12.48)\end{aligned}$$

If we differentiate Z with respect to its source terms, we obtain the Green's function:

$$-\frac{\delta^2 \ln Z}{\delta\bar{j}_{\lambda n}\delta j_{\lambda' n'}} = [\underline{G}]_{\lambda n, \lambda' n'} = \delta_{\lambda\lambda'}\delta_{nn'}\frac{1}{i\omega_n - \epsilon_\lambda}$$

12.5 Hubbard Stratonovich transformation

The "Hubbard Stratonovich" transformation maps certain classes of interacting fermion problem, onto non-interacting electrons moving through an effective field. Let us suppose that the interaction part of the Hamiltonian involves the product of two fermion bilinears, $H = H_o + H_I$, where

$$H_I = -g\int d^3x A^\dagger(x)A(x),$$

in the continuum, or on a lattice,

$$H_I = -g\sum_j A^\dagger{}_j A_j,$$

Examples of such bilinears might be the pair density

$$A(x) = \psi_\downarrow(x)\psi_\uparrow(x), \qquad A^\dagger(x) = \psi_\uparrow{}^\dagger(x)\psi^\dagger{}_\downarrow(x),$$

in a superconductor, or the spin-raising and lowering operators in a magnetism problem.

$$A(x) \equiv S^-(x) = \psi^\dagger{}_\downarrow(x)\psi_\uparrow(x), \qquad A^\dagger(x) \equiv S^+(x) = \psi^\dagger{}_\uparrow(x)\psi_\downarrow(x),$$

The Hubbard Stratonovich transformation replaces the combination $-gA(x)$ by an effective field $-gA(x) \rightarrow \Delta(x)$, in the following way

$$-gA^\dagger(x)A(x) \rightarrow A^\dagger(x)\Delta(x) + \bar{\Delta}(x)A(x) + \frac{\bar{\Delta}(x)\Delta(x)}{g}$$

A similar type of replacement occurs in the mean-field treatment of interactions, where Δ is taken to be a static field By elevating Δ to the status of a field, this transformation becomes *exact*. You may think of Δ as the exchange boson which mediates the original interaction.

Let us begin by reminding ourselves about Gaussian integrals. Suppose $\Delta = \Delta_1 - i\Delta_2$ and $\bar{\Delta} = \Delta_1 + i\Delta_2$ then since

$$\int d\Delta_1 d\Delta_2 e^{-(\Delta_1^2+\Delta_1^2)/g} = \pi g,$$

by writing $d\Delta d\bar{\Delta} = 2id\Delta_1 d\Delta_2$, we obtain

$$\int \frac{d\Delta d\bar{\Delta}}{2\pi i g} e^{-\bar{\Delta}\Delta/g} = 1. \tag{12.49}$$

Now suppose that $\Delta(x, \tau)$ is a function of space and time, defined on a grid in space time that can be made infinitely fine. We can naturally generalize (12.49) as follows

$$\int \mathcal{D}[\bar{\Delta}, \Delta] \exp\left[\int d^3x \int_0^\beta d\tau \frac{\bar{\Delta}(x)\Delta(x)}{g}\right] = 1, \tag{12.50}$$

where

$$\mathcal{D}[\bar{\Delta}, \Delta] \equiv \prod_{\tau,\mathbf{j}} \frac{d\bar{\Delta}(x_j, \tau) d\Delta(x_j, \tau)}{\mathcal{N}}$$

Here $\mathcal{N} = 2\pi i g/(\Delta x^3 \Delta\tau)$ is a normalization and we have taken the continuum limit, $(\delta x, \Delta\tau) \rightarrow 0$, replacing the discrete sum over the grid $\sum_{x_j,\tau_j} \bar{\Delta}(x_j)\Delta(x_j)$ by a continuous integral $\int d^3x \int_0^\beta d\tau \bar{\Delta}(x)\Delta(x)$.

Now consider the following path integral

$$Z = \int \mathcal{D}[\bar{c}, c] e^{-\int_0^\beta d\tau \left[\bar{c}(\partial_\tau + \underline{h})c + H_I\right]}$$

By introducing the unit identity (12.50) into the fermionic path integral, we obtain

$$Z = \int \mathcal{D}[\bar{c}, c] \int \mathcal{D}[\bar{\Delta}, \Delta] e^{-\int_0^\beta d\tau \left[\bar{c}(\partial_\tau + \underline{h})c + H'_I\right]} \tag{12.51}$$

where

$$H'_I = \int d^3x \left\{ \frac{\bar{\Delta}(x)\Delta(x)}{g} - g\bar{A}(x)A(x) \right\} \tag{12.52}$$

Now if we shift the Δ field as follows

$$\begin{array}{rcl} \Delta(x) & \rightarrow & \Delta(x) - gA(x), \\ \bar{\Delta}(x) & \rightarrow & \bar{\Delta}(x) - g\bar{A}(x), \end{array}$$

the measure is unchanged. Making this substitution in (12.52), we obtain

$$H_I' = \int d^3x \Big\{ \bar{A}(x)\Delta(x) + \bar{\Delta}(x)A(x) + \frac{\bar{\Delta}(x)\Delta(x)}{g} \Big\}. \tag{12.53}$$

In other words, we have absorbed the interaction, replacing it by an effective field which couples to the fermion bilinear A. If we now invert the order of integration inside the path integral (12.51), we now obtain

$$\begin{array}{rcl} Z & = & \int \mathcal{D}[\bar{\Delta}, \Delta] e^{-\int d^3 d\tau \frac{\bar{\Delta}(x)\Delta(x)}{g}} \int \mathcal{D}[\bar{c}, c] e^{-\tilde{S}} \\ \tilde{S} & = & \int_0^\beta d\tau \bar{c}\partial_\tau c + H_{eff}[\bar{\Delta}, \Delta] \end{array} \tag{12.54}$$

where

$$H_{eff}[\bar{\Delta}, \Delta] = H_o + \int d^3x \Big\{ \bar{A}(x)\Delta(x) + \bar{\Delta}(x)A(x) \Big\}$$

represents the action for electrons moving in the fluctuating field $\Delta(x)$. The weight function

$$e^{-\int d^3x d\tau \frac{\bar{\Delta}(x)\Delta(x)}{g}}$$

is a Gaussian distribution function for a white noise field with correlation function [1]

$$\langle \Delta(x)\Delta(x') \rangle = g\delta^{(4)}(x - x').$$

It is these white noise fluctuations that mediate the interaction between the fermions, much as an exchange boson mediates interactions in particle physics. More schematically,

$$Z = \sum_{\{\Delta\}} e^{-\int d^4x \frac{|\Delta|^2}{g}} [\text{ Path integral of fermions moving in field } \Delta \text{ }]$$

---

[1] To show this, it is helpful to consider the generating functional

$$\Lambda[\bar{j}, j] = \int \mathcal{D}[\bar{\Delta}, \Delta] \exp\Big[- \int d^3x \int_0^\beta d\tau \frac{\bar{\Delta}(x)\delta(x)}{g} - \bar{j}(x)\Delta(x) - \bar{\Delta}(x)j(x) \Big]$$

By changing variables, $\Delta(x) \rightarrow \Delta(x) + gj(x)$, we can absorb the terms linear in j, to obtain

$$\Lambda[\bar{j}, j] = \exp\Big[\int d^3x \int_0^\beta d\tau g\bar{j}(x)j(x) \Big]$$

Differentiating this with respect to $j(x)$, we find that

$$\left. \frac{\partial^2 \ln\Lambda[j, \bar{j}]}{\partial\bar{j}(x)\partial j(x')} \right|_{j,\bar{j}=0} = \langle \Delta(x\bar{\Delta}(x')) \rangle = gd^{(4)}(x - x')$$

where the summation represents a sum over all possible configurations $\{\Delta\}$ of the auxiliary field Δ. Of course, the coupling of the auxiliary field to the fermions modifies its distribution function. Since the fermionic action inside the path integral is actually Gaussian, we can formerly integrate out the fermions as follows

$$e^{-S_\psi[\bar{\Delta},\Delta]} = \int \mathcal{D}[\bar{c},c]e^{-\tilde{S}} = \det[\partial_\tau + \underline{h}_{eff}[\bar{\Delta},\Delta]] \tag{12.55}$$

where $\underline{h}_{eff}$ is the matrix representation of H_{eff}. The Full path integral may thus be written

$$Z = \int \mathcal{D}[\bar{\Delta},\Delta]e^{-S_{eff}[\bar{\Delta},\Delta]}$$

where

$$\begin{aligned} S_{eff}[\bar{\Delta},\Delta] &= \int d^3xd\tau\frac{\bar{\Delta}(x)\Delta(x)}{g} - \ln\det[\partial_\tau + \underline{h}_{eff}[\bar{\Delta},\Delta]] \\ &= \int d^3xd\tau\frac{\bar{\Delta}(x)\Delta(x)}{g} - \mathrm{Tr}\ln[\partial_\tau + \underline{h}_{eff}[\bar{\Delta},\Delta]] \end{aligned} \tag{12.56}$$

where we have made the replacement $\ln\det \rightarrow \mathrm{Tr}\det$. This quantity is called the "effective action" of the field Δ. The additional fermionic contribution to this action can profoundly change the distribution of the field Δ. For example, if S_{eff} develops a minima away around $\Delta = \Delta_o \neq 0$, the $\Delta = -A/g$ will acquire a "vacuum expectation value". This makes the Hubbard Stratonovich transformation an invaluable tool for studying the development of broken symmetry in interacting Fermi systems.

12.6 Superconductivity and BCS theory

12.6.1 Introduction: Superconductivity pre-history

As a specific illustration of the above approach, we shall now develop the BCS theory of superconductivity using the path integral method.

Before we start, a brief diversion about the history of superconductivity. Superconductivity - the phenomenon whereby the resistance of metal spontaneously drops to zero upon cooling below its critical temperature, was discovered by Kamerlingh Onnes in 1906. However, it took more than 50 years to fully develop the conceptual framework required to understand this collective phenomenon. During this time, many great physicists, including Bohr, Pauli and Feynman tried, yet failed to develop a microscopic theory of the phenomenon.

Some highlights in the development of the theory of superconductivity were

- Discovery of the Meissner effect in 1933 by Meissner and Ochsenfeld. When a superconductor is cooled in a small magnetic field, the flux is spontaneously excluded as it becomes superconducting. The Meissner effect demonstrates that a superconductor is, in essence a perfect diamagnet.

- London's observation in 1937, that perfect diamagnetism develops if the wavefunction develops a rigidity which prevents the paramagnetic component of the current evolving to screen out the diamagnetic current. (See earlier discussions) Using this reasoning, London deduced the famous relationship

$$\vec{j} = -\frac{n_s e^2}{m}\vec{A}, \qquad (\vec{\nabla} \cdot A = 0).$$

- Development of the Landau Ginzburg theory in 1951. Landau and Ginzburg extended the Landau theory of phase transitions, proposing that superconductivity involves a complex order parameter $\Psi(x)$. Using arguments of gauge invariance, LG reasoned that the Free energy must contain a gradient term of the form

$$f = \int d^3x \frac{1}{2m^*}|(-i\hbar\vec{\nabla} - e^*\vec{A})\psi(x)|^2$$

  Although we now know that $e^* = 2e$, in the original version of the theory, Landau erroneously convinced Ginzburg that he had an argument based on gauge invariance, that proves $e^* = e$. The vitally important aspect of this free energy function is that once $\psi \neq 0$, the electromagnetic field develops a mass giving rise to a super-current

$$\vec{j} = -\frac{\delta f}{\delta\vec{A}(x)} = -\frac{(e^*)^2}{m^*}|\psi|^2\vec{A}(x)$$

The BCS Hamiltonian is one of the earliest examples of "model Hamiltonians". By the early fifties, the observation of the isotope effect by Bernie Serin at Rutgers University, had lead to the realization that the mechanism of superconductivity in conventional metals was driven by the electron phonon interaction. Frohlich had proposed his Hamiltonian for the electron phonon interaction, and had discovered that these interactions can give rise to sliding charge density waves. Frohlich's theoretical prediction of charge density waves was twenty five years ahead of its time, but it also misled him into thinking that charge density waves could provide the explanation of the Meissner effect. Frohlich's error was to neglect the effect of pining, which in any disordered materials, prevents incommensurate charge density waves from sliding freely.

In the early fifties, Bardeen and Pine's recognized that to make progress with the theory of superconductivity, it would be necessary to simplify the Hamiltonian by carrying out a canonical transformation that eliminates the phonon degrees of freedom, giving rise to an effective electron-electron interaction. The Bardeen Pine Hamiltonian is the immediate predecessor of the BCS model

12.6.2 The BCS Hamiltonian

We start with the BCS Hamiltonian

$$H = \sum_{\mathbf{k}\sigma} \epsilon_{\mathbf{k}\sigma} c^\dagger{}_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} - \frac{g_0}{V} A^\dagger A$$

where

$$A = \sum_{\mathbf{k},|\epsilon_{\mathbf{k}}|<\omega_D} c_{-\mathbf{k}\downarrow} c_{\mathbf{k}\uparrow}, \qquad A^\dagger = \sum_{\mathbf{k}} c^\dagger{}_{\mathbf{k}\uparrow} c^\dagger{}_{-\mathbf{k}\downarrow},$$

are the operators that annihilate or create a uniform pair density. Note how the interaction between electrons is limited to within an energy ω_D of the Fermi energy. This "simplified" pairing Hamiltonian is the one originally used by BCS. Notice how the interaction

$$H_I = -\frac{g_0}{V} \sum_{\mathbf{k},\mathbf{k}'} c^\dagger{}_{\mathbf{k}\uparrow} c^\dagger{}_{-\mathbf{k}\downarrow} c_{-\mathbf{k}'\downarrow} c_{\mathbf{k}'\uparrow},$$

involves pairs of infinite spatial extent (all momenta summed over). This feature enhances the mean-field properties of the model to the point where mean-field theory actually gives the exact solution.

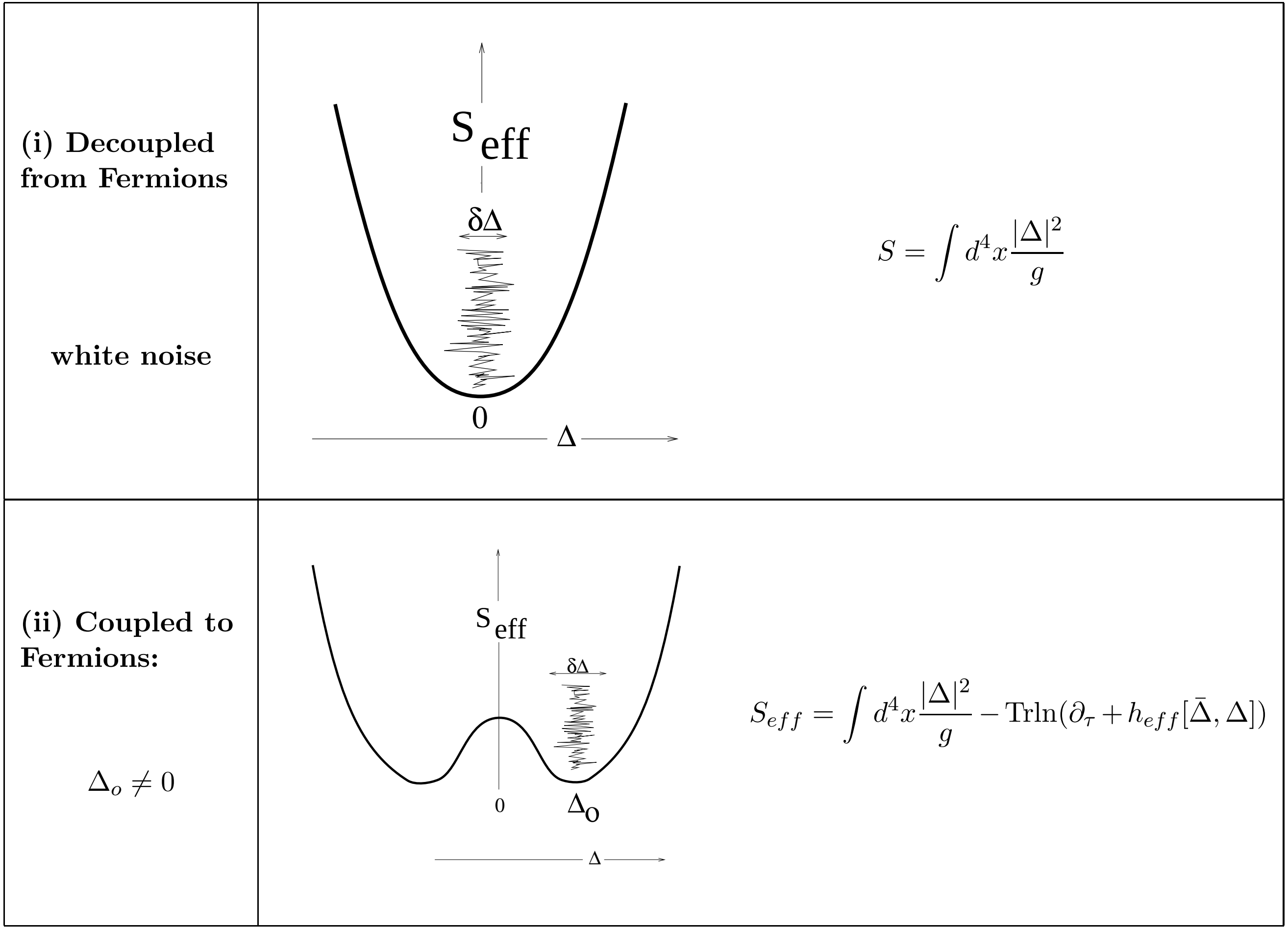


Fig. 3 Effective action for auxilliary field.

The volume normalizing factor $1/V$ is required so that this term grows linearly, rather than quadratically with volume V. We shall redefine $g = g_0/V$ to simplify our maniupations, re-instating the volume at the end of the calculation.

The appearance of just one A and $A^\dagger$ in the Hamiltonian makes it particularly easy to apply the methods introduced in the last section. We begin by writing the problem as a path integral

$$Z = \int \mathcal{D}[\bar{c}, c] e^{-S}$$

where

$$S = \int_0^\beta \sum_{\mathbf{k}\sigma} \bar{c}_{\mathbf{k}\sigma}(\partial_\tau + \epsilon_{\mathbf{k}}) c_{\mathbf{k}\sigma} - g\bar{A}A$$

Next we introduce the identity

$$\int \mathcal{D}[\bar{\Delta}, \Delta] \exp\left[\frac{1}{g}\int_0^\beta d\tau \bar{\Delta}(\tau)\Delta(\tau)\right] = 1 \qquad (12.57)$$

into the path integral. By shifting the variables $\Delta \to \Delta - gA$, $\bar{\Delta} \to \bar{\Delta} - g\bar{A}$, we obtain

$$\begin{aligned} Z &= \int \mathcal{D}[\bar{\Delta}, \Delta, \bar{c}, c] e^{-S} \\ S &= \int_0^\beta d\tau \left\{ \sum_{\mathbf{k}\sigma} \bar{c}_{\mathbf{k}\sigma}(\partial_\tau + \epsilon_{\mathbf{k}}) c_{\mathbf{k}\sigma} + \Delta A + \bar{A}\Delta + \frac{1}{g}\bar{\Delta}\Delta \right\} \end{aligned} \qquad (12.58)$$

where $\Delta(\tau)$ is a function of time only. In a Nambu notation, this can be re-written

$$S = \int_0^\beta d\tau \left\{ \sum_{\mathbf{k}} \bar{\psi}_{\mathbf{k}}(\partial_\tau + \underline{h}_{\mathbf{k}})\psi_{\mathbf{k}} + \frac{1}{g}\bar{\Delta}\Delta \right\}$$

where

$$\psi_{\mathbf{k}} = \begin{pmatrix} c_{\mathbf{k}\uparrow} \\ \bar{c}_{-\mathbf{k}.\downarrow} \end{pmatrix}$$

defines the Nambu spinor and

$$\underline{h}_{\mathbf{k}} = \begin{bmatrix} \epsilon_{\mathbf{k}} & \Delta(\tau) \\ \bar{\Delta}(\tau) & -\epsilon_{\mathbf{k}} \end{bmatrix} = \epsilon\tau_3 + \Delta_1\tau_1 + \Delta_2\tau_2$$

is the matrix Hamiltonian. If we now "integrate out" the Fermions, we obtain

$$e^{-S_{eff}[\bar{\Delta},\Delta]} = \prod_{\mathbf{k}} \det[\partial_\tau + \underline{h}_{\mathbf{k}}(\tau)] e^{-\int_0^\beta d\tau \frac{\bar{\Delta}\Delta}{g}}$$

for the effective action, where we have separated the fermionic determinant into a product over each decoupled momentum. Thus

$$S_{eff}[\bar{\Delta}, \Delta] = \int_0^\beta d\tau \frac{\bar{\Delta}\Delta}{g} + \sum_{\mathbf{k}} \mathrm{Trln}(\partial_\tau + \underline{h}_{\mathbf{k}}).$$

where we have replaced lndet → Trln. Except for certain uniform, or almost uniform configurations of Δ, we can not calculate S_{eff} explicitly. It turns out however, that these configurations dominate the path integral in the limit $V \to \infty$. To see this consider the path integral

$$Z = \int \mathcal{D}[\bar{\Delta}, \Delta] e^{-S_{eff}[\bar{\Delta},\Delta]}$$

The effective action is actually extensive in the volume, V, so that as $V \to \infty$, S/V is a constant. This means that when we find the configuration of $\Delta = \Delta_o$ which minimizes S_{eff}, the cost of fluctuations $\delta\Delta$ around this configuration will also be of order $O(V)$, i.e. the amplitude for a small fluctuation is given by

$$e^{-S} = e^{-S_o + O(V)\times|\delta\Delta|^2}$$

The appearance of V in the coefficient of this Gaussian distribution implies the variance of small fluctuations around the minimum will be of order O(1/V), so that to a good approximation,

$$Z = e^{-S_{eff}[\bar{\Delta}_o,\Delta_o] + O(1)}$$

This is why the mean-field approximation to the path integral is essentially exact for the BCS model.

Since the original problem is translationally invariant, we expect the configurations that minimize the action to also be uniform. The mean-field approximation to the path integral is made by replacing the integral over the Δ field by its uniform "saddle-point" value, obtained by replacing $\Delta(\tau)$ with a uniform field $\Delta(\tau) = \Delta_1 - i\Delta_2$. In this case, we can use momentum and frequency eigenstates for the Nambu fields

$$\psi_{\mathbf{k}}(\tau) = \frac{1}{\sqrt{\beta}} \sum_n \psi_{\mathbf{k}n} e^{-i\omega_n \tau}$$

In this basis,

$$\partial_\tau + h \to [-i\omega_n + \underline{h}_{\mathbf{k}}]$$

so that the determinant

$$\det[\partial_\tau + \underline{h}_{\mathbf{k}}] = \prod_n \det[-i\omega_n + \underline{h}_{\mathbf{k}}] = \prod_n [\omega_n^2 + \epsilon_{\mathbf{k}}^2 + |\Delta|^2]$$

and the effective action for a uniform field is

$$F_{eff} = \frac{S_{eff}}{\beta} = -T \sum_{\mathbf{k}\mathbf{n}} \ln[\omega_n^2 + \epsilon_{\mathbf{k}}^2 + |\Delta|^2] + \frac{|\Delta|^2}{g}$$

We see that this is nothing more than the mean-field free-energy for the BCS model. Minimizing F_{eff} w.r.t Δ gives us the gap equations

$$\frac{\partial F_{eff}}{\partial \bar{\Delta}} = -\sum_{\mathbf{k}n} \frac{\Delta}{\omega_n^2 + E_{\mathbf{k}}^2} + V\frac{\Delta}{g_0} = 0 \qquad (12.59)$$

$$\Rightarrow \frac{1}{g_0} = \frac{1}{\beta V} \sum_{\mathbf{k}n} \frac{1}{\omega_n^2 + E_{\mathbf{k}}^2} \qquad (12.60)$$

where

$$E_{\mathbf{k}} = \sqrt{\epsilon_{\mathbf{k}}^2 + |\Delta|^2}$$

is the quasiparticle energy and we have re-instated $g_0 = g/V$.

We could have carried out the Matsubara sum at any stage in the above manipulation. Using the contour integration method,

$$F_{eff} = -\sum_{\mathbf{k}} \oint \frac{dz}{2\pi i} f(z) \ln[E_{\mathbf{k}}^2 - z^2] + V\frac{|\Delta|^2}{g_0}$$

where the integral runs anti-clockwise around the poles of the Fermi function. The logarithm inside the integral has a branch cut running from $z = -E_{\mathbf{k}}$to $z = +E_{\mathbf{k}}$, where the imaginary part of the logarithm changes by 2π. Distorting the contour integral around this branch cut, we obtain

$$\int \frac{dx}{2\pi i} f(x)\{\ln[E_{\mathbf{k}}^2 - (x+i\delta)^2] - \ln[E_{\mathbf{k}}^2 - (x-i\delta)^2]\} = -\int_{-E_{\mathbf{k}}}^{E_{\mathbf{k}}} dx f(x) = -2T\ln\left[2\cosh(\beta E_{\mathbf{k}}/2)\right] \quad (12.61)$$

The Free energy then becomes

$$F_{eff} = -2TV \int \frac{d^3k}{(2\pi)^3} \ln\left[2\cosh(\beta E_{\mathbf{k}}/2)\right] + V\frac{|\Delta|^2}{g_0}.$$

Differentiating w.r.t. $\bar{\Delta}$ then gives

$$\begin{aligned} \frac{1}{g_0} &= \int_{|\epsilon_{\mathbf{k}}|<\omega_D} \frac{d^3k}{(2\pi)^3}\left[\frac{\tanh(\beta E_{\mathbf{k}}/2)}{2E_{\mathbf{k}}}\right] \\ &= N(0)\int_0^{\omega_D} d\epsilon \left[\frac{\tanh(\beta\sqrt{\epsilon^2+\Delta^2}/2)}{\sqrt{\epsilon^2+\Delta^2}}\right] \end{aligned}$$

Note that in a real superconductor, the attractive interaction, derived from phonons, is restricted to a narrow momentum shell near the Fermi surface. This means that the momentum sums appearing in the original model need to be restricted to within an shell around the Fermi surface where $|\epsilon_{\mathbf{k}}| < \omega_D$, where ω_D is the Debye energy.

12.6.3 Computing Tc carefully

T=0

$$1 = gN(0)\int_0^{\omega_D} \frac{d\epsilon}{\sqrt{\epsilon^2+\Delta^2}} = gN(0)\left[\sinh^{-1}\left(\frac{\omega_D}{\Delta}\right)\right] = gN(0)\ln\left(\frac{\omega_D}{\Delta}\right)$$

so

$$\boxed{2\Delta = \omega_D e^{-\frac{1}{gN(0)}}}$$

12.6.4 The Nambu Greens function

12.6.5 The structure of the Boguilubov quasiparticle and the BCS wavefunction

12.6.6 Twisting the phase: the Anderson Higg's mechanism

A Appendix: Grassman Calculus

A.1 Differentiation and Integration

Differentiation is defined to have the normal linear properties of the differential operator. We define

$$\partial \equiv \frac{\partial}{\partial c}, \quad \bar{\partial} \equiv \frac{\partial}{\partial \bar{c}} \tag{12.62}$$

so that

$$\partial c = \bar{\partial}\bar{c} = 1, \tag{12.63}$$

and thus if $f(\bar{c}, c)$ is defined as above, then

$$\begin{array}{rcl} \partial f & = & \tilde{f}_1 - f_{12}\bar{c} \\ \bar{\partial} f & = & f_1 + f_{12}c \end{array} \tag{12.64}$$

where the minus sign in the first expression occurs because the $\bar{\partial}$ operator must anticommute with c. But how do we define integration? This proves to be much easier for Grassman variables, than for regular c-numbers. The great sparseness of the space of functions dramatically restricts the number of linear operations we can apply to functions, forcing differentiation and integration to become the *same* operation :

$$\int dc \equiv \partial, \qquad \int d\bar{c} \equiv \bar{\partial} \tag{12.65}$$

In other words,

$$\int d\bar{c}\bar{c} = 1, \qquad \int dcc = 1, \qquad \int d\bar{c} = \int dc = 0$$

A.2 Change of variable

Suppose we change variables, writing

$$\begin{pmatrix} c \\ \bar{c} \end{pmatrix} = A \begin{pmatrix} \xi \\ \bar{\xi} \end{pmatrix}$$

where A is c-number matrix. If we make this substitution in the polynomial f, we form a new polynomial

$$g(\xi, \bar{\xi}) = f(c, \bar{c}).$$

Equating each term in the function, we have

$$f_{12}c\bar{c} = g_{12}\xi\bar{\xi} = (f_{12}detA)\xi\bar{\xi}.$$

Now we would like to know the Jacobian for this transformation, which is defined so that

$$d\bar{c}dc = J\left(\frac{\bar{c}, c}{\bar{\xi}, \xi}\right) d\bar{\xi}d\xi$$

Now

$$\int d\bar{c}dcf(c,\bar{c}) = f_{12} = g_{12}(detA)^{-1}, \qquad \int d\bar{\xi}d\xi g(\xi,\bar{\xi}) = g_{12}$$

For a linear transformation the Jacobian should be just a number, so by comparing the above, we see that

$$J\left(\frac{\bar{c}, c}{\bar{\xi}, \xi}\right) = (detA)^{-1}$$

This result can be easily generalized to a large number of variables, so that

$$J\left(\frac{c_1 \ldots c_r}{\xi_1 \ldots \xi_r}\right) = \left|\frac{\partial c_1 \ldots c_r}{\partial \xi_1 \ldots \xi_r}\right|^{-1}$$

which is precisely the inverse of the bosonic Jacobian. This has important implications for super-symmetric field theories, where the Jacobian of the bosons and fermions precisely cancels. For our purposes however, the most important point, is that for a Unitary transformation, the Jacobian is unity.

A.3 Gaussian Integrals

The basic Gaussian integral is simply

$$\int d\bar{c}dce^{-a\bar{c}c} = \int d\bar{c}dc(1 - a\bar{c}c) = a$$

If now we introduce a set of N variables, then

$$\int \prod_j d\bar{c}_j dc_j \exp -[\sum_j a_j \bar{c}_j c_j] = \prod_j a_j$$

Suppose now, we carry out a unitary transformation, for which the Jacobian is unity, then since

$$c = U\xi, \qquad \bar{c} = \bar{\xi}U^\dagger,$$

the integral then becomes

$$\int \prod_j d\bar{\xi}_j d\xi_j \exp[-\bar{\xi} \cdot A \cdot \xi] = \prod_j a_j$$

where $A_{ij} = \sum_l U^\dagger{}_{il} a_l U_{lj}$ is the matrix with eigenvalues a_l. It follows that

$$\int \prod_j d\bar{\xi}_j d\xi_j \exp[-\bar{\xi} \cdot A \cdot \xi] = \mathrm{det} A$$

Finally, by shifting the variables $\xi \rightarrow \xi - A^{-1} j$, where j is an arbitrary vector, we find that

$$Z[j] = \int \prod_j d\bar{\xi}_j d\xi_j \exp[-\bar{\xi} \cdot A \cdot \xi + \bar{j} \cdot \xi + \bar{\xi} \cdot j] = \mathrm{det} A \exp[\bar{j} \cdot A^{-1} \cdot j]$$

This is the basic Gaussian integral for Grassman variables. Notice that using the result $\mathrm{lndet}[A] = \mathrm{Trln}[A]$, it is possible to take the logarithm of both sides to obtain

$$S[j] = -\mathrm{ln} Z[j] = -\mathrm{Trln}[A] - \bar{j} \cdot A^{-1} \cdot j.$$

The main use of this integral, is for evaluating the Path integral for free field theories. In this case, the matrix $A \rightarrow -G^{-1}$ becomes the inverse propagator for the fermions, and $\xi_n \rightarrow \psi(i\omega_n)$ is the Fourier component of the Fermi field at Matsubara frequency $i\omega_n$.

Exercises

1. Repeat the calculation of section 3. without taking the continuum limit. Show that the path integral for a single fermion with a large, but finite number of time slices is given by
$$Z_N = \prod_{-N/2 \leq n < N/2} (\epsilon - i\omega_n J_o(\omega_n \Delta\tau/2))$$
where $J_o(x) = sinx/x$, so that in the limit $\Delta\tau \to 0$, the partition function reverts to the form obtained from the continuum action.

2. Using path integrals, calculate the partition function for an electron in a magnetic field, with the action
$$S = \int d\tau \bar{f}_\alpha \Big(\delta_{\alpha\beta}\partial_\tau + \vec{\sigma}_{\alpha\beta} \cdot \vec{B} \Big) f_\beta$$
Why is your answer not the same as the partition function of a spin 1/2 in a magnetic field?

3. Suppose
$$\mathcal{M} = e^{\frac{1}{2}\sum_{i,j} A_{ij} c^\dagger{}_i c^\dagger{}_j}$$
where A_{ij} is an $N \times N$ antisymmetric matrix, and the $c^\dagger{}_j$ are a set of N canonical Fermi creation operators. Using coherent states, calculate
$$\mathrm{Tr}[\mathcal{M}\mathcal{M}^\dagger]$$
where the trace is over the 2^N dimensional Hilbert space of fermions. (Hint: notice that $\mathcal{M}\mathcal{M}^\dagger$ is already normal ordered, so that by using the trace formula, you can rewrite this in terms of a simple Grassman integral.)

4. Calculate, to Gaussian order, the change in the BCS effective action for a fluctuation in the gap function of the following form
$$\Delta(\tau) = \Delta_0 + \frac{1}{\sqrt{\beta}} \sum_n \delta\Delta_n e^{-i\nu_n\tau}$$
where $\nu_n = 2\pi T n$ is the Bose Matsubara frequency and Δ_0 is a value of Δ which minimizes the effective action. Use your result to confirm that the BCS Free energy per unit volume is accurate to $O(1/V)$, where V is the volume.

5. Re-derive table 1. for the case of bosonic coherent states.
$$|b\rangle = e^{b\hat{b}^\dagger}|0\rangle$$
where the Grassman variable is now replaced by a conventional c-number b.

B Exercises for chapter 12

1. (a) Suppose $H = \epsilon c^\dagger c$ represents a single fermion state. Consider the approximation to the partition function obtained by dividing up the period $\tau \in [0, \beta]$ into N equal time-slices,

$$Z_N = \mathrm{Tr}[(e^{-\Delta\tau H})^N] \tag{12.66}$$

where $\Delta\tau = \beta/N$. By using coherent states $|c\rangle = e^{\hat{c}^\dagger c}|0\rangle$, and approximating the matrix element from time τ_j to time τ_{j+1}, where $\tau_j = j\Delta\tau$ by

$$\langle \bar{c}_{j+1}| e^{-\Delta\tau H} |c_j\rangle = e^{\alpha \bar{c}_{j+1} c_j} + O(\Delta\tau^2) \tag{12.67}$$

where $\alpha = (1 - \Delta\tau\epsilon)$, (Fig. 1.)

(12.68)

show that Z_3 can be written as a "toy functional integral",

$$Z_3 = \int d\bar{c}_3 dc_3 d\bar{c}_2 dc_2 d\bar{c}_1 dc_1 \exp\left\{ -(\bar{c}_3, \bar{c}_2, \bar{c}_1) \begin{bmatrix} 1 & -\alpha & 0 \\ 0 & 1 & -\alpha \\ \alpha & 0 & 1 \end{bmatrix} \begin{pmatrix} c_3 \\ c_2 \\ c_1 \end{pmatrix} \right\} \tag{12.69}$$

(b) Evaluate Z_3.

(c) Generalize the result to N time slices and obtain an expression for Z_N. What is the limiting value of your result as $N \to \infty$?

2. The one dimensional electron gas is prone to the development of charge-density wave instabilities. The treatment of these instabilities bears close resemblance to the BCS theory of superconductivity. Suppose we have a one-dimensional conductor, described by the Hamiltonian

$$\begin{aligned} H - \mu N &= H_o + H_I, \\ H_o &= -t \sum_{j,\ \sigma} \left(\psi^\dagger{}_{j+1\ \sigma} \psi_{j\ \sigma} + \psi^\dagger{}_{j\ \sigma} \psi_{j+1\ \sigma} \right), \\ H_I &= -g \sum_j n_{j\uparrow} n_{j\downarrow} \end{aligned} \tag{12.70}$$

where $g > 0$ and $\psi^\dagger{}_{j\sigma}$ creates an electron with spin $\sigma = \pm\frac{1}{2}$ at site j. The separation between sites is taken to be unity and the chemical potential has been chosen to be *zero*, giving a half-filled band.

(a) Show that H_o can be diagonalized in the form

$$H_o = -\sum_{k\ \sigma} (2t\cos k) c^\dagger{}_{k\sigma} c_{k\sigma}, \tag{12.71}$$

where $c_{k\sigma} = \frac{1}{\sqrt{N}} \sum_j \psi_{j\sigma} e^{-ikj}$, $k = \frac{2\pi}{N}(0,\ 1,\ \ldots N-1)$. Please note that the band is exactly half-filled, so that the Fermi surfaces are separated by a distance π in momentum space and the average electron density is 1 per site.

(b) Suppose a staggered potential $V_j = -(-1)^j \Phi$ is applied to the conductor. This will induce a staggered charge density to the sample

$$\langle n_{j\sigma} \rangle = \frac{1}{2} + (-1)^j \Delta_j / g \tag{12.72}$$

At low temperatures, the staggered order will remain even after the applied potential is removed. Why? If the RMS fluctuations in the staggered charge density can be ignored, show that the interaction Hamiltonian can be recast in the form

$$H_I \rightarrow \sum_j \left((-1)^j \Delta_j \hat{n}_j + \frac{\Delta_j^2}{g} \right) + O(\delta \hat{n}_j^2). \tag{12.73}$$

(c) How can the above transformation be elevated to the status of an exact result using a path integral? (Note that the order parameter is no longer complex- does this change your discussion?)

(d) Calculate the excitation spectrum in the presence of the uniformly staggered order parameter $\Delta_j = \Delta$. (Hint: write the mean field Hamiltonian in momentum space and treat the terms that scatter from one-side of the Fermi surface in an analogous fashion to the pairing terms in superconductivity. You may find it useful to work with the spinor $\Psi_{k\sigma} = \begin{pmatrix} c_{k\sigma} \\ c_{k+\pi\sigma} \end{pmatrix}$.)

(e) Calculate the Free energy $F[\Delta]$ and sketch your result as a function of temperature. Write down the gap equation for the value of $\Delta(T)$ that develops spontaneously at low temperatures.

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