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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 àpriori 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 $\nabla \to \nabla + i(e/\hbar)\vec{A}$, $U(x) \to U(x) - eV_{ext}(\vec{x})$. 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

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

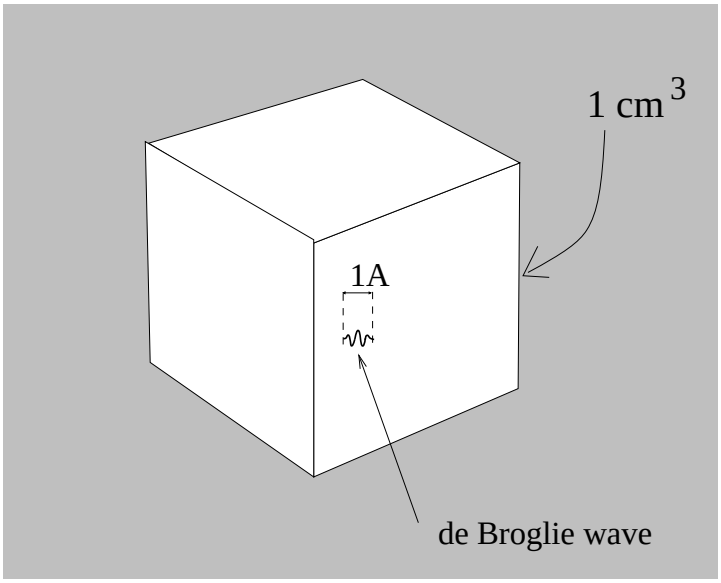


Figure 2.1: The typical size of a de Broglie wave is $10^{-10}m$, to be compared with a typical scale $1cm$ of a macroscopic crystal.

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

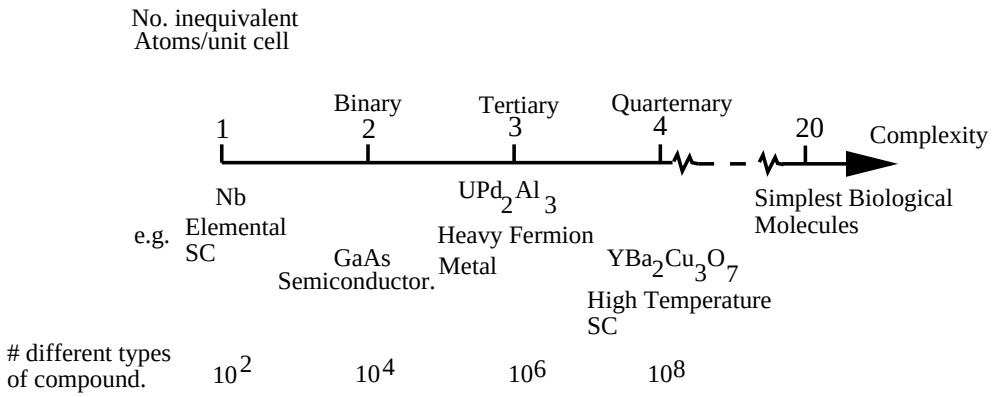


Figure 2.2: Examples of crystals of increasing complexity. As the number of inequivalent atoms per unit cell grows, the complexity of the material and the potential for new types of behavior grows.

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.

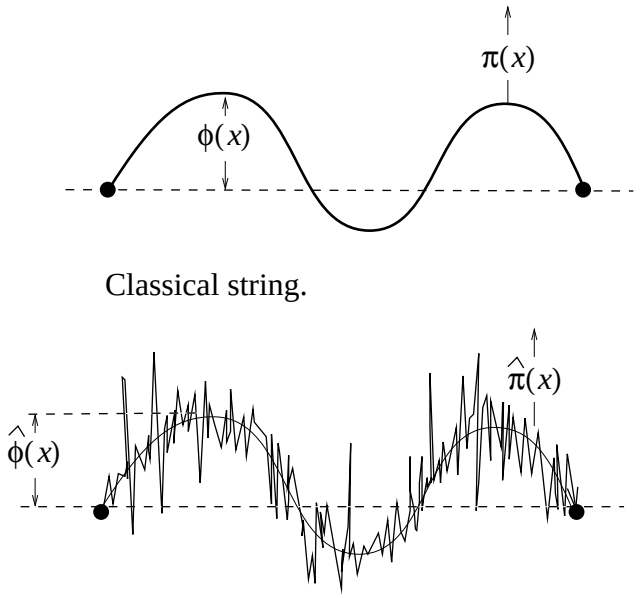


Figure 3.1: Contrasting a classical, and a quantum string.

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.

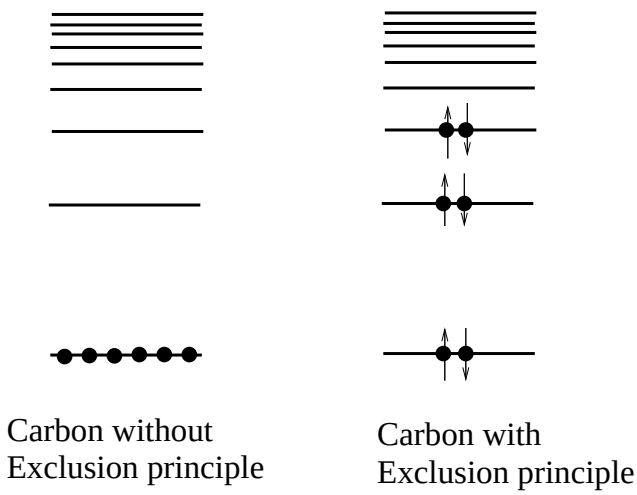


Figure 3.2: Without the exclusion principle, all electrons would occupy the same atomic orbital. There would be no chemistry, no life.

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

$$e^{2i\Theta} = 1 \Rightarrow e^{i\Theta} = \pm 1 \begin{cases} \text{bosons} \\ \text{fermions} \end{cases} \tag{3.6}$$

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

[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

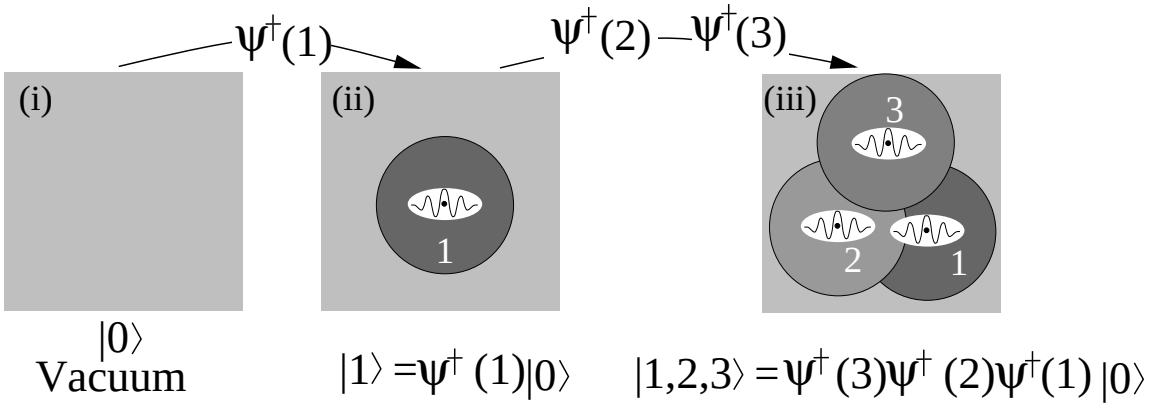


Figure 3.3: Action of creation operator on vacuum to create (i) a one particle and (ii) a three particle state

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,

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

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

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

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

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

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

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

(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,

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

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?

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.

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

The first part of this procedure is essentially identical for both quantum, and classical oscillators. The second-stage is nothing more than the second-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

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

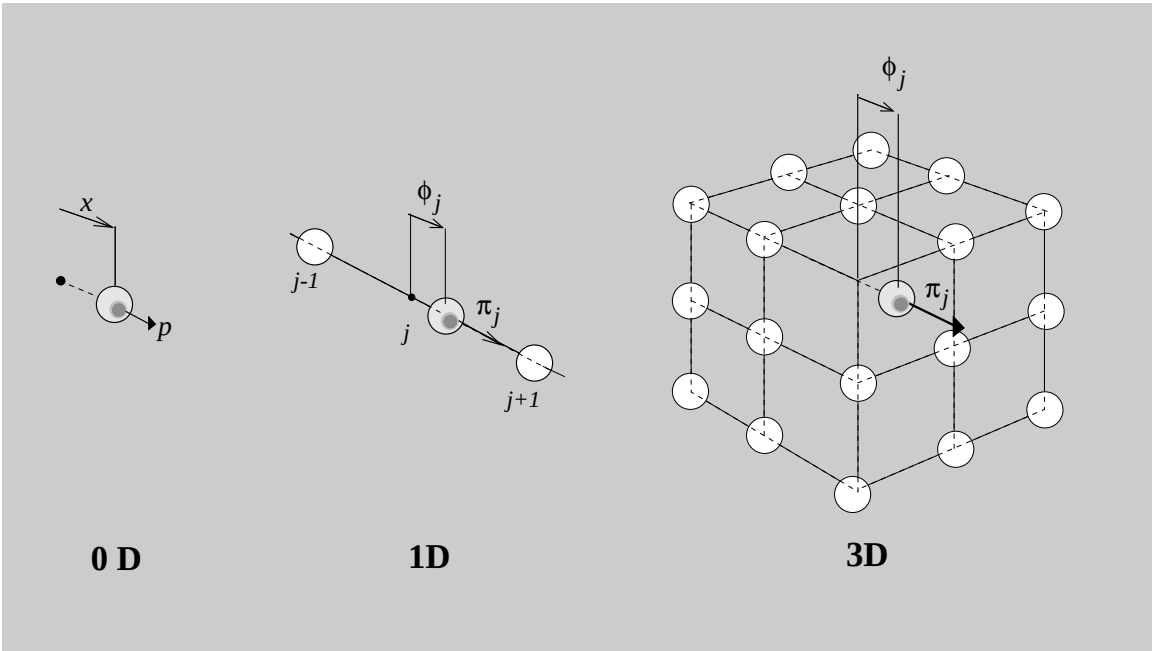


Figure 4.1: Family of zero, one and three-dimensional Harmonic crystals.

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

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

where ω is the frequency of the oscillator.

The second-quantized approach re-interprets 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.

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

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

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

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

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

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

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

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

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

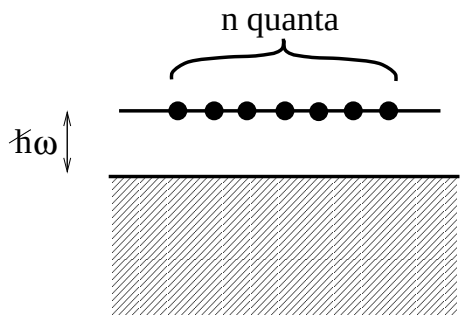


Figure 4.2: Illustrating the excitation picture for a single harmonic oscillator.

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

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

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

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

- 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 $\beta = 1/k_B T$, 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,

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

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, lets imagine we are discussing the displacement of an atom in the x-direction from its equilibrium position. Lets start in one dimension, and imagine that the displacement of the

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

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

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

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

$$\begin{aligned} \phi_q &= \tfrac{1}{\sqrt{N_s}}\textstyle\sum_j e^{-iqR_j}\phi_j \\ \pi_q &= \tfrac{1}{\sqrt{N_s}}\textstyle\sum_q e^{-iqR_j}\pi_j \end{aligned} \tag{4.47}$$

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

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

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

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

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

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

Adding the two terms inside the Hamiltonian then gives

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

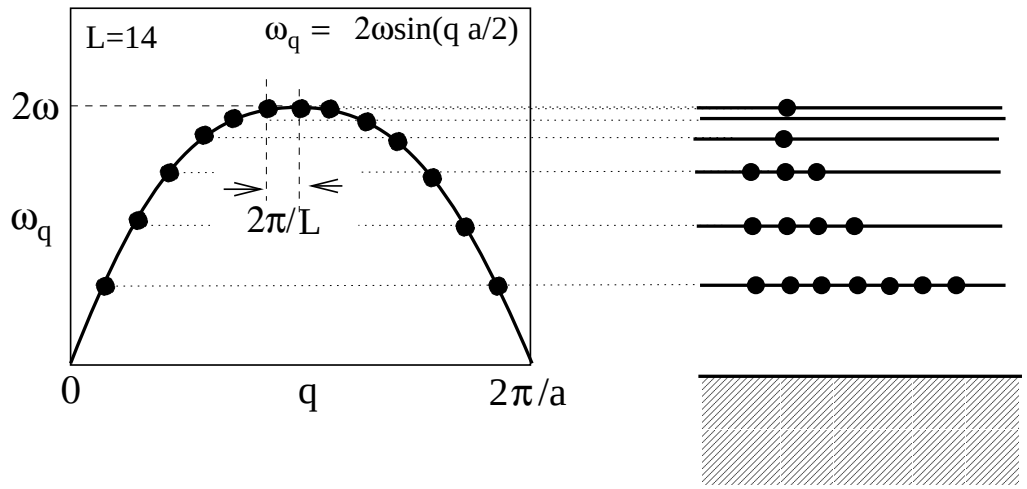


Figure 4.3: Illustrating the excitation picture for a chain of coupled oscillators, length L=14.

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,

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

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 $E_o = \sum_q \hbar\omega_q$ 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

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

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

$$N_s^{-1}\sum_j e^{-i(\mathbf{q}-\mathbf{q}')\cdot R_j} = \delta_{\mathbf{q}-\mathbf{q}'} \tag{4.61}$$

  where now,

$$\mathbf{q} = \frac{2\pi}{L}(i_i, i_2 \ldots i_D) \tag{4.62}$$

  and $\mathbf{R_j}$ is a site on the lattice.

- The zero-point energy $E_o = \sum_q \hbar\omega_q$ 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

$$\Delta q = \frac{2\pi}{L} \tag{4.63}$$

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

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

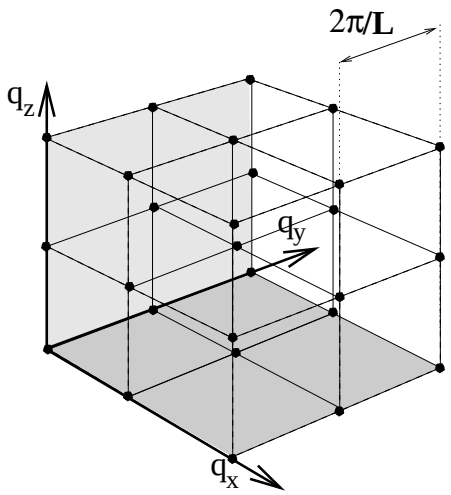


Figure 4.4: Illustrating the grid of allowed momenta for a three-dimensional crystal of dimensions L^3. In the limit $L \to \infty$, the grid becomes a continuum, with $(L/2\pi)^3$ points per unit volume of momentum space.

where $q_j = 2\pi \frac{j}{L} j$, 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:

$$\sum_q \{\ldots\} \longrightarrow L \int_0^{2\pi/a} \frac{dq}{2\pi} \{\ldots\} \tag{4.65}$$

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

$$(\Delta q)^D = \frac{(2\pi)^D}{L^D} \tag{4.66}$$

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

$$\sum_q \{\ldots\} = L^D \sum_q \frac{(\Delta q)^D}{(2\pi)^D} \{\ldots\} \longrightarrow L^D \int_{0<q_i<2\pi/a} \frac{d^D q}{(2\pi)^D} \{\ldots\} \tag{4.67}$$

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

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

$$\langle \vec{x} | \vec{k} \rangle \longrightarrow e^{i\vec{x}\cdot\vec{k}} \tag{4.68}$$

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

$$\langle \vec{k}'|\vec{k}\rangle = \int d^D x e^{i(\vec{k}-\vec{k}')\cdot\vec{x}} = L^D \delta_{\vec{k}-\vec{k}'}, \tag{4.69}$$

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

$$\int d^D x e^{i(\vec{k}-\vec{k}')\cdot\vec{x}} = (2\pi)^D \delta^D(\vec{k}-\vec{k}') \tag{4.70}$$

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

$$L^D \delta_{\vec{k}\vec{k}'} \longrightarrow (2\pi)^D \delta^D(\vec{k}-\vec{k}') \tag{4.71}$$

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

$$H = \sum_j \frac{\pi_j^2}{2m} + \sum_{j,\vec{a}=(\hat{x},\hat{y},\hat{z})} \frac{m\omega_o^2}{2}(\Phi_j - \Phi_{j+\vec{a}})^2 \tag{4.72}$$

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

$$\hat{V} = \frac{1}{2}\sum_{i,j} V_{i-j}\phi_i\phi_j \tag{4.73}$$

where

$$V_{\mathbf{R}} = m\omega_o^2 \sum_{\vec{a}=(\hat{x},\hat{y},\hat{z})} (2\delta_{\mathbf{R}} - \delta_{\mathbf{R}-\vec{a}} - \delta_{\mathbf{R}+\vec{a}}) \tag{4.74}$$

The Fourier transform of this expression is

$$\begin{aligned} V_{\mathbf{q}} &= \sum_{\mathbf{R}} V_{\mathbf{R}} e^{-i\mathbf{q}\cdot\mathbf{R}} \\ &= m\omega_o^2 \sum_{\vec{a}=(\hat{x},\hat{y},\hat{z})} (2 - e^{-i\mathbf{q}\cdot\mathbf{a}} - e^{i\mathbf{q}\cdot\mathbf{a}}) \\ &= m\omega_o^2 \sum_{l=x,y,z} [2 - \cos(q_l a)] \end{aligned} \tag{4.75}$$

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

$$\omega_{\mathbf{q}} = 2\omega_o[\sin^2(q_x a/2) + \sin^2(q_y a/2) + \sin^2(q_z a/2)]^{\frac{1}{2}} \tag{4.76}$$

Fourier transforming the fields

$$\phi_j = \frac{1}{\sqrt{N_s}} \sum_{\mathbf{q}} \phi_{\mathbf{q}} e^{i\mathbf{q}\cdot\mathbf{x}}$$
$$\pi_j = \frac{1}{\sqrt{N_s}} \sum_{\mathbf{q}} \pi_{\mathbf{q}} e^{i\mathbf{q}\cdot\mathbf{x}} \tag{4.77}$$

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

$$H = \sum_{\mathbf{q}} \left[\frac{\pi_{\mathbf{q}}\pi_{-\mathbf{q}}}{2m} + \frac{m\omega_{\mathbf{q}}^2}{2}\phi_{\mathbf{q}}\phi_{-\mathbf{q}} \right] \tag{4.78}$$

Defining the creation and annihilation operator

$$b_{\mathbf{q}} = \sqrt{\frac{m\omega_{\mathbf{q}}}{2\hbar}}\big(\phi_{\mathbf{q}} + \frac{i}{m\omega_{\mathbf{q}}}\pi_{\mathbf{q}}\big), \qquad b^{\dagger}{}_{\mathbf{q}} = \sqrt{\frac{m\omega_{\mathbf{q}}}{2\hbar}}\big(\phi_{-\mathbf{q}} - \frac{i}{m\omega_{\mathbf{q}}}\pi_{-\mathbf{q}}\big), \tag{4.79}$$

we reduce the Hamiltonian to its standard form

$$H = \sum_{\mathbf{q}} \hbar\omega_{\mathbf{q}}\big(\hat{n}_{\mathbf{q}} + \frac{1}{2}\big) \tag{4.80}$$

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

$$E_o = \sum_{\mathbf{q}} \frac{\hbar\omega_{\mathbf{q}}}{2} \longrightarrow V \int \frac{d^3q}{(2\pi)^3} \frac{\hbar\omega_{\mathbf{q}}}{2} \tag{4.81}$$

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

$$\begin{aligned} E_o &= V \prod_{l=1,3} \int_0^{2\pi/a} \frac{dq_l}{2\pi} \hbar\omega_o \sqrt{\sum_{l=1,3} \sin^2(q_l a/2)} \\ &= N_s \hbar\omega_o I_3 \end{aligned} \tag{4.82}$$

where

$$I_3 = \int_{0<u_1,u_2,u_3<\pi} \frac{d^3u}{\pi^3} \sqrt{\sum_{l=1,3} \sin^2(u_l)} = 1.19 \tag{4.83}$$

and N_s is the number of sites.

<u>*Remarks*</u>

- 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.

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

$$\hat{H} = \sum_{j=1,N_s} \left[\frac{\pi_j^2}{2m} + \frac{T}{2a}(\phi_j - \phi_{j+1})^2 \right] \tag{4.84}$$

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

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

$$\begin{aligned} a\sum_j &\to \int dx, \\ \frac{(\phi_j - \phi_{j+1})^2}{a^2} &\to (\nabla_x \phi(x))^2, \end{aligned} \tag{4.85}$$

Making the replacement

$$\pi_j/a \to \tilde{\pi}(x) \tag{4.86}$$

we obtain

$$H = \int dx \left[\frac{T}{2}(\nabla_x \phi)^2 + \frac{1}{2\rho}\tilde{\pi}(x)^2 \right] \tag{4.87}$$

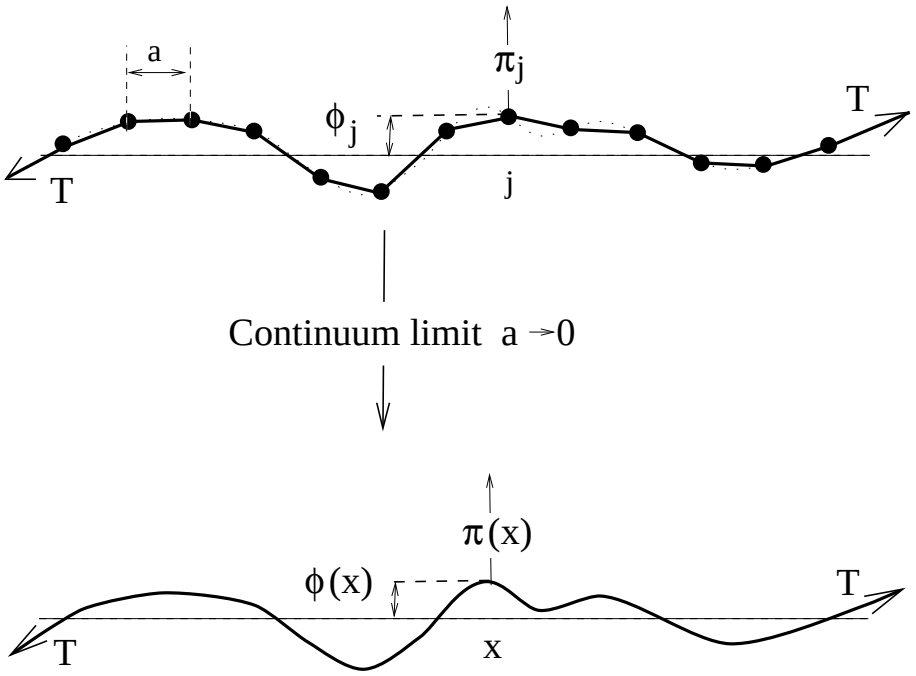


Figure 4.5: Illustrating a (a) discrete and a (b) continuous string. By taking the length between units in the string to zero, maintaining the density per unit length and the tension, we arrive at the continuum limit.

On the discrete lattice, the commutation relations

$$[\phi_i, \tilde{\pi}_j] = i\hbar\tilde{\delta}(x_i - x_j), \tag{4.88}$$

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

$$[\phi(x), \tilde{\pi}(y)] = i\hbar\delta(x - y) \tag{4.89}$$

We now make the jump to Fourier space, writing

$$\phi(x) = \int \frac{dq}{2\pi}\phi_q e^{iqx}e^{-\epsilon|q|/2} \tag{4.90}$$

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 ϕ_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

$$[\phi_q, \pi_{-q'}] = i\hbar 2\pi\delta(q-q') \tag{4.91}$$

When we transform the Hamiltonian, we obtain

$$H = \int \frac{dq}{2\pi}\left[\frac{\pi_{\mathbf{q}}\pi_{-\mathbf{q}}}{2\rho} + \frac{\rho\omega_{\mathbf{q}}^2}{2}\phi_{\mathbf{q}}\phi_{-\mathbf{q}}\right]e^{-\epsilon|q|} \tag{4.92}$$

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

$$\begin{aligned}\phi_q &= \sqrt{\frac{\hbar}{2\rho\omega_q}}[a_q + a^\dagger{}_{-q}] \\ \pi_q &= -i\sqrt{\frac{\hbar}{2\rho\omega_q}}[a_q - a^\dagger{}_{-q}]\end{aligned} \tag{4.93}$$

we find that the creation and annihilation operators satisfy

$$[a_q, a^\dagger{}_{q'}] = 2\pi\delta(q-q'). \tag{4.94}$$

We may now rewrite the Hamiltonian as

$$H = \int_{-\infty}^{\infty}\frac{dq}{2\pi}\frac{\hbar\omega_{\mathbf{q}}}{2}(b^\dagger{}_q b_q + b_{-q}b^\dagger{}_{-q})e^{-\epsilon|q|} \tag{4.95}$$

If we re-order the Boson operators, we obtain

$$H = \int_{\infty}^{\infty}\frac{dq}{2\pi}\hbar\omega_{\mathbf{q}}(b^\dagger{}_q b_q + \overbrace{2\pi\delta(0)}^{\text{“}L\text{”}}\frac{1}{2})e^{-|\epsilon q|/2} \tag{4.96}$$

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,

$$E_{ZP} = L\int\frac{dq}{2\pi}\hbar c|q||e^{-\epsilon|q|\epsilon} = L\hbar(\frac{c}{\epsilon}) \tag{4.97}$$

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

$$: H := \hbar c \int_{-\infty}^{\infty} |q| \hat{n}_q \tag{4.98}$$

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

$$\phi(x,t) = \int \frac{dq}{2\pi} \sqrt{\frac{\hbar}{2\rho\omega_q}} [a_q(t) + a_{-q}(t)] e^{iqx} e^{-\epsilon|q|/2} \tag{4.99}$$

where, as in the case of the Harmonic oscillator

$$a_q(t) = a_q e^{-i\omega_q t}, \qquad {a^\dagger}_q(t) = a_q e^{i\omega_q t}, \tag{4.100}$$

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

$$S(x) = \frac{1}{2}\langle 0|(\phi(x) - \phi(0))^2|0\rangle. \tag{4.101}$$

for a one-dimensional string.

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

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

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:

$$\begin{aligned} S(x) &= \int \frac{dqdq'}{(2\pi)^2} \frac{\hbar}{2\rho c\sqrt{|q||q'|}} \langle 0|[a_q + {a^\dagger}_{-q}][a_{-q'} + {a^\dagger}_{q'}]|0\rangle (e^{iqx} - 1) e^{-|q|\epsilon} \\ &= \frac{\hbar}{2\rho c} \int \frac{dq}{2\pi} e^{-|q|\epsilon} \left(\frac{e^{iqx} - 1}{|q|} \right) \\ &= \left(\frac{\hbar}{\rho c} \right) \left[\frac{1}{4\pi} \ln\left(\frac{\epsilon^2}{\epsilon^2 + x^2} \right) \right] \end{aligned} \tag{4.103}$$

where to obtain the last step, we first calculate

$$\frac{dS}{dx} = -\frac{\hbar}{\rho c} \int_0^{\infty} \frac{dq}{2\pi} e^{-|q|\epsilon} \sin(qx) = -\left(\frac{\hbar}{2\pi\rho c} \right) \frac{x}{x^2 + \epsilon^2} \tag{4.104}$$

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

$$S(x) = \frac{a\hbar}{2\rho}\int \frac{dq}{2\pi}\left(\frac{e^{iqx}-1}{\omega_q}\right) \tag{4.105}$$

  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,

$$S(x) \sim \int d^D q\left(\frac{e^{iqx}-1}{|q|}\right) \sim \frac{1}{x^{D-1}} \tag{4.106}$$

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

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

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

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:

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

where the $\pm$ 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

$$[ab, c]_\pm = a[b, c]_\pm \mp [a, c]_\pm \tag{5.21}$$

we may verify that

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

so that

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

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

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

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

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

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

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

The commutation algebra of the new operators is now

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

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:

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

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

$$\psi(x) = \langle x|\psi(t)\rangle = \sum_n \langle x|n\rangle\psi_n \tag{5.29}$$

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

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

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

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

to invert these relations:

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

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.

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

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

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

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

$$H = \int d^D x d^D x' \psi^\dagger(x)\langle x|H|x'\rangle\psi(x') \tag{5.35}$$

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

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

so that the Hamiltonian becomes

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

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

$$N = \sum_l \psi^\dagger{}_l \psi_l \tag{5.38}$$

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

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

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

$$\psi^{\dagger 2}_l = \frac{1}{2}\{\psi^\dagger{}_l,\ \psi^\dagger{}_l\} = 0 \tag{5.40}$$

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

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

A specific example for fermions, is

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

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

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

By contrast, a bosonic state is symmetric, for example

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

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

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

so that

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

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

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

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:

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

Now the corresponding "bra" state is given by

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

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

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

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, $(12\ldots N) \to (P_1 P_2 \ldots P_N)$

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

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

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

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

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

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

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

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 $|x_1,\ldots x_N\rangle$ is given by

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

Solution: To prove this, we need the intermediate result

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

We now calulate

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

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

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

where the remainder is

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

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

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

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,

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

In otherwords, the state $|x_1 \ldots x_N\rangle$ 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

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

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

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

We shall also Fourier transform the interaction

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

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

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

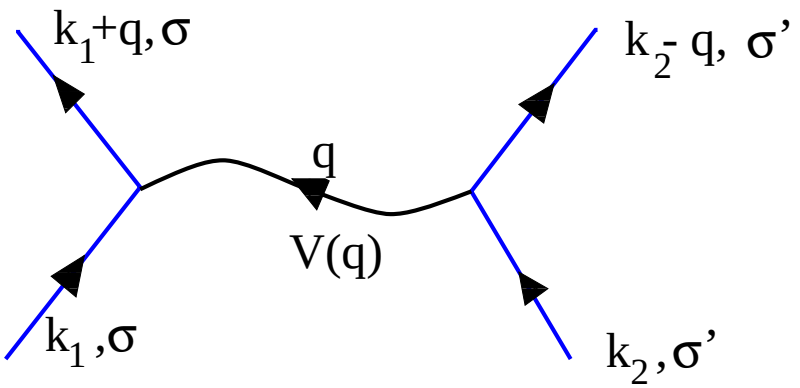


Figure 5.1: Scattering of two particles, showing transfer of momentum. $\mathbf{q}$.

where the spatial integrals take the form

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

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

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

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 $\mathbf{q}$:

$$\begin{array}{lll} \text{particle 1} & \mathbf{k}_1 & \longrightarrow \quad \mathbf{k}_1+\mathbf{q} \\ \text{particle 2} & \mathbf{k}_2 & \longrightarrow \quad \mathbf{k}_2-\mathbf{q} \end{array} \quad (5.86)$$

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

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

so the interaction in momentum space is

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

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 $d^3x = r^2 d\phi d\cos\theta \to 2\pi r^2 d\cos\theta$, so that

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

so that for an arbitrary spherically symmetric potential

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

In this case,

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

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

$$\hat{V} = \frac{1}{2}\sum_{lmnp} c^\dagger{}_l c^\dagger{}_m c_n c_p \langle lm|V|pn\rangle \tag{5.97}$$

where

$$\langle lm|V|pn\rangle = \int_{x,x'} \Phi_l^*(x)\Phi_p(x)\Phi_m^*(x')\Phi_n^*(x')V(x-x') \qquad (5.98)$$

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 $\longrightarrow$ 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	$\sum_{i<j} V(x_i - x_j)$	$\hat{V} = \frac{1}{2}\int_{x,x'} V(x-x') : \hat{\rho}(x)\hat{\rho}(x') :$ $= \frac{1}{2}\sum V(\mathbf{q}) c^\dagger{}_{\mathbf{k}+\mathbf{q}} c^\dagger{}_{\mathbf{k}'-\mathbf{q}} c_{\mathbf{k}'} c_{\mathbf{k}}$
Many Body Wavefunction	$\Psi(x_1, x_2 \ldots x_N)$	$\langle 0\|\hat{\psi}(x_1)\ldots\hat{\psi}(x_N)\|0\rangle$
Schrodinger Eqn	$\left(\sum \mathcal{H}_i + \sum_{i<j} V_{ij}\right)\Psi = i\hbar\dot{\Psi}$	$[\mathcal{H}^{(0)} + \int_{x'} \rho(x')V(x'-x)]\psi(x) = i\hbar\dot{\psi}(x)$

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,

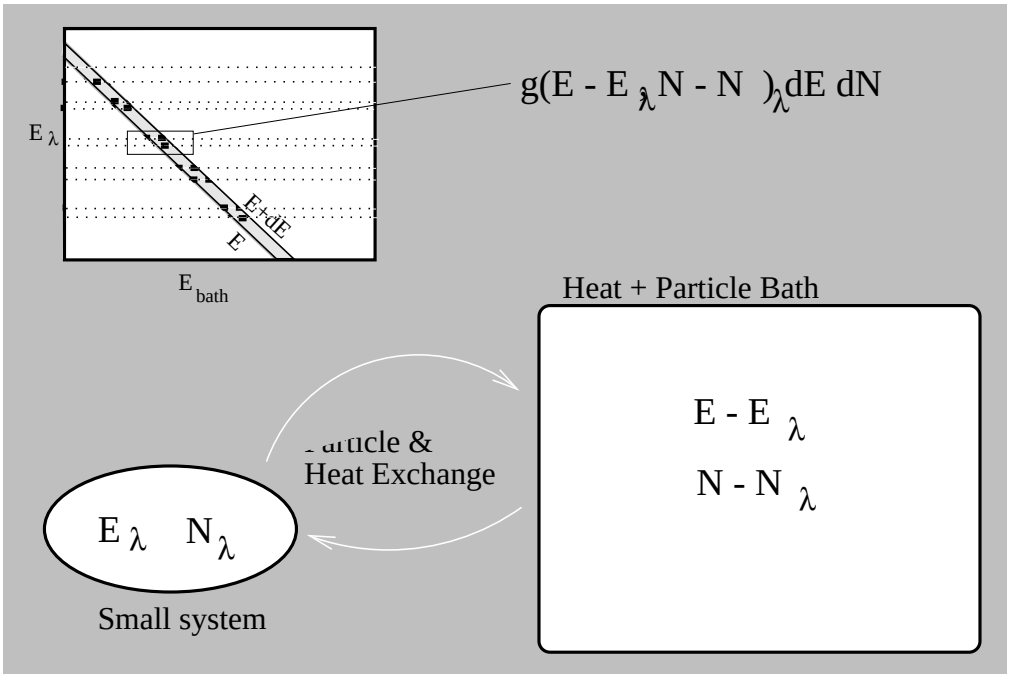


Figure 5.2: Illustrating equilibrium between a small system and a large heat bath. Inset illustrates how the number of states with energy E_λ, particle number N_λ is proportional to the density of states in the big system.

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

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

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:

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

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

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

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

Thermodynamic Relations

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

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

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

(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

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

(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

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

The corresponding Free energy is given by

$$F = \mp k_B T \sum_\lambda \ln[1 \pm e^{-\beta(\epsilon_\lambda - \mu)}], \qquad \begin{cases} fermions \\ bosons \end{cases} \tag{5.131}$$

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.

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

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

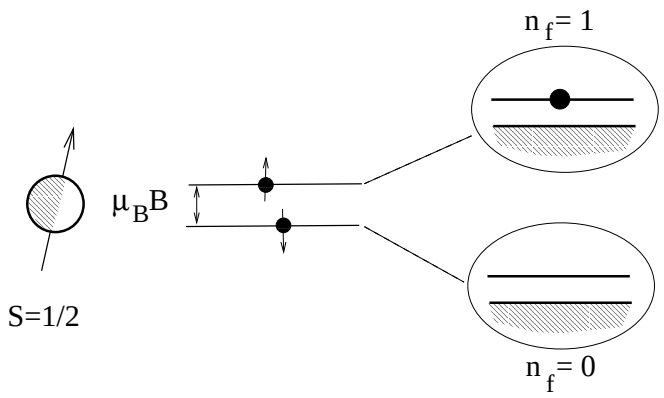


Figure 6.1: Showing how the "up" and "down" states of a spin-1/2 can be treated as a one particle state which is either full, or empty.

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

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

$$\left.\begin{array}{rcl} S_j^z &=& {f^\dagger}_j f_j - \frac{1}{2}, \\ S_j^+ &=& {f^\dagger}_j e^{i\pi \sum_{l<j} n_j}, \\ S_j^+ &=& f_j e^{i\pi \sum_{l<j} n_j} \end{array}\right\} \textbf{Jordan Wigner transformation} \tag{6.9}$$

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:

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

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

$$\begin{aligned} [S_j^{(\pm)}, S_k^{(\pm)}] &= [f_j^{(\dagger)} e^{i\phi_j}, f_k^{(\dagger)} e^{i\phi_k}] \\ &= [f_j^{(\dagger)}, f_k^{(\dagger)} e^{i\pi n_j}] \\ &= \{f_j^{(\dagger)}, f_k^{(\dagger)}\} e^{i\pi n_j} - f_k^{(\dagger)} \{f_j^{(\dagger)}, e^{i\pi n_j}\} = 0. \end{aligned} \tag{6.11}$$

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

$$H = -J \sum [S_j^x S_{j+1}^x + S_j^y S_{j+1}^y] - J_z \sum_j S_j^z S_{j+1}^z \tag{6.12}$$

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

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

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

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

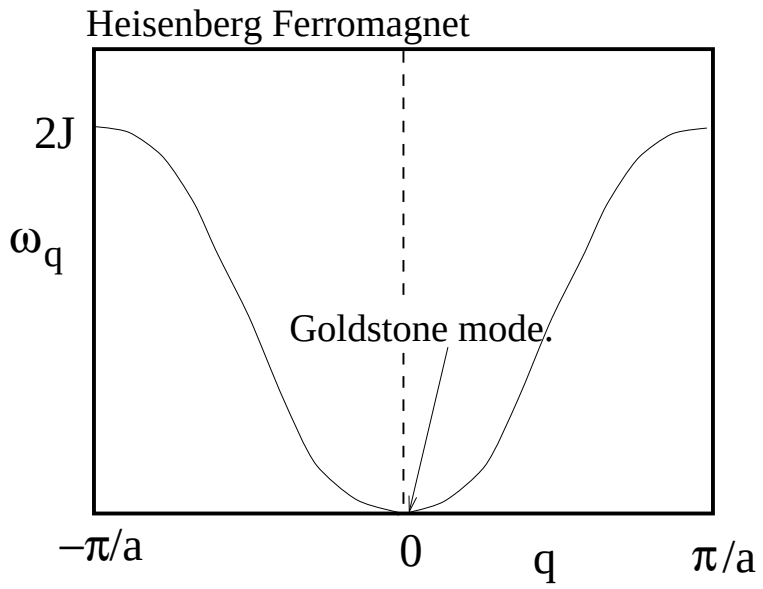


Figure 6.2: Excitation spectrum of the one dimensional Heisenberg Ferromagnet.

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

$$H = \sum_k \omega_k {s^\dagger}_k s_k - \frac{J_z}{2N_s} \sum_{k,k',q} \cos(qa)\ {s^\dagger}_{k-q} {s^\dagger}_{k'+q} s_{k'} s_k. \tag{6.21}$$

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 $J_z = 0$.

- *Heisenberg Ferromagnet.* $J_z = J$

  In this case, the spectrum

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

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 ?? 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

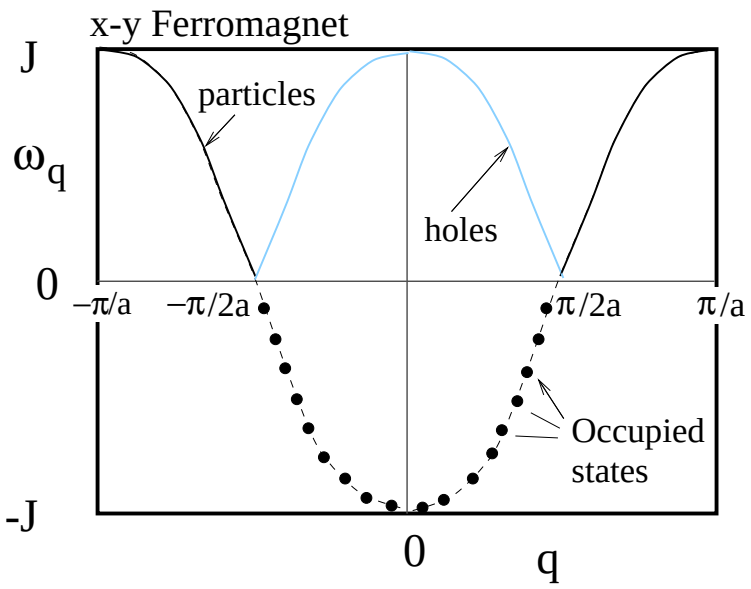


Figure 6.3: Excitation spectrum of the one dimensional x-y Ferromagnet, showing how the negative energy states are filled, the negative energy dispersion curve is "folded over" to describe the positive hole excitation energy.

"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

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

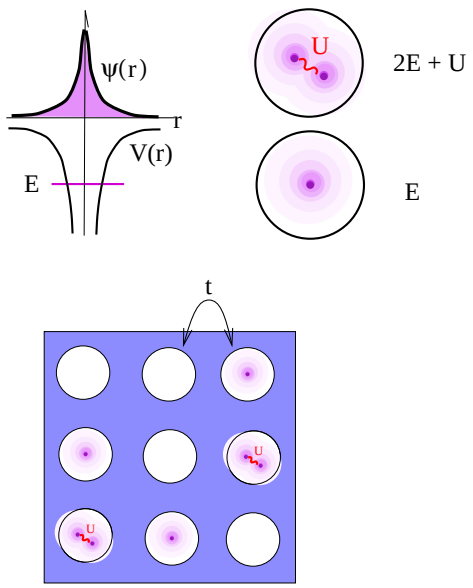


Figure 6.4: Illustrating the Hubbard Model. When two electrons of opposite spin occupy a single atom, this gives rise to a Coulomb repulsion energy U. The amplitude to hop from site to site in the crystal is t.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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.

6.3.2 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

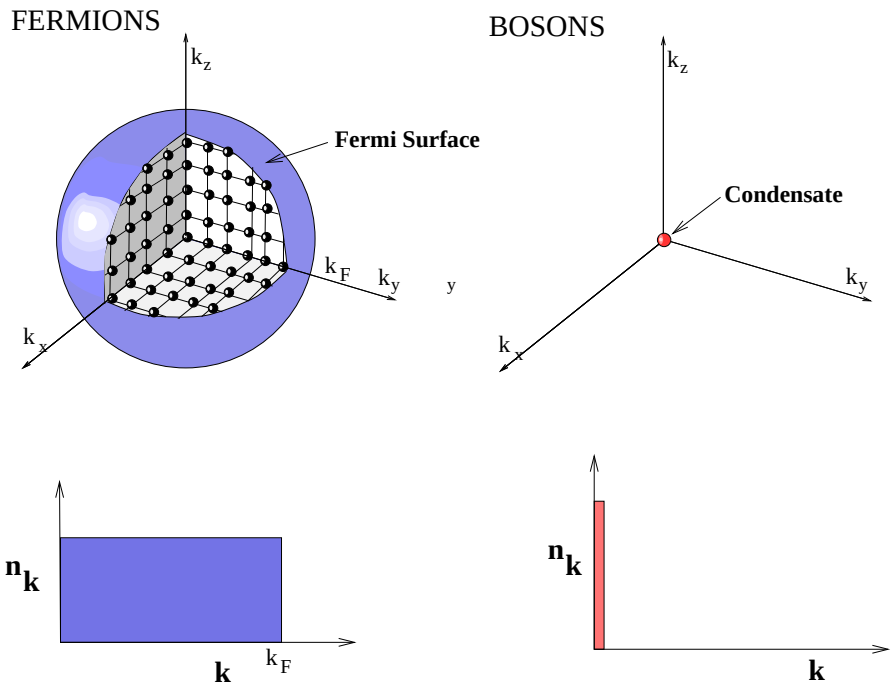


Figure 6.5: Contrasting the ground-states of non-interacting Fermions and non-interacting Bosons. Fermions form a degenerate Fermi gas, with all one-particle states below the Fermi energy individually occupied. Bosons form a Bose Einstein condensate, with a macroscopic number of bosons in the zero momentum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

6.3.3 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 $\sum_{\mathbf{k}\sigma} \to 2V \int_{\mathbf{k}}$. 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 $f(x) \to \theta(-x)$, 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

$$a^{\dagger}{}_{\mathbf{k}\sigma} = \begin{cases} c^{\dagger}{}_{\mathbf{k}\sigma} & (k > k_F) \qquad \text{particle} \\ \sigma c_{-\mathbf{k}-\sigma} & (k > k_F) \qquad \text{hole} \end{cases} \tag{6.56}$$

Beneath the Fermi surface, we must replace $c^\dagger_{\mathbf{k}\sigma}c_{\mathbf{k}\sigma} \to 1 - a^\dagger_{\mathbf{k}\sigma}a_{\mathbf{k}\sigma}$, 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

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

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

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

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 $PV = Nk_BT$, 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 $d^3k \sim k^2 \to k_F^3/3$, whereas the second term contains an integral over $\epsilon_k d^3k \sim k^4 \to k_F^5/5$, 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 $Z_{\mathbf{k_F}} < 1$.

6.3.4 Fluid of Bosons

For a fluid of Bosons, the density of particles 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

$$\begin{aligned} x &= \beta\epsilon_{\mathbf{k}} = \beta\frac{\hbar^2k^2}{2m}, \qquad \left(\frac{m}{\beta\hbar^2}\right)dx = kdk \\ \frac{d^3k}{(2\pi)^3} &\rightarrow \frac{4\pi k^2dk}{(2\pi)^3} = \frac{1}{\sqrt{2}\pi^2}\left(\frac{m}{\beta\hbar^2}\right)^{3/2}\sqrt{x}dx \end{aligned} \tag{6.65}$$

we can rewrite the Boson density in the form

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

where

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

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,

$$\left(\frac{\tilde{\lambda}_T}{a}\right)^3 = \frac{1}{\sqrt{2}\pi^2}\int_0^\infty dx\sqrt{x}\frac{1}{e^x-1} = \frac{\zeta(\frac{3}{2})}{(2\pi)^{3/2}} = 0.166 \tag{6.68}$$

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

$$\rho_o(T) = \rho\left[1 - \left(\frac{T}{T_o}\right)^{3/2}\right] \tag{6.74}$$

<u>*Remarks*</u>

- 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

$$\begin{aligned} g^{\pm}(z) &= \pm\int_0^{\infty} dx\sqrt{x}\ln[1 \pm e^{-(x-z)}] \\ h^{\pm}(z) &= \int_0^{\infty} dx\sqrt{x}\frac{1}{e^{(x-z)} \pm 1} \end{aligned} \tag{6.77}$$

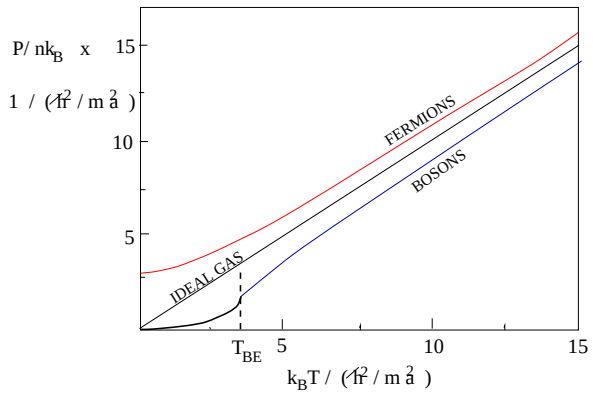


Figure 6.6: Pressure dependence in a Fermi or Bose gas, where temperature is measured in units of $\hbar^2/ma^2$ Showing P/nk_B

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

$$F = \mp(2S+1)k_BTV\int_{\mathbf{k}}\ln[1\pm e^{-\beta(\epsilon_{\mathbf{k}}-\mu)}] \tag{6.78}$$

where S is the spin of the particle. Making the change of variables,

$$\begin{aligned} x &= \beta\epsilon_{\mathbf{k}} = \beta\frac{\hbar^2k^2}{2m}, \\ \frac{d^3k}{(2\pi)^3} &\rightarrow \frac{1}{\tilde{\lambda}_T^3\sqrt{2}\pi^2}\sqrt{x}dx \end{aligned} \tag{6.79}$$

where $\tilde{\lambda}_T = \hbar/\sqrt{mk_BT}$ is the rescaled Thermal de Broglie wavelength, we obtain

$$F = \mp(2S+1)k_BT\frac{V}{\tilde{\lambda}_T^3}\frac{1}{\sqrt{2}\pi^2}\int dx\sqrt{x}\ln[1\pm e^{-(x+\mu\beta)}] \tag{6.80}$$

Taking the derivative with respect to volume, and chemical potential, we obtain the following results for the Pressure and the particle density.

$$\begin{aligned} P &= -\frac{\partial F}{\partial V} = \pm(2S+1)\frac{k_BT}{\tilde{\lambda}_T^3}\frac{1}{\sqrt{2}\pi^2}\int dx\sqrt{x}\ln[1\pm e^{-(x+\mu\beta)}] \\ n &= -\frac{\partial F}{V\partial\mu} = \frac{(2S+1)}{\tilde{\lambda}_T^3}\frac{1}{\sqrt{2}\pi^2}\int dx\sqrt{x}\frac{1}{e^{(x+\mu\beta)}\pm 1} \end{aligned} \tag{6.81}$$

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 in the form

$$k_B T = \frac{\hbar^2}{ma^2}[h^{\pm}(\mu/\beta)]^{-2/3} \tag{6.82}$$

So that both the pressure and the temperature can be plotted parametrically as a function of $\mu\beta$. Fig 6.6 shows the results of such a plot.

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.

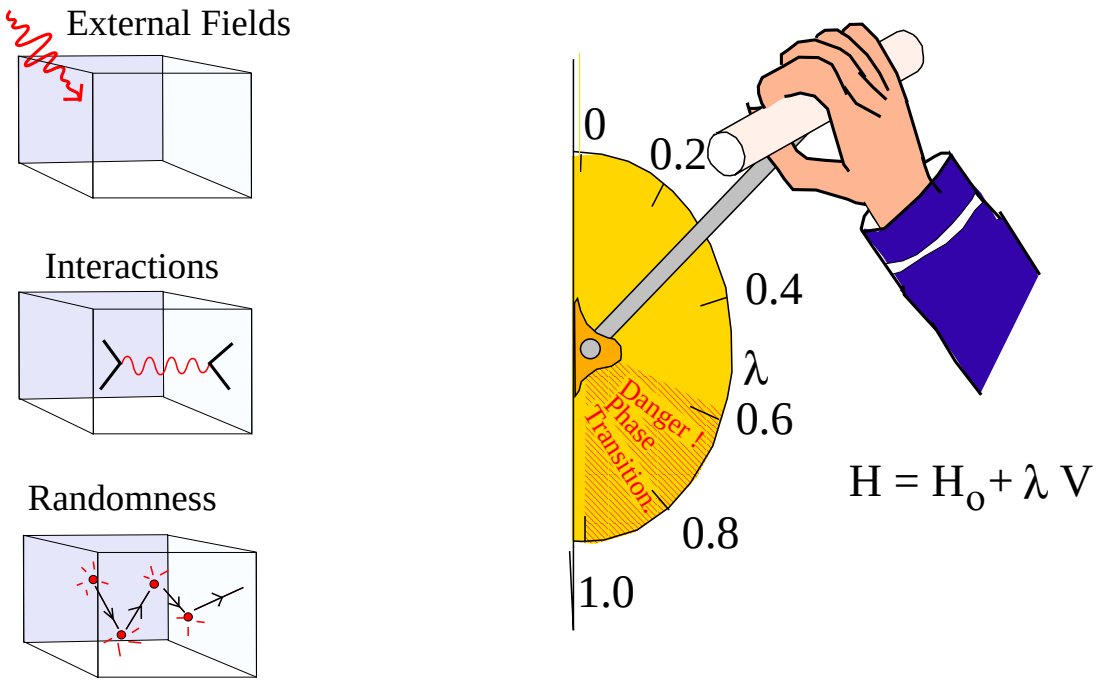


Figure 7.1: "Dialing up the interaction". Motivating the need to be able to treat perturbations to a non-interacting Hamiltonian by dialing up the strength of the perturbation.

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 $i\frac{\partial}{\partial t}\|\psi_S(t)\rangle = H\|\psi_S(t)\rangle$	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 $i\frac{\partial}{\partial t}\|\psi_I(t)\rangle = V_I(t)\|\psi_I(t)\rangle$	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

$$\left.\begin{array}{rcl} |\psi_I(t)\rangle &=& e^{iH_o t}|\psi_S(t)\rangle, \\ O_I(t) &=& e^{iH_o t}O_S e^{-iH_o t} \end{array}\right\} \text{Removes rapid state evolution due to } H_o \qquad (7.6)$$

The evolution of the wavefunction is thus

$$\left.\begin{aligned} |\psi_I(t)\rangle &= U(t)|\psi_I(t)\rangle, \\ U(t) &= e^{iH_o t}e^{-iHt} \end{aligned}\right] \tag{7.7}$$

or more generally,

$$\begin{aligned} |\psi_I(t)\rangle &= S(t,t')|\psi_I(t')\rangle, \\ S(t) &= U(t)U^\dagger(t') \end{aligned} \tag{7.8}$$

The time evolution of $U(t)$ can be derived as follows

$$\begin{aligned} i\frac{\partial U}{\partial t} &= i\left(\frac{\partial e^{iH_o t}}{\partial t}\right)e^{-iHt} + ie^{iH_o t}\left(\frac{\partial e^{-iHt}}{\partial t}\right) \\ &= e^{iH_o t}(-H_o + H)e^{-iHt} \\ &= [e^{iH_o t}Ve^{-iH_o t}]U(t) \\ &= V_I(t)U(t) \end{aligned} \tag{7.9}$$

so that

$$i\frac{\partial S(t_2,t_1)}{\partial t_1} = V(t_2)S(t_2,t_1) \tag{7.10}$$

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 $\{O_1(t_1), O_2(t_2)\ldots O_N(t_N)\}$ is a set of operators at different times $\{t_1, t_2 \ldots t_N\}$. If P is the permutation that orders the times, so that $t_{P_1} > t_{P_2}\ldots t_{P_N}$, then if the operators are entirely bosonic, containing an even number of fermionic operators,the time ordering operator is defined as

$$T\big[O_1(t_1)O_2(t_2)\ldots O_N(t_N)\big] = O_{P_1}(t_{P_1})O_{P_2}(t_{P_2})\ldots O_{P_N}(t_{P_N}) \tag{7.11}$$

For later use, we note that if the operator set contains fermionic operators, composed of an odd number of fermionic operators, then

$$T\big[F_1(t_1)F_2(t_2)\ldots F_N(t_N)\big] = (-1)^P F_{P_1}(t_{P_1})F_{P_2}(t_{P_2})\ldots F_{P_N}(t_{P_N}) \tag{7.12}$$

where P is the number of pairwise permutations of fermions involved in the time ordering process.

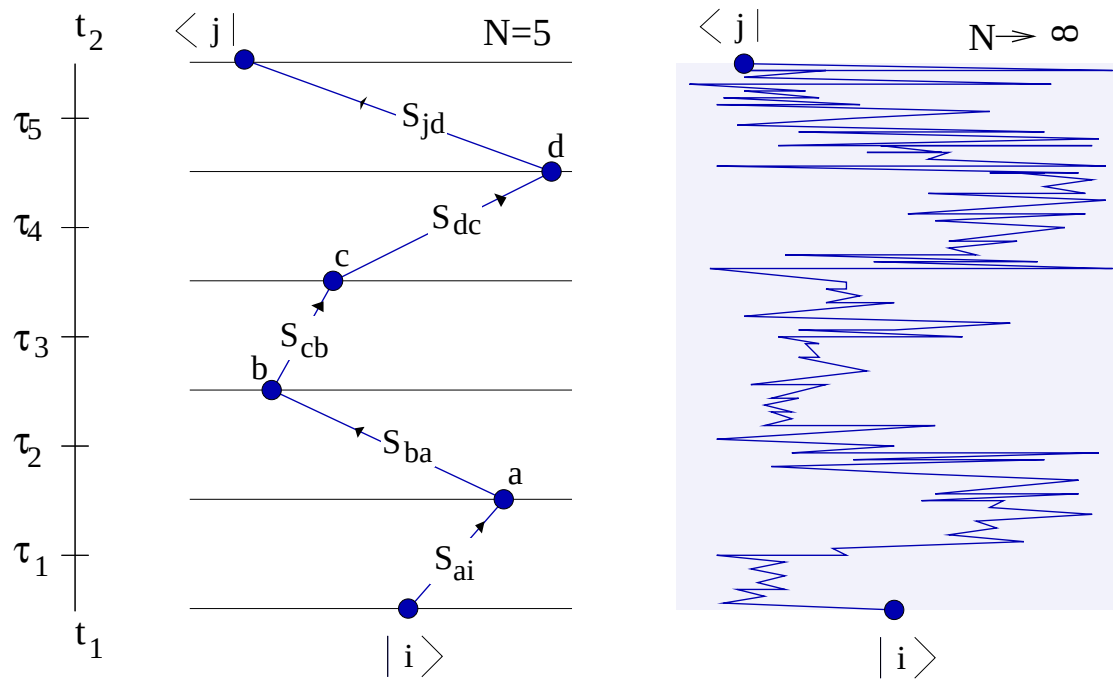


Figure 7.2: Each contribution to the time-ordered exponential corresponds to the amplitude to follow a particular path in state space. The S-matrix is given by the limit of the process where the number of time segments is sent to infinity.

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:

$$S(t_2, t_1) \quad = \quad S(t_2, \tau_N - \tfrac{\Delta t}{2}) S(\tau_{N-1} + \tfrac{\Delta t}{2}, \tau_{N-1} - \tfrac{\Delta t}{2}) \ldots S(\tau_1 + \tfrac{\Delta t}{2}, t_1) \qquad (7.13)$$

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

$$S(t_2, t_1) = e^{-iV(\tau_N)\Delta t} e^{-iV(\tau_{N-1})\Delta t} \ldots e^{-iV(\tau_1)\Delta t} + O(1/N) \qquad (7.15)$$

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

$$T[e^{A(t_1)}e^{A(t_2)}] = T[e^{A(t_1)+A(t_2)}] \tag{7.17}$$

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,

$$S(t_2,t_1) = Lim_{N\to\infty} T[e^{-i\sum_j V(\tau_j)\Delta t}] \tag{7.18}$$

The limiting value of this time-ordered exponential is written as

$$\boxed{S(t_2,t_1) = T\left[\exp\left\{-i\int_{t_1}^{t_2} V(t)dt\right\}\right], \qquad \textbf{Time-ordered exponential}} \tag{7.19}$$

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

$$S_{fi}(t_2,t_2) = \sum_{\text{path}=\{p_1,\ldots p_{N_1}\}} S_{f,p_{N-1}}(\tau_N)\ldots S_{p_2p_1}(\tau_2)S_{p_1i}(\tau_1) \tag{7.20}$$

  Each term in this sum is the amplitude to go along the path of states

$$\text{path } i \;\to\; f: \;\; i \to p_1 \to p_2 \to \ldots p_{N-1} \to f. \tag{7.21}$$

  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,

$$S(t_2,t_1) = \sum_{n=0,\infty} \frac{(-i)^n}{n!}\int_{t_1}^{t_2} d\tau_1\ldots d\tau_n T[V(\tau_1)\ldots V(\tau_n)] \tag{7.22}$$

  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

$$S(t_2,t_1)=\sum_{n=0,\infty}(-i)^n\int_{t_1,\ \{\tau_n>\tau_{n-1}\ldots>\tau_1\}}^{t_2}d\tau_1\ldots d\tau_n V(\tau_n)\ldots V(\tau_1) \tag{7.23}$$

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

$$\langle 0|Te^{i\int_{-\infty}^{\infty}dt[\bar{z}(t)b(t)+b^\dagger(t)z(t)]}|0\rangle=\exp\left[-i\int_{-\infty}^{\infty}dtdt'\bar{z}(t)G(t-t')z(t')\right]. \tag{7.26}$$

where $G(t-t')=-i\theta(t-t')e^{-i\omega(t-t')}$ is our first example of a one particle "Green's function".

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

$$G(t-t')=-i\langle\phi|Tb(t)b^\dagger(t')|\phi\rangle. \tag{7.27}$$

- By expanding the time-ordered exponential as a power-series in z and $\bar{z}$, we find that the n-th order term is

$$(-i)^n \int_{-\infty}^{\infty} \prod_{r=1,n} dt_r dt'_r \bar{z}(t_r) z(t'_r) \times \text{ coeff} \tag{7.28}$$

where

$$\text{coeff} = G(t_1, \ldots t_r; t'_1 \ldots t'_r) = (-i)^n \langle \phi | T b(t_1) \ldots b(t_n) b^\dagger(t_n) \ldots b^\dagger(t_1) | \phi \rangle \tag{7.29}$$

is called the n-particle Greens function. 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 $\{t'_r\}$ with final times $\{t_r\}$ by a single-particle Green's function,

$$G(t_1, \ldots t_r; t'_1 \ldots t'_r) = \sum_P \prod_r G(t_r - t'_{P_r}), \tag{7.30}$$

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.

- This result can be generalized to an arbitrary number of oscillators by replacing $(z,\ \bar{z}) \to (z_r, \bar{z}_r)$, whereapon

$$\begin{aligned} \langle \quad 0 \quad | T \exp\left[i \int_{-\infty}^{\infty} dt [\bar{z}_r(t) b_r(t) + b_r{}^\dagger(t) z_r(t)] \right] |0\rangle \\ = \quad \exp\left[-i \int_{-\infty}^{\infty} dt dt' \bar{z}_r(t) G_{rs}(t-t') z_s(t') \right] \end{aligned} \tag{7.31}$$

where now, $G_{rs}(t-t') = -i\langle \phi | T b_r(t) b^\dagger{}_s(t') | \phi \rangle = -i\delta_{rs}\theta(t-t') e^{-i\omega_r(t-t')}$, 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

$$\langle \quad 0 \quad | T \exp\left[i \int_{-t_1}^{t_2} dt [\bar{z}(t) b(t) + b^\dagger(t) z(t)] \right] |0\rangle \tag{7.32}$$

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

$$S_N = e^{A_N + B_N} \times \ldots e^{A_r + B_r} \times \ldots e^{A_1 + B_1} \tag{7.33}$$

where we have used the short-hand notation,

$$\begin{aligned} A_r &= i\bar{z}(\tau_r)b(\tau_r)\Delta\tau, \\ B_r &= ib^\dagger(\tau_r)z(\tau_r)\Delta\tau \end{aligned} \tag{7.34}$$

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

$$e^{\alpha+\beta} = e^\beta e^\alpha e^{[\alpha,\beta]/2} \tag{7.35}$$

and the related result ,

$$e^\alpha e^\beta = e^\beta e^\alpha e^{[\alpha,\beta]} \tag{7.36}$$

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 B_r. Fortunately, the commutator

$$[A_r, B_s] = -\Delta\tau^2\bar{z}(\tau_r)z(\tau_s)e^{-i\omega(\tau_r-\tau_s)} \tag{7.37}$$

is a c-number, so we can use the above theorem. We first normal order each term in the product, writing $e^{A_r+B_r} = e^{B_r}e^{A_r}e^{[A_r,B_r]/2}$ so that

$$S_N = e^{B_N}e^{A_N}\ldots e^{B_1}e^{A_1}e^{\sum_r[A_r,B_r]/2} \tag{7.38}$$

Now we move the general term e^{A_r} to the right-hand side, picking up the residual commutators along the way to obtain

$$S_N = \overbrace{e^{\sum_r B_r}e^{\sum_r A_r}}^{:S_N:}\exp[\sum_{r\geq s}[A_r, B_s](1-\frac{1}{2}\delta_{rs})] \tag{7.39}$$

The vacuum expectatation value of the first term is unity, so that

$$\begin{aligned} S(t_2,t_1) &= \lim_{\Delta\tau\to 0}\exp\Big[-\sum_{s\leq r}\Delta\tau^2\bar{z}(\tau_r)z(\tau_s)e^{-i\omega(\tau_r-\tau_s)}(1-\frac{1}{2}\delta_{rs})\Big] \\ &= \exp\Big[-\int_{t_1}^{t_2}d\tau d\tau'\bar{z}(\tau)\theta(\tau-\tau')e^{-i\omega(\tau-\tau')}z(\tau')\Big] \end{aligned} \tag{7.40}$$

So placing $G(t-t') = -i\theta(\tau-\tau')e^{-i\omega(\tau-\tau')}z(\tau')$,

$$S(t_2,t_1) = \exp\Big[-i\int_{t_1}^{t_2}d\tau d\tau'\bar{z}(\tau)G(t-t')z(\tau')\Big] \tag{7.41}$$

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

$$p = \exp\big[-4g^2 \sin^2(\omega T/2)\big] \tag{7.42}$$

where ω is the frequency of the oscillator

$$g^2 = \frac{V_{spring}}{\hbar\omega} \tag{7.43}$$

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

$$G_{\lambda\lambda'}(t-t') = -i\langle\phi|T\psi_\lambda(t)\psi^\dagger{}_{\lambda'}(t')|\phi\rangle \tag{7.44}$$

where $|\phi\rangle$ is the true ground-state and

$$T\psi_\lambda(t)\psi^\dagger{}_{\lambda'}(t') = \begin{cases} \psi_\lambda(t)\psi^\dagger{}_{\lambda'}(t') & (t > t') \\ \pm\psi^\dagger{}_{\lambda'}(t')\psi_\lambda(t) & (t < t') \end{cases} \qquad \pm \begin{cases} \text{Bosons} \\ \text{Fermions} \end{cases} \tag{7.45}$$

defines the time-ordering for fermions and bosons. Diagramattically, this quantity is represented as follows

$$G_{\lambda\lambda'}(t-t') = \quad \lambda,t \longleftarrow \lambda',t' \tag{7.46}$$

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

$$G_{\mathbf{k}\sigma,\mathbf{k}'\sigma'}(t-t') = \delta_{\sigma\sigma'}\delta_{\mathbf{k}\mathbf{k}'}G(\mathbf{k},t-t') \tag{7.47}$$

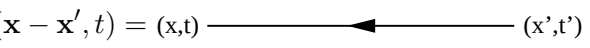
is diagonal, (where in the continuum limit, $\delta_{\mathbf{k}\mathbf{k}'} \to (2\pi)^D\delta^{(D)}(\mathbf{k}-\mathbf{k}')$). In this case, we denote

$$G(\mathbf{k},t-t') = -i\langle\phi|T\psi_{\mathbf{k}\sigma}(t)\psi^\dagger{}_{\mathbf{k}\sigma}(t')|\phi\rangle = \quad t \xleftarrow{\mathbf{k}} t' \tag{7.48}$$

We can also define Green's function in real time,

$$G(\mathbf{x}-\mathbf{x}',t) = -i\langle\phi|T\psi_\sigma(\mathbf{x},t)\psi^\dagger{}_\sigma(\mathbf{x}',t')|\phi\rangle \tag{7.49}$$

which we denote diagramatically, by

$G(\mathbf{x}-\mathbf{x}',t) =$ 

(7.50)

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:

$$\begin{aligned} G(\mathbf{x}-\mathbf{x}',t) &= \int_{\mathbf{k},\mathbf{k}'} e^{i(\mathbf{k}\cdot\mathbf{x}-\mathbf{k}'\cdot\mathbf{x}')} \overbrace{-i\langle\phi|T\psi_{\mathbf{k}\sigma}(t)\psi^\dagger{}_{\mathbf{k}'\sigma}(0)|\phi\rangle}^{\delta_{\mathbf{k}\mathbf{k}'}G(\mathbf{k},t-t')} \\ &= \int \frac{d^3k}{(2\pi)^3} G(\mathbf{k},t) e^{i\mathbf{k}\cdot(\mathbf{x}-\mathbf{x}')} \end{aligned} \tag{7.51}$$

It is also often convenient to Fourier transform in time, so that

$$G(\mathbf{k},t) = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} G(\mathbf{k},\omega) e^{-i\omega t} \tag{7.52}$$

The quantity

$$\begin{aligned} G(\mathbf{k},\omega) &= \int_{-\infty}^{\infty} dt G(\mathbf{k},t) e^{i\omega t} \\ &= \quad \mathbf{k},\omega \end{aligned} \tag{7.53}$$

is known as the propagator. We can then relate the Green's function in real space to its propagator, as follows

$$-i\langle\phi|T\psi_\sigma(\mathbf{x},t)\psi_\sigma(\mathbf{x}',t')|\phi\rangle = \int \frac{d^3k d\omega}{(2\pi)^4} G(\mathbf{k},\omega) e^{i[(\mathbf{k}\cdot(\mathbf{x}-\mathbf{x}')-\omega(t-t')]} \tag{7.54}$$

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

$$H = \hat{H}_o - \mu N = \sum_\sigma \epsilon_{\mathbf{k}} c^\dagger{}_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma}. \tag{7.55}$$

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

$$|\phi\rangle = \prod_{\sigma|\mathbf{k}|<k_f} c^\dagger{}_{\mathbf{k}\sigma}|0\rangle \tag{7.56}$$

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

$$\begin{aligned}\langle\phi|c_{\mathbf{k}\sigma}(t)c^\dagger{}_{\mathbf{k}'\sigma'}(t')|\phi\rangle &= \delta_{\sigma\sigma'}\delta_{\mathbf{k}\mathbf{k}'}e^{-i\epsilon_{\mathbf{k}}(t-t')}\langle\phi|c_{\mathbf{k}\sigma}c^\dagger{}_{\mathbf{k}\sigma}|\phi\rangle \\ &= \delta_{\sigma\sigma'}\delta_{\mathbf{k}\mathbf{k}'}(1-n_{\mathbf{k}})e^{-i\epsilon_{\mathbf{k}}(t-t')}\end{aligned} \tag{7.57}$$

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

$$\langle\phi|c^\dagger{}_{\mathbf{k}'\sigma'}(t')c_{\mathbf{k}\sigma}(t)|\phi\rangle = \delta_{\sigma\sigma'}\delta_{\mathbf{k}\mathbf{k}'}n_{\mathbf{k}}e^{-i\epsilon_{\mathbf{k}}(t-t')} \tag{7.58}$$

so that

$$\begin{aligned}G(\mathbf{k},t) &= -i[(1-n_{\mathbf{k}})\theta(t) - n_{\mathbf{k}}\theta(-t)]e^{-i\epsilon_{\mathbf{k}}t} \\ &= \begin{cases} -i\theta_{|\mathbf{k}|-|\mathbf{k}_F|}e^{-i\epsilon_{\mathbf{k}}t} & (t>0) \quad \text{“electrons”} \\ i\theta_{|\mathbf{k}_F|-|\mathbf{k}_F|}e^{-i\epsilon_{\mathbf{k}}t} & (t<0) \quad \text{holes = “electrons moving backwards in time”} \end{cases}\end{aligned} \tag{7.59}$$

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

$$\begin{aligned}G(\mathbf{k},\omega) &= -i\int_{-\infty}^{\infty} dt e^{i(\omega-\epsilon_{\mathbf{k}})t} \quad \overbrace{e^{-|t|\delta}}^{\text{cnvgnce factor}} \quad \Big[\theta_{k-k_F}\theta(t) - \theta_{k_F-k}\theta(-t)\Big] \\ &= -i\Big[\frac{\theta_{k-k_F}}{\delta - i(\omega-\epsilon_{\mathbf{k}})} - \frac{\theta_{k_F-k}}{\delta + i(\omega-\epsilon_{\mathbf{k}})}\Big] = \frac{1}{\omega - \epsilon_{\mathbf{k}} + i\delta_{\mathbf{k}}}\end{aligned} \tag{7.60}$$

where $\delta_{\mathbf{k}} = \text{sign}(\text{k} - \text{k}_\text{F})$. The free fermion propagator is then

$$G(\mathbf{k},\omega) = \frac{1}{\omega - \epsilon_{\mathbf{k}} + i\delta_{\mathbf{k}}} = \quad \mathbf{k},\omega \quad \longleftarrow \tag{7.61}$$

[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!

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

$$\begin{aligned}\langle\hat{\rho}(x)\rangle &= \sum_\sigma \langle {\psi^\dagger}_\sigma \psi_\sigma\rangle = -\sum_\sigma \langle\phi|T\psi_\sigma(x,0^-){\psi^\dagger}_\sigma(x,0)|\phi\rangle \\ &= -i(2S+1)G(\mathbf{x},0^-)|_{\mathbf{x}=0} \end{aligned} \tag{7.62}$$

where S is the spin of the fermion. We can also use it to calculate the Kinetic energy density, which is given as follows

$$\begin{aligned}\langle\hat{T}(x)\rangle &= -\frac{\hbar^2}{2m}\sum_\sigma \langle {\psi^\dagger}_\sigma \nabla_x^2\psi_\sigma(x)\rangle = \frac{\hbar^2\nabla_x^2}{2m}\sum_\sigma \langle\phi|T\psi_\sigma(x,0^-){\psi^\dagger}_\sigma(\vec{x}',0)|\phi\rangle\Big|_{\mathbf{x}-\mathbf{x}'=\mathbf{0}} \\ &= i(2S+1)\,\frac{\hbar^2\nabla^2}{2m}G(\mathbf{x},0^-)\Big|_{\mathbf{x}=0} \end{aligned} \tag{7.63}$$

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.

Solution: We begin by writing $\langle\hat{\rho}(x)\rangle = -i(2S+1)G(\vec{0},0^-)$. Writing this out explicitly we obtain

$$\langle\rho(x)\rangle = (2S+1)\int\frac{d^3k}{(2\pi)^3}\left[\int\frac{d\omega}{2\pi i}e^{i\omega\delta}\frac{1}{\omega-\epsilon_{\mathbf{k}}+i\delta_{\mathbf{k}}}\right] \tag{7.64}$$

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. **??**. 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

$$\int\frac{d\omega}{2\pi i}e^{i\omega\delta}\frac{1}{\omega-\epsilon_{\mathbf{k}}+i\delta_{\mathbf{k}}} = \theta_{k_F-|\mathbf{k}|} \tag{7.65}$$

and hence

$$\rho = (2S+1)\int_{k<k_F}\frac{d^3k}{(2\pi)^3} = (2S+1)\frac{V_F}{(2\pi)^3} \tag{7.66}$$

In a similar way, the kinetic energy density is written

$$\begin{aligned}\langle T(x)\rangle &= (2S+1)\int\frac{d^3k}{(2\pi)^3}\frac{\hbar^2k^2}{2m}\left[\int\frac{d\omega}{2\pi i}e^{i\omega\delta}\frac{1}{\omega-\epsilon_{\mathbf{k}}+i\delta_{\mathbf{k}}}\right] \\ &= (2S+1)\int_{k<k_F}\frac{d^3k}{(2\pi)^3}\frac{\hbar^2k^2}{2m} = \frac{2}{5}\epsilon_F\rho \end{aligned} \tag{7.67}$$

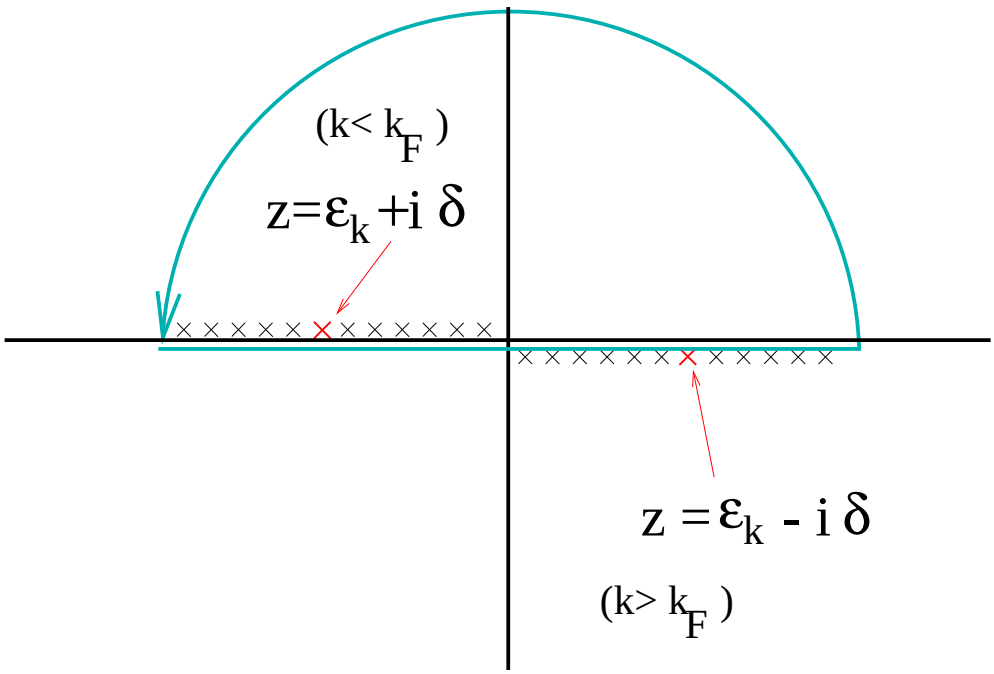


Figure 7.3: Showing how the path of integration in (7.65) picks up the pole contributions from the occupied states beneath the Fermi surface.

7.2.2 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

$$G(\mathbf{k},\omega) = \sum_{\lambda} \frac{|M_\lambda|^2}{\omega - \epsilon_\lambda + i\delta_\lambda} \tag{7.68}$$

where $\delta_\lambda = \delta \text{sign}(\epsilon_\lambda)$ and the total pole strength

$$\sum_{\lambda} |M_\lambda|^2 = 1 \tag{7.69}$$

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

$$\epsilon_\lambda = \begin{cases} E_\lambda - E_g & (|\lambda\rangle \in |N+1\rangle) \\ E_g - E_\lambda & (|\lambda\rangle \in |N-1\rangle) \end{cases} \tag{7.70}$$

and the corresponding matrix elements are

$$M_\lambda = \begin{cases} \langle\lambda|c^\dagger{}_{\mathbf{k}\sigma}|\phi\rangle, & (|\lambda\rangle \in |N+1\rangle), \\ \\ \langle\lambda|c_{\mathbf{k}\sigma}|\phi\rangle, & (|\lambda\rangle \in |N-1\rangle). \end{cases} \tag{7.71}$$

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,

$$A(\mathbf{k},\omega) = \frac{1}{\pi}\mathrm{Im}G(\mathbf{k},\omega - i\delta), \qquad \textbf{Spectral Function} \tag{7.72}$$

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 (7.68) to write

$$A(\mathbf{k},\omega) = \sum |M_\lambda|^2 \delta(\omega - \epsilon_\lambda) \tag{7.73}$$

where now, the normalization of the pole-strengths means that

$$\int_{-\infty}^{\infty} A(\mathbf{k},\omega)d\omega = \sum_\lambda |M_\lambda|^2 = 1 \tag{7.74}$$

Since the excitation energies are always positive, ϵ_λ is positive for electron states and negative for electron states, so

$$A(\mathbf{k},\omega) = \theta(\omega)\rho_e(\mathbf{k},\omega) + \theta(-\omega)\rho_h(\mathbf{k},-\omega) \tag{7.75}$$

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

$$G(\mathbf{k},t) = -i\sum_\lambda \Big[\langle\phi|c_{\mathbf{k}\sigma}(t)\overbrace{|\lambda\rangle\langle\lambda|}^{=1}c^\dagger{}_{\mathbf{k}\sigma}(0)|\phi\rangle\theta(t) + i\langle\phi|c^\dagger{}_{\mathbf{k}\sigma}(0)\overbrace{|\lambda\rangle\langle\lambda|}^{=1}c_{\mathbf{k}\sigma}(t)|\phi\rangle\theta(-t)\Big]$$

By using energy eigenstates, we are able to write

$$\begin{aligned} \langle\phi|c_{\mathbf{k}\sigma}(t)|\lambda\rangle &= \langle\phi|e^{iHt}c_{\mathbf{k}\sigma}e^{-iHt}|\lambda\rangle = \langle\phi|c_{\mathbf{k}\sigma}|\lambda\rangle e^{i(E_g-E_\lambda)t} \\ \langle\lambda|c_{\mathbf{k}\sigma}(t)|\phi\rangle &= \langle\lambda\phi|e^{iHt}c_{\mathbf{k}\sigma}e^{-iHt}|\phi\rangle = \langle\lambda|c_{\mathbf{k}\sigma}|\phi\rangle e^{i(E_\lambda-E_g)t} \end{aligned} \tag{7.76}$$

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:

$$G(\mathbf{k},t) \ = \ -i\sum_{\lambda}\Big[|\langle\lambda|c^{\dagger}{}_{\mathbf{k}\sigma}|\phi\rangle|^2 e^{-i(E_\lambda - E_g)t}\theta(t) + |\langle\lambda|c_{\mathbf{k}\sigma}|\phi\rangle|^2 e^{-i(E_g-E_\lambda)t}\theta(-t)\Big],$$

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 $\epsilon_{\mathbf{k}} \to E_\lambda - E_g$ in the first term, and $\epsilon_{\mathbf{k}} \to E_g - E_\lambda$ in the second term. We can use this observation to quickly carry out the Fourier transform, whereapon

$$G(\mathbf{k},\omega) \ = \ \sum_{\lambda}\left[\frac{|\langle\lambda|c^{\dagger}{}_{\mathbf{k}\sigma}|\phi\rangle|^2}{\omega - (E_\lambda - E_g)) + i\delta} + \frac{|\langle\lambda|c_{\mathbf{k}\sigma}|\phi\rangle|^2}{\omega - (E_g - E_\lambda) - i\delta}\right]$$

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

$$\begin{aligned}
\sum_{\lambda}|M_\lambda|^2 \ &= \ \sum_{\lambda}|\langle\lambda|c^{\dagger}{}_{\mathbf{k}\sigma}|\phi\rangle|^2 + |\langle\lambda|c_{\mathbf{k}\sigma}|\phi\rangle|^2 \\
&= \ \sum_{\lambda}\langle\phi|c_{\mathbf{k}\sigma}\overbrace{|\lambda\rangle\langle\lambda|}^{=1}c^{\dagger}{}_{\mathbf{k}\sigma}|\phi\rangle + \langle\phi|c^{\dagger}{}_{\mathbf{k}\sigma}\overbrace{|\lambda\rangle\langle\lambda|}^{=1}c_{\mathbf{k}\sigma}|\phi\rangle \\
&= \ \langle\phi|\overbrace{\{c_{\mathbf{k}\sigma}, c^{\dagger}{}_{\mathbf{k}\sigma}\}}^{=1}|\phi\rangle = 1
\end{aligned} \tag{7.77}$$

7.2.3 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

$$H = \sum_{\mathbf{q}}\omega_{\mathbf{q}}[b^{\dagger}{}_{\mathbf{q}}b_{\mathbf{q}} + \frac{1}{2}] \tag{7.78}$$

where physical field operator is related to a sum of creation and annihilation operators:

$$\begin{aligned}
\phi(x) \ &= \ \int_q \phi_{\mathbf{q}}e^{i\mathbf{q}\cdot\mathbf{x}} \\
\phi_{\mathbf{q}} \ &= \ \frac{\hbar}{2m\omega_{\mathbf{q}}}[b_{\mathbf{q}} + b^{\dagger}{}_{-\mathbf{q}}]
\end{aligned} \tag{7.79}$$

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

$$-i\langle\phi|Tb_{\mathbf{q}}(t)b^{\dagger}{}_{\mathbf{q}}(0)|\phi\rangle = -i\theta(t)e^{-i\omega_{\mathbf{q}}t},$$

$$-i\langle\phi|Tb^{\dagger}{}_{-\mathbf{q}}(t)b_{-\mathbf{q}}(0)|\phi\rangle = -i\theta(-t)e^{i\omega_{\mathbf{q}}t}, \tag{7.80}$$

so that

$$D(\mathbf{q},t) = -i\langle\phi|\phi(\mathbf{q},t)\phi(-\mathbf{q},t)|\phi\rangle = -i\frac{\hbar}{2m\omega_{\mathbf{q}}}[\theta(t)e^{-i\omega_{\mathbf{q}}t} + \theta(-t)e^{i\omega_{\mathbf{q}}t}] \tag{7.81}$$

If we Fourier transform this quantity, we obtain the boson propgator,

$$\begin{aligned} D(\mathbf{q},\nu) &= \int_{-\infty}^{\infty} dt e^{-\delta|t|+i\nu t} D(\mathbf{q},t) \\ &= -i\frac{\hbar}{2m\omega_{\mathbf{q}}}\left[\frac{1}{\delta - i(\nu-\omega_{\mathbf{q}})} + \frac{1}{\delta + i(\nu-\omega_{\mathbf{q}})}\right] \end{aligned} \tag{7.82}$$

or

$$D(\mathbf{q},\nu) = \frac{\hbar}{2m\omega_{\mathbf{q}}}\left[\frac{2\omega_{\mathbf{q}}}{\nu^2 - (\omega_{\mathbf{q}} - i\delta)^2}\right], \qquad \text{Bose propagator} \tag{7.83}$$

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.

$$D(\mathbf{q},\nu) = \frac{\hbar}{2m\omega_{\mathbf{q}}}\left[\frac{\overbrace{1}^{\text{emission}}}{\nu - (\omega_{\mathbf{q}} - i\delta)} + \frac{\overbrace{1}^{\text{absorption}}}{-\nu - (\omega_{\mathbf{q}} - i\delta)}\right] \tag{7.84}$$

- 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

$$H_{int} = g\int d^3x \phi(\mathbf{x})\rho(\mathbf{x}) \tag{7.85}$$

The exchange of virtual bosons between particles gives rise to *retarded* interactions,

$$V(\mathbf{q},t-t') = \frac{g^2}{\hbar}D(\mathbf{q},t-t'), \tag{7.86}$$

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 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:

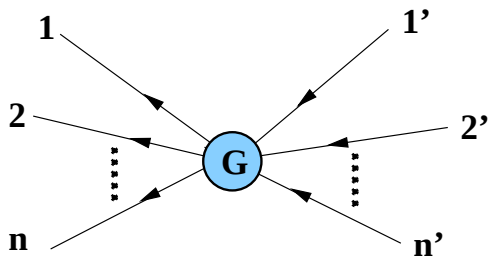
$$\overbrace{\{1', 2' \ldots n'\}}^{\text{initial particle positions}} \xrightarrow{G} \overbrace{\{1', 2' \ldots n'\}}^{\text{final particle positions}} \tag{7.87}$$

where $1' \equiv (\mathbf{x}', t'), etc.$ and $1 \equiv (\mathbf{x}, t), etc.$. The n-particle Green's function is defined as

$$G(1, 2, \ldots n; 1', 2', \ldots n') = (-i)^n \langle \phi | T\psi(1)\psi(2) \ldots \psi(n)\psi^\dagger(n') \ldots \psi^\dagger(1') | \phi \rangle$$

and represented diagramatically as

$G(1, 2, \ldots n; 1', 2', \ldots n') =$



(7.88)

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 $(1, 2, \ldots n)$. The amplitude for this process is

$$G(\mathbf{r} - P'_{\mathbf{r}}) \tag{7.89}$$

and the overall amplitude for all n-particles to go from locations P'_r to positions r is then

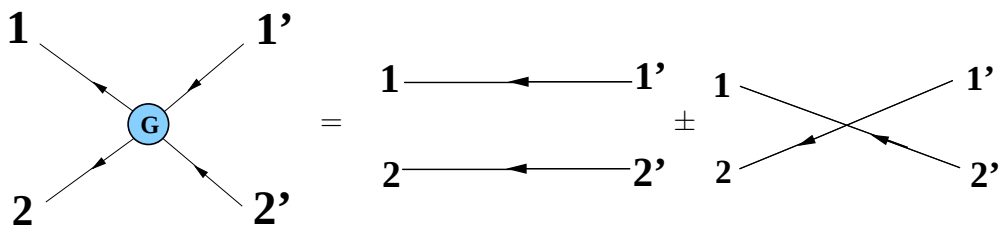
$$\zeta^p G(1 - P'_1) G(2 - P'_2) \ldots G(n - P'_n) \tag{7.90}$$

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:

$$G(\mathbf{1}, \mathbf{2}, \ldots \mathbf{n}; \mathbf{1}', \mathbf{2}', \ldots \mathbf{n}') = \sum \zeta^P \prod_{r=1,n} G(\mathbf{r} - P'_r) \tag{7.91}$$

For example, the two-body Green's function is given by

$$G(\mathbf{1},\mathbf{21}',\mathbf{2}') \;=\; G(\mathbf{1},\mathbf{1}')G(\mathbf{2},\mathbf{2}') \pm G(\mathbf{1},\mathbf{2}')G(\mathbf{2},\mathbf{1}')$$



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

$$\langle\phi|T\ldots\overbrace{\psi(1)\ldots\psi^\dagger(2)}\ldots|\phi\rangle \;\longrightarrow\; \langle\phi|T\psi(1)\psi^\dagger(2)|\phi\rangle = iG(1-2)$$

$$\langle\phi|T\ldots\overbrace{\psi^\dagger(2)\ldots\psi(1)}\ldots|\phi\rangle \;\longrightarrow\; \langle\phi|T\psi^\dagger(2)\psi(1)|\phi\rangle = \pm iG(1-2)$$

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

$$\langle\phi|T\psi(1)\psi(2)\ldots\psi(n)\ldots\psi^\dagger(P_2')\ldots\psi^\dagger(P_1')\ldots\psi^\dagger(P_n')|\phi\rangle$$

$$= \;\zeta^P G(\mathbf{1}-P_1')G(\mathbf{2}-P_2')\ldots G(\mathbf{n}-P_n') \tag{7.92}$$

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

$$\langle\phi|\;\; T\;\; \psi(1)\psi(2)\ldots\psi^\dagger(n')|\phi\rangle =$$

$$\sum_{\text{All contractions}} \langle\phi|T\psi(1)\psi(2)\ldots\psi(n)\ldots\psi^\dagger(P_2')\ldots\psi^\dagger(P_1')\ldots\psi^\dagger(P_n')|\phi\rangle$$

Example: Show how the expansion of the generating functional can be used to derive Wick's theorem.

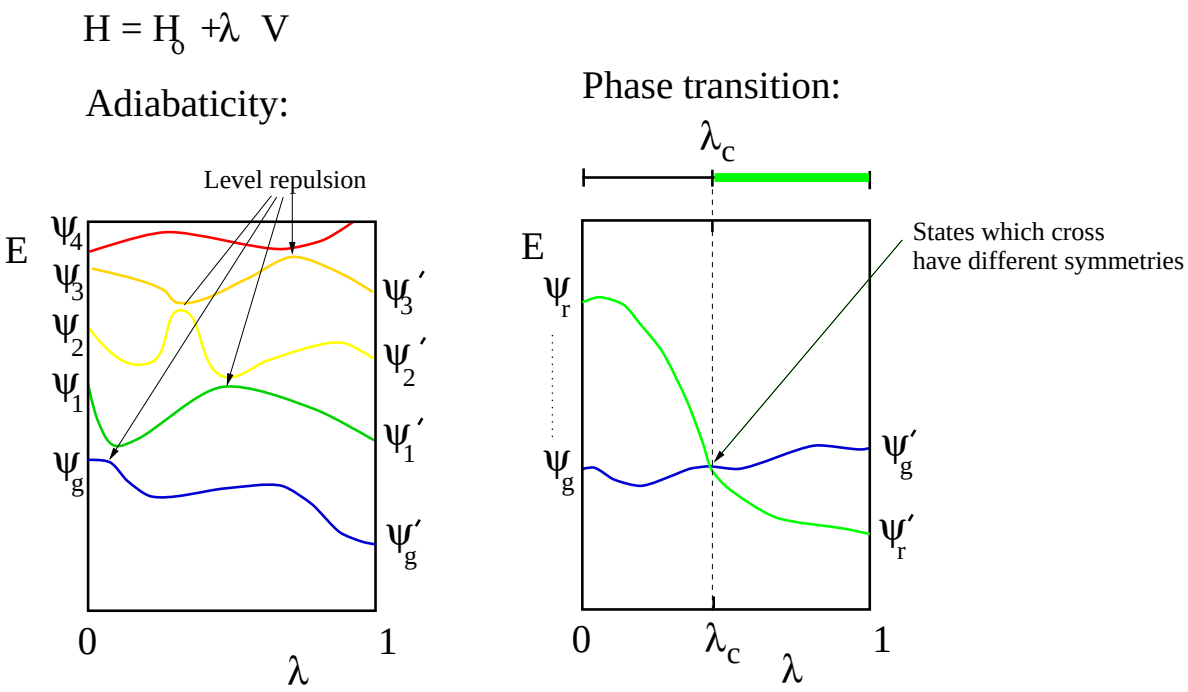


Figure 7.4: Illustrating the evolution of the Hilbert space as the Hamiltonian is adiabatically evolved. In the first case, the ground-state can be adiabatically evolved all the way to $\lambda = 1$. In the second case, a phase transition occurs at $\lambda = \lambda_c$, where a previously excited state, with a different symmetry to the ground-state crosses below the ground-state.

7.4 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 from H_o to H, i.e, if $\hat{V} = H - H_o$, we imagine that the state time-evolves according to the Hamiltonian

$$\begin{aligned} H(t) &= H_o + \lambda(t)V \\ \lambda(t) &= e^{-|t|\delta} \end{aligned} \tag{7.93}$$

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.

7.4.1 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

$$\begin{aligned} \langle 0|TA(t_1)B(t_2)\dots R(t_r)|0\rangle_H &= \langle +\infty|TS[\infty,-\infty]A(t_1)B(t_2)\dots R(t_r)|-\infty\rangle_I \\ S[\infty,-\infty] &= T\exp\Big[-i\int_{-\infty}^{\infty} V(t')dt'\Big] \end{aligned} \tag{7.94}$$

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

$$\langle +\infty| = \frac{\langle -\infty|}{\langle -\infty|+\infty\rangle} \tag{7.95}$$

and the Gell-Mann Lowe formula becomes

$$\langle 0|TA(t_1)B(t_2)\dots R(t_r)|0\rangle_H = \frac{\langle -\infty|TS[\infty,-\infty]A(t_1)B(t_2)\dots R(t_r)|-\infty\rangle_I}{\langle -\infty|S[\infty,-\infty]|-\infty\rangle} \tag{7.96}$$

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,

$$|\psi_I(t)\rangle = U(t)|\psi_H\rangle \tag{7.97}$$

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

$$A_H(t) = U^\dagger(t)A_I U(t) \tag{7.98}$$

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,

$$\langle -\infty|S^\dagger(t_1,-\infty) = \langle\infty|S(\infty,t_1) \tag{7.99}$$

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,

$$\langle 0|T[A(t_1)\dots R(t_r)]|0\rangle_H = \langle +\infty|T[S(\infty,-\infty)A_I(t_1)B(t_2)\dots R_I(t_r)]|-\infty\rangle \qquad (7.100)$$

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.

7.4.2 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

$$N(0) = 2\frac{(4\pi)p^2}{(2\pi\hbar)^3}\frac{dp}{dE}\bigg|_{p=p_F} = \frac{mp_F}{\pi^2\hbar^3} \qquad (7.101)$$

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,

$$\chi = g\mu_B(N_\uparrow - N_\downarrow)/B = \mu_f^2 N(0) \qquad (7.102)$$

is the "Pauli paramagnetic susceptibility" . In a degenerate Fermi liquid, the energy is given by

$$E(T) - \mu N = \sum_{\mathbf{k}\sigma=\pm\mathbf{1/2}} \epsilon_{\mathbf{k}} \frac{1}{e^{\beta\epsilon_{\mathbf{k}}}+1} \qquad (7.103)$$

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

$$\begin{aligned} C_V = \frac{dE}{dT} &= N(0)\int_{-\infty}^{\infty} d\epsilon \epsilon \frac{d}{dT}\left(\frac{1}{e^{\beta\epsilon}+1}\right) \\ &= N(0)k_B^2 T \overbrace{\int_{-\infty}^{\infty} dx \frac{x^2}{(e^x+1)(e^{-x}+1)}}^{\pi^2/3} = \overbrace{\frac{\pi^2}{3}N(0)k_B^2\, T}^{=\gamma} \end{aligned} \tag{7.104}$$

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:

$$\frac{\chi}{\gamma} = g^2 \frac{3\mu_B^2}{\pi^2 k_B^2} \tag{7.105}$$

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

$$\begin{aligned} m^* &= (3.1) m_{(\mathrm{He}^3)}, \\ (g^*)^2 &\approx 3(g^2)_{(\mathrm{He}^3)}, \end{aligned} \tag{7.106}$$

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.*[**?**]

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

$$\Psi = |n_{\mathrm{p}_1\sigma_1},\ n_{\mathrm{p}_2\sigma_2}, \ldots\rangle \tag{7.107}$$

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

$$\mathrm{Ground-state}\ \Psi_{\mathrm{o}} \qquad : \quad n_{\mathrm{p}\sigma} = \begin{cases} 1 & (\mathrm{p} < \mathrm{p_F}) \\ 0 & (\text{otherwise } \mathrm{p} > \mathrm{p_F}) \end{cases} \tag{7.108}$$

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:

$$\mathrm{Quasi-particle}: \ \Psi_{\mathrm{p_o}} \qquad n_{\mathrm{p}} = \begin{cases} 1 & (\mathrm{p} < \mathrm{p_F} \text{ and } \mathrm{p} = \mathrm{p_o}) \\ 0 & (\text{otherwise}) \end{cases} \tag{7.109}$$

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

$$\epsilon_{\mathrm{p_o}} = E(p_o) - E_o \tag{7.110}$$

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:

$$(\mathrm{p}_1, \mathrm{p}_2) \to (\mathrm{p}_1 - \mathrm{q}, \mathrm{p}_2 + \mathrm{q}) \qquad (\mathrm{q} = 0 \qquad \text{On Fermi surface.}) \tag{7.111}$$

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 $\delta n_{\mathrm{p}\sigma} = n_{\mathrm{p}\sigma} - n^{(o)}_{\mathrm{p}\sigma}$ from equilibrium. This leads to the Landau energy functional for the Fermi surface,

$$E(\{n_{\mathrm{p}\sigma}\}) = E_0 + \sum_{\mathrm{p}\sigma} \epsilon_{\mathrm{p}} \delta n_{\mathrm{p}\sigma} + \frac{1}{2} \sum_{\mathrm{p},\mathrm{p}',\sigma,\sigma'} f_{\mathrm{p}\sigma,\mathrm{p}'\sigma'} \delta n_{\mathrm{p}\sigma} \delta n_{\mathrm{p}'\sigma'} + \ldots \tag{7.112}$$

where

$$\epsilon_{\mathrm{p}} \ = \ \frac{\delta E}{\delta n_{\mathrm{p}\sigma}}$$

$$f_{\mathrm{p}\sigma,\mathrm{p}'\sigma'} = \frac{\delta^2 E}{\delta n_{\mathrm{p}\sigma}\delta n_{\mathrm{p}'\sigma'}} \tag{7.113}$$

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

$$\frac{\delta E}{\delta n_{\mathrm{p}\sigma}} = \epsilon_{\mathrm{p}} + \sum_{\mathrm{p}'\sigma'} f_{\mathrm{p}\sigma,\mathrm{p}',\sigma'}\delta n_{\mathrm{p}'\sigma'}. \tag{7.114}$$

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

$$f_{\mathrm{p}\sigma,\mathrm{p}',\sigma'} = f^s_{\mathrm{p},\mathrm{p}'} + f^a_{\mathrm{p},\mathrm{p}'}\sigma\sigma'. \tag{7.115}$$

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

$$N(0)f^{s,a}_{\mathrm{p},\mathrm{p}'} = F^{s,a}_{\mathrm{p},\mathrm{p}'} = \sum_{l=0}^{\infty}(2l+1)F^{s,a}_l P_l(\cos\theta_{\vec{\mathrm{p}},\vec{\mathrm{p}}'}) \tag{7.116}$$

where

$$N(0) = \frac{m^* p_F}{\pi^2\hbar^3} \tag{7.117}$$

is the density of one-particle quasiparticle states at the Fermi energy. The parameters F^s_l and F^a_l 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.

$$S = -k_B\sum_{\mathbf{p},\sigma}[n_{\mathbf{p}\sigma}\ln n_{\mathbf{p}\sigma} + (1-n_{\mathbf{p}\sigma})\ln(1-n_{\mathbf{p}\sigma})] \tag{7.118}$$

The complete free energy is then the sum of (7.114) and (7.118). Taking the variation with respect to small changes in $n_{\mathbf{p}\sigma}$, we obtain

$$\delta F = \sum_{\mathbf{p}\sigma}\delta n_{\mathbf{p}\sigma}\left[\epsilon_{\mathbf{p}} + k_B T\ln\left(\frac{n_{\mathbf{p}\sigma}}{1-n_{\mathbf{p}\sigma}}\right)\right] + \emptyset(\delta {n_{\mathbf{p}\sigma}}^2) \tag{7.119}$$

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.

$$n_{\mathbf{p}\sigma} = \frac{1}{e^{\beta\epsilon_{\mathbf{p}}} + 1} \tag{7.120}$$

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. This changes its inertia, modifying its energy, as follows

$$\begin{aligned} m &\longrightarrow m^* \\ \epsilon(\mathrm{p}) &= \frac{\mathrm{p}^2}{2m^*} - \epsilon_F. \end{aligned} \tag{7.121}$$

Landau was able to relate the renormalized mass m^* to the interactions. He did this by considering two situations

1. One quasiparticle added at momentum $m\mathbf{u}$ above a stationary Fermi sea.
2. One quasiparticle added at the Fermi energy, above a Fermi sea moving backwards at velocity $-\mathbf{u}$.

Using the "Galilean" equivalence of the two situations, he argued that the momentum carried by the quasiparticle could be written

$$\vec{\mathrm{p}} = m\vec{v}(1 + \frac{1}{3}F_1^s) \tag{7.122}$$

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 $\vec{v} = \vec{\mathrm{p}}/m^*$, it follows that $\vec{\mathrm{p}} = \frac{m}{m^*}(1 + \frac{1}{3}F_1^s)\vec{\mathrm{p}}$ or

$$\frac{m^*}{m} = 1 + \frac{1}{3}F_1^s \tag{7.123}$$

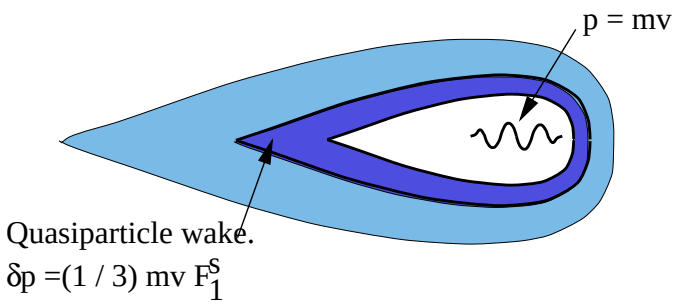


Figure 7.5: Illustrating the wake of particle-hole excitations that moves with a quasiparticle.

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 $\mathbf{u}$, to leading order in $\mathbf{u}$, the energy and momenta are

$$(E', \mathbf{P}') = (E - \mathbf{P}\cdot\mathbf{u}, \mathbf{P} - M\mathbf{u}) \tag{7.124}$$

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

$$\begin{aligned} E &= E[n_{\mathbf{p}\sigma}], \\ \mathbf{P} &= \sum_{\mathbf{p},\sigma} \mathbf{p} n_{\mathbf{p}\sigma}. \end{aligned} \tag{7.125}$$

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.

$$n'_{\mathbf{p}\sigma} = n_{\mathbf{p}+m\mathbf{u}\sigma} = n_{\mathbf{p}\sigma} + m\mathbf{u}\cdot\nabla_{\mathbf{p}}\mathbf{n}_{\mathbf{p}\sigma} \tag{7.126}$$

This means that the energy in the moving frame is given by

$$E' = E[n'_{\mathbf{p}\sigma}] = E[n_{\mathbf{p}\sigma}] + \sum_{\mathbf{p}\sigma} \frac{\delta E}{\delta n_{\mathbf{p}\sigma}} m\mathbf{u}\cdot\nabla_{\mathbf{p}}\mathbf{n}_{\mathbf{p}\sigma} \tag{7.127}$$

The second term can be integrated by parts to yield

$$E[n'_{\mathbf{p}\sigma}] = E[n_{\mathbf{p}\sigma}] - \mathbf{u}\cdot\sum_{\mathbf{p}\sigma} m\mathbf{v}_{\mathbf{p}\sigma}\mathbf{n}_{\mathbf{p}\sigma} \tag{7.128}$$

where we have identified the group velocity of each quasiparticle by

$$\mathbf{v}_{\mathbf{p}\sigma} = \nabla_{\mathbf{p}}\left(\frac{\delta E}{\delta n_{\mathbf{p}\sigma}}\right) \tag{7.129}$$

By comparing (7.128) with (7.124) we thus see that in the original Lab frame there are two ways of writing the momentum

$$\mathbf{P} = \sum_{\mathbf{p}\sigma} \mathbf{p} n_{\mathbf{p}\sigma} = m\sum_{\mathbf{p}\sigma} \mathbf{v}_{\mathbf{p}\sigma} n_{\mathbf{p}\sigma} \tag{7.130}$$

This is not as absurdly simple as it seems, for this seemingly innocuous little equation hides the fact that $\mathbf{v}_{\mathbf{p}\sigma}$ depends on the distribution of particles.

If we now examine the variation of the right-hand-side of (7.130) with respect to the quasiparticle occupancies, we obtain

$$\delta\mathbf{P} = m\sum_{\mathbf{p}\sigma}\mathbf{v}_{\mathbf{p}\sigma}\delta n_{\mathbf{p}\sigma} + (\delta\mathbf{v}_{\mathbf{p}\sigma})n_{\mathbf{p}\sigma} \tag{7.131}$$

Using (7.114), we see that

$$\delta(v_{\mathbf{p}\sigma}) = \sum_{\mathbf{p}'\sigma'}\nabla_{\mathbf{p}}\left(\frac{\delta^2 E}{\delta n_{\mathbf{p}\sigma}\delta n_{\mathbf{p}'\sigma'}}\right)\delta n_{\mathbf{p}'\sigma'} = \sum_{\mathbf{p}\sigma'}\nabla_{\mathbf{p}} f_{\mathbf{p}\sigma,\mathbf{p}'\sigma'}\delta n_{\mathbf{p}'\sigma'} \tag{7.132}$$

so that

$$\begin{aligned}\delta\mathbf{P} &= m\sum_{\mathbf{p}\sigma}\delta n_{\mathbf{p}\sigma}\left(\mathbf{v}_{\mathbf{p}\sigma} + (\nabla_{\mathbf{p}'} f_{\mathbf{p}\sigma,\mathbf{p}'\sigma'})n_{\mathbf{p}'\sigma'}\right)\\ &= \sum_{\mathbf{p}\sigma}\delta n_{\mathbf{p}\sigma}\left(m\mathbf{v}_{\mathbf{p}\sigma} - \overbrace{m f_{\mathbf{p}\sigma,\mathbf{p}'\sigma'}\nabla_{\mathbf{p}'}n_{\mathbf{p}'\sigma'}}^{\mathbf{p}_{\rm wake}}\right)\end{aligned} \tag{7.133}$$

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 $\mathbf{p}$ on the Fermi surface, we obtain

$$\mathbf{p}_{\rm wake} = -m\sum_{\mathbf{p}\sigma'} f_{\mathbf{p}\sigma,\mathbf{p}'\sigma'}\nabla_{\mathbf{p}'}n^{(0)}_{\mathbf{p}'\sigma'} \quad = \quad 2m\int_{\mathbf{p}'} f^s_{\mathbf{p}\mathbf{p}'}\mathbf{v}_{\mathbf{p}'}\delta(\epsilon_{\mathbf{p}'}) \tag{7.134}$$

Replacing

$$2\int_{\mathbf{p}'}\delta(\epsilon_{\mathbf{p}'}) = N(0)\int\frac{d\Omega_{\hat{\mathbf{p}}'}}{4\pi} \tag{7.135}$$

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

$$\mathbf{p}_{\rm wake} \quad = \quad m\mathbf{v}\int\frac{d\Omega_{\hat{\mathbf{p}}'}}{4\pi}\overbrace{N(0)f^s(\cos\theta)}^{F^s(\cos\theta)}\cos\theta \tag{7.136}$$

where $\cos\theta = \hat{\mathbf{p}}\cdot\hat{\mathbf{p}}'$. Using the Legendre decomposition of the interaction (7.116), this is then

$$p_{wake} = m\mathbf{v}\overline{F^s(\cos\theta)\cos\theta} = \frac{1}{3}m\mathbf{v}F^s_1 \tag{7.137}$$

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

$$C_V^* = \frac{m^*}{m} C_V \tag{7.138}$$

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,

$$\chi^* = \frac{m^*}{m(1 - F_0^a)} \chi \tag{7.139}$$

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. 7.6(b)).

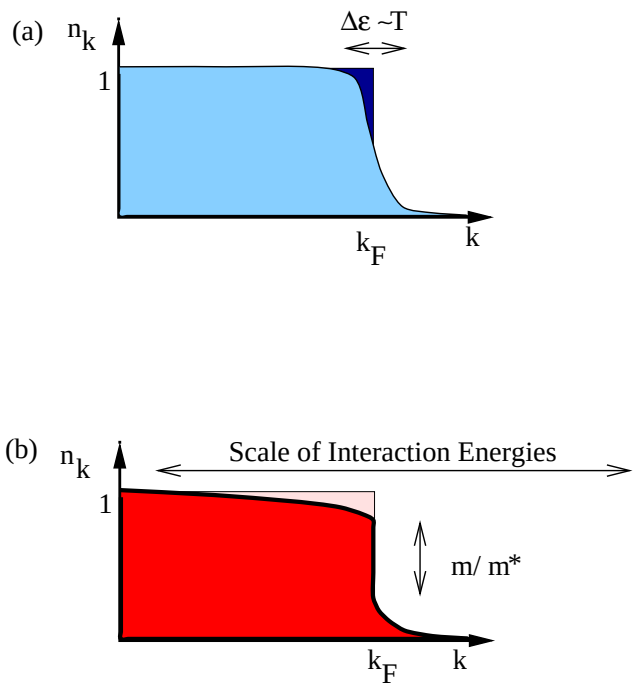


Figure 7.6: (a) A temperature T that is smaller than the Fermi energy, slightly "blurs" the Fermi surface; (b) even though the interaction energy is greater than the temperature, often greater than the Fermi energy, in a Fermi liquid, the exclusion principle stabilizes the jump in occupancy at the Fermi surface.

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.

$$\begin{aligned}\langle\phi|T\psi(1)\psi^\dagger(2)|\phi\rangle &= \frac{\langle\phi_o|T\hat{S}\psi(1)\psi^\dagger(2)|\phi_o\rangle}{\langle\phi_o|\hat{S}|\phi_o\rangle} \\ \hat{S} &= T\exp\left[-i\int_{-\infty}^{\infty}V(t')dt'\right] \end{aligned} \tag{8.1}$$

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

$$S = \langle\phi_o|\hat{S}|\phi_o\rangle = \sum\{\text{Unlinked Feynman Diagrams}\} \tag{8.2}$$

- The logarithm of the $S-$ matrix, which is directly related to the shift in the ground-state energy due to interactions.

$$E - E_o = \lim_{\tau\to\infty}\frac{\partial}{\partial\tau}\ln\langle\phi_o|S[\tau/2,-\tau/2]|\phi_o\rangle = i\sum\{\text{Linked Feynman Diagrams}\} \tag{8.3}$$

- Green's functions.

$$G(1-2) = \sum\{\text{Two-legged Feynman Diagrams}\} \tag{8.4}$$

- Response functions. These are a different type of Green's function, of the form

$$\mathcal{R}(1-2) = -i\langle\phi|[A(1),B(2)]|\phi\rangle\theta(t_1-t_2) \tag{8.5}$$

Before we start discussing Feynman diagrams, a word on how how they were derived. Feynman initially derived his diagramatic expansion as a mnemonic device for calculating scattering amplitudes. His approach was heuristic: each diagram had 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 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.

$$\langle\phi_o|\hat{S}|\phi_o\rangle = \sum_{n=0}^{\infty}\frac{(-i)^n}{n!}\int_{-\infty}^{\infty}dt_1\ldots dt_n \sum_{\text{Contractions}} \langle\phi_o|V(t_1)V(t_2)\ldots V(t_n)|\phi_o\rangle \tag{8.6}$$

8.0.3 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

$$\hat{S}[\bar{z},z] = T\exp\left[i\int d1[\psi^\dagger(1)z(1)+\bar{z}(1)\psi(1)]\right]. \tag{8.7}$$

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 expecation value of this S-matrix is then

$$S[\bar{z},z] = \langle\phi|\hat{S}[\bar{z},z]|\phi\rangle = \exp\left[-i\int d1d2\bar{z}(1)G(1-2)z(2)\right] \tag{8.8}$$

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

$$\int d1d2\bar{z}(1)G(1-2)z(2) = \bar{z} \longleftarrow z \tag{8.9}$$

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

$$S[\bar{z},z] = \exp\Big[-i\bar{z} \longleftarrow z\Big] \tag{8.10}$$

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

$$\begin{aligned} -i\frac{\delta}{\delta\bar{z}(1)} &\rightarrow \psi(1) \\ -i\frac{\delta}{\delta\bar{z}(1)}\langle\phi|T\hat{S}\{\ldots\}|\phi\rangle &= \langle\phi|T\hat{S}\{\psi(1)\ldots\}|\phi\rangle \end{aligned} \tag{8.11}$$

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

$$-i\zeta\frac{\delta}{\delta z(1)} \rightarrow \psi^\dagger(1) \tag{8.12}$$

Here our familiar $\zeta = -1$ for fermions, appears because in this case z anticommutes with the field operators $\psi^\dagger(1)z(1) = -z(1)\psi^\dagger(1)$. For example, the field operator has an expectation value

$$\begin{aligned} \langle\psi(1)\rangle &= \frac{\langle\phi|\hat{S}[\bar{z},z]\psi(1)|\phi\rangle}{\langle\phi|\hat{S}[\bar{z},z]|\phi\rangle} = -i\frac{\delta}{\delta\bar{z}(1)}\ln S[\bar{z},z] \\ &= -\int G(1-2)z(2)d2 \\ &\equiv -[1 \longleftarrow z] \end{aligned} \tag{8.13}$$

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. If we now differentiate (8.13) w.r.t. z(2), we obtain

$$-i\,\frac{\delta}{\delta z(2)}\langle\psi(1)\rangle\Big|_{z=\bar{z}=0} = \langle\phi|T\psi(1)\psi^\dagger(2)|\phi\rangle = iG(1-2) \tag{8.14}$$

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.

$$\langle\phi|T\hat{S}[\bar{z},z]F[\psi^\dagger,\psi]|\phi\rangle = F\left[-i\zeta\frac{\delta}{\delta z},-i\frac{\delta}{\delta\bar{z}}\right]\exp\left[-i\bar{z} \longleftarrow z\right]. \tag{8.15}$$

If we now set $F[\psi^\dagger,\psi] = Te^{-i\int V[\psi^\dagger,\psi]dt}$, then

$$S_I[\bar{z},z] = \langle\phi|Te^{-i\int_{-\infty}^{\infty}dt\left(V(\psi^\dagger,\psi)+\text{source terms}\right)}|\phi\rangle \tag{8.16}$$

can be written completely algebraically, in the form

$$S_I[\bar{z},z] = e^{-i\int_{-\infty}^{\infty}V(-i\zeta\frac{\delta}{\delta z},-i\frac{\delta}{\delta\bar{z}})dt}\exp\left[-i\bar{z} \longleftarrow z\right] \tag{8.17}$$

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

$$\mathcal{S}_I[\bar{\alpha}, \alpha] = e^{-(i)^{(n+1)}\int_{-\infty}^{\infty} V(\frac{\delta}{\delta\bar{\alpha}}, \frac{\delta}{\delta\alpha})dt} \exp\Big[\bar{\alpha} \longleftarrow \alpha\Big]$$

where we have written

$$V(-i\zeta\frac{\delta}{\delta z}, -i\frac{\delta}{\delta\bar{z}}) = i^n V(\frac{\delta}{\delta\bar{\alpha}}, \frac{\delta}{\delta\alpha}) \tag{8.18}$$

for an interaction involving n creation and n annihilation operators (n-particle interaction). We should like to recast this in a still more graphical form. For a one-particle scattering potential ($n = 1$), we write

$$-(i)^2 V(\frac{\delta}{\delta\bar{\alpha}}, \frac{\delta}{\delta\alpha}) = \int d^3x U(x) \frac{\delta}{\delta\bar{\alpha}(x)} \frac{\delta}{\delta\alpha(x)} \tag{8.19}$$

which we denote as

$\frac{\delta}{\delta\alpha(1)}$

$\frac{\delta}{\delta\bar{\alpha}(1)}$ (8.20)

whereas for a two-particle interaction,

$$-(i)^3 V(\frac{\delta}{\delta\bar{\alpha}}, \frac{\delta}{\delta\alpha}) = i\frac{1}{2}\int d^3x d^3x' V(x - x') \frac{\delta}{\delta\bar{\alpha}(x)} \frac{\delta}{\delta\bar{\alpha}(x')} \frac{\delta}{\delta\alpha(x')} \frac{\delta}{\delta\alpha(x)} \tag{8.21}$$

which we denote as

$\frac{\delta}{\delta\alpha(2)}$ $\frac{\delta}{\delta\alpha(1)}$

$\frac{1}{2}$

$\frac{\delta}{\delta\bar{\alpha}(2)}$ $\frac{\delta}{\delta\bar{\alpha}(1)}$ (8.22)

Schematically then, our Feynman diagram expansion can be written as

$$\mathcal{S}_I[\bar{\alpha}, \alpha] = \exp\Big[\begin{matrix}\frac{\delta}{\delta\alpha(1)} \\ \\ \frac{\delta}{\delta\bar{\alpha}(1)}\end{matrix}\Big] \exp\Big[\bar{\alpha} \longleftarrow \alpha\Big]$$

for scattering off a one-body potential, and

$$\mathcal{S}_I[\bar{\alpha},\alpha] = \exp\Big[\frac{1}{2}\frac{\delta}{\delta\alpha(2)}\frac{\delta}{\delta\bar{\alpha}(2)}\times\frac{\delta}{\delta\alpha(1)}\frac{\delta}{\delta\bar{\alpha}(1)}\Big]\exp\Big[\bar{\alpha}\longleftarrow\alpha\Big]$$

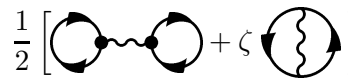
for the S-matrix of interacting particles. These equations provide the basis for a Feynman diagram expansion. The differential operators acting on the bare S-matrix, glue the scattering vertices to the ends of the propagators, and thereby generate a sum of all possible Feynman diagrams. Formally, we must expand the exponentials on both sides, e.g.

$$\mathcal{S}_I[\bar{\alpha},\alpha] = \sum_{n,m}\frac{1}{n!m!}\Big[\frac{1}{2}\frac{\delta}{\delta\alpha(2)}\frac{\delta}{\delta\bar{\alpha}(2)}\times\frac{\delta}{\delta\alpha(1)}\frac{\delta}{\delta\bar{\alpha}(1)}\Big]^n\Big[\bar{\alpha}\longleftarrow\alpha\Big]^m \tag{8.23}$$

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. The Feynman rules tell us how to convert the diagrams into scattering amplitures. These rules are summarized in table 8.1.

Let us look at some of the leading diagrams that appear in this process. For instance

$$\frac{1}{2!}\Big[\frac{1}{2}\frac{\delta}{\delta\alpha(2)}\frac{\delta}{\delta\bar{\alpha}(2)}\times\frac{\delta}{\delta\alpha(1)}\frac{\delta}{\delta\bar{\alpha}(1)}\Big]\Big[\bar{\alpha}\longleftarrow\alpha\Big]^2 \;=\; \frac{1}{2}\Big[$$



$$+\,\zeta$$

$$\Big].$$

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. 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

$$\zeta(2S+1) \tag{8.24}$$

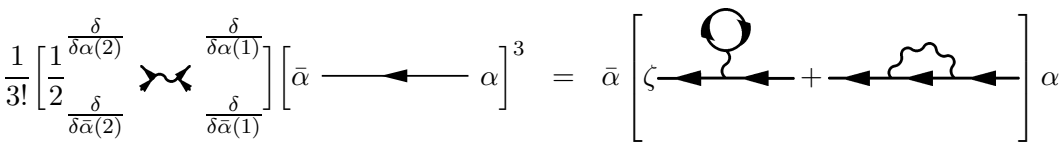
per fermion loop. This is the origin of the factor ζ in the second linked cluster diagram above. The algebraic rendition of these Feynman diagrams is then

$$\frac{1}{2}\int d1d2V(1-2)\Big[(2S+1)^2G(0,0^-)^2+\zeta(2S+1)G(1-2)G(2-1)\Big] \tag{8.25}$$

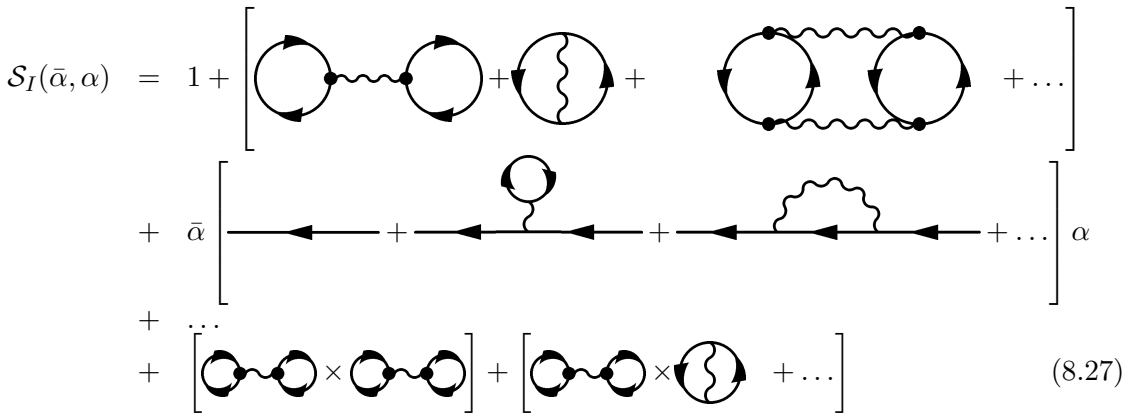
Notice finally, that the first Hartree diagram contains a propagator which "bites its own tail". This comes from a contraction of the density operator,

$$-i\sum_\sigma\langle\ldots\sigma\psi_\sigma{}^\dagger(\mathbf{x},t)\psi_\sigma(\mathbf{x},t)\ldots\rangle = -(2S+1)G(\mathbf{x},0^-) \tag{8.26}$$

and since the creation operator lies to the left of the destruction operator, for fermions, we pick up a minus sign. 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



(8.27)

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.

8.0.4 Symmetry factors

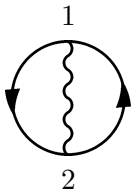
Remarkably, in making the contractions of the S-matrix, the prefactors in terms like eq. (10.17) are almost completely absorbed by the combinatorics. The number of ways of making the contractions of the two terms in (10.17) are given by

$$\frac{2^n n! m!}{p} \tag{8.28}$$

where the term in the denominator is the "symmetry factor". The topology of each Feynman is invariant under certain group of permutations of the vertices. p is the dimension of this

group. The denominator p arises because the quantity $2^n n! m$ overcounts the p permutations of the vertices that leave the diagram unchanged.

Consider the simplest diagram,

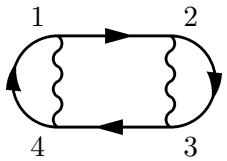


(8.29)

This diagram is topologically invariant under the group of permutations

$$\mathcal{G} \;=\; \{(12),(21)\} \tag{8.30}$$

so $p = 2$. In a second example

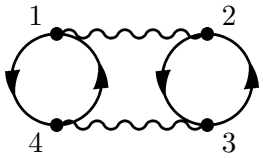


(8.31)

the invariance group is

$$\mathcal{G} \;=\; \{(1234),(3412)\} \tag{8.32}$$

so once again, $p = 2$. By contrast, for the diagram



(8.33)

the invariance group is

$$\mathcal{G} \;=\; \{(1234),(3412),(2143),(4312)\} \tag{8.34}$$

so that $p = 4$.

8.0.5 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:

$$\ln S_I[\bar{z}, z] = \sum \{\text{Linked Cluster Diagrams}\} \tag{8.35}$$

To show this result, we shall employ a trick called the "replica trick", which takes advantage of the relation

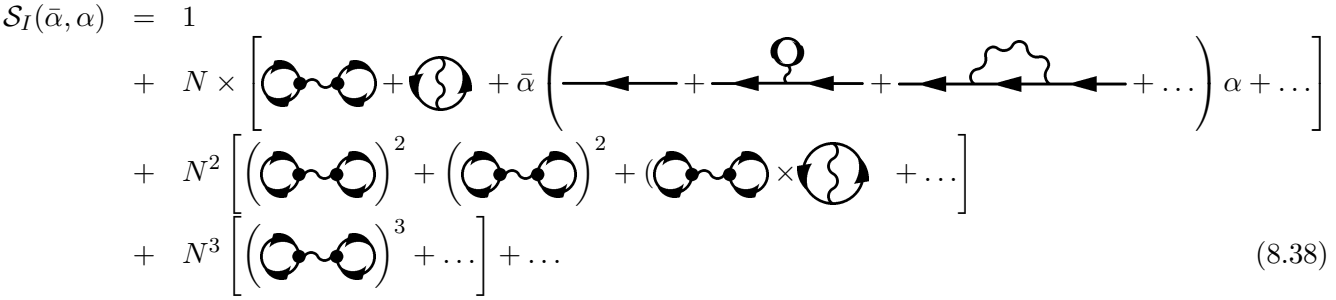
$$\ln S = \lim_{n\to 0}\left[\frac{S^n - 1}{n}\right] \tag{8.36}$$

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

$$(S_I[\bar{z}, z])^N = \langle\phi|Te^{-i\int_{-\infty}^{\infty} dt \sum_\lambda (V(\psi_\lambda{}^\dagger, \psi_\lambda) + \text{source terms})}|\phi\rangle \tag{8.37}$$

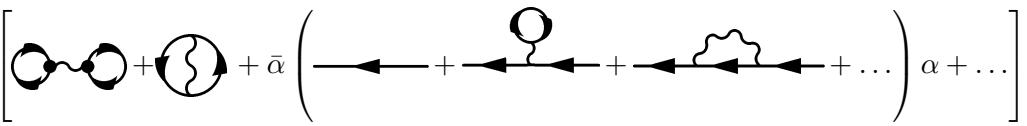
When we expand this, we will generate exactly the same Feynman diagrams as in S, excepting that now, for each linked Feynman diagram, we will have to multiply the amplitude by N. The diagram expansion for interacting fermions will look like

$\mathcal{S}_I(\bar{\alpha}, \alpha) = 1$



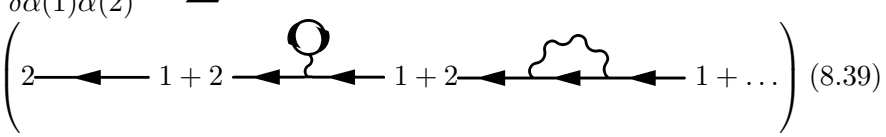
(8.38)

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



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

$$G(1-2) = \frac{\delta \ln \mathcal{S}_I(\bar{\alpha}, \alpha)}{\delta\alpha(1)\bar{\alpha}(2)} = \sum\{\text{Two leg diagrams}\}$$



(8.39)

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,

$$G(1-2) = -i\frac{\langle\phi|TS\psi(1)\psi^\dagger(2)|\phi\rangle}{\langle\phi|S|\phi\rangle} \tag{8.40}$$

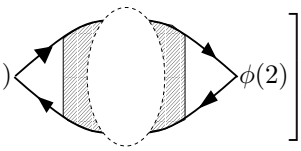
we would have to consider the quotient of two sets of Feynman diagrams, coming from the contractions of the denominator and numerator. Remarkably, the unlinked diagrams of the S matrix in the numerator cancel the unlinked diagrams appearing in the Wick expansion of the denominator, leaving us with this 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

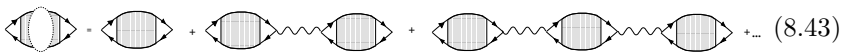
Example: By introducing a chemical potential source term into the original Hamiltonian,

$$H = \int d^3x \delta\phi(x,t)\hat{\rho}(x) \tag{8.41}$$

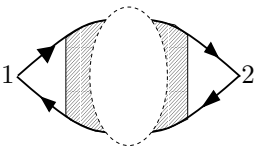
show that the change in the logarithm of the S-matrix is

$$\ln S[\phi] = \ln S[0] + \frac{1}{2}\left[\phi(1)\right.$$  $$\left.\phi(2)\right] \tag{8.42}$$

where

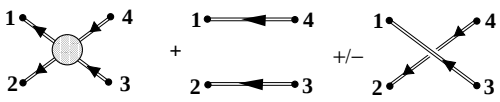
 (8.43)

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

$$i\langle\phi|T\delta\rho(1)\delta\rho(2)|\phi\rangle = -i\frac{\delta^2}{\delta\phi(1)\delta\phi(2)}\ln S[\phi] = 1$$  $$2 \tag{8.44}$$

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

$$\frac{1}{S[\bar{\alpha},\alpha]}\frac{\delta^4 S}{\delta\bar{\alpha}(1)\delta\bar{\alpha}(2)\delta\alpha(3)\delta\alpha(4)} = -\langle\phi|T[\psi(1)\psi(2)\psi^\dagger(3)\psi^\dagger(4)]|\phi\rangle$$

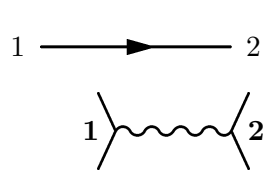
$$=$$ 

(8.45)

Show that the last term, which is the connected two-particle Green's function, is the quartic term coefficient in the expansion of $\ln S[\bar{\alpha},\alpha]$.

8.0.6 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:



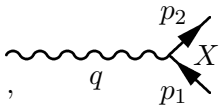
$$= G(X_1 - X_2) = \int \frac{d^d p}{(2\pi)^d} G(p) e^{ip(X_1 - X_2)}$$

$$= V(X_1 - X_2) = \int \frac{d^d q}{(2\pi)^d} V(q) e^{iq(X_1 - X_2)} \tag{8.46}$$

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

$$\alpha(X) = \int \frac{d^d p}{(2\pi)^d} e^{ipX} \alpha(p). \tag{8.47}$$

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.



$$= \int d^d X e^{i(p_1 - p_2 - q)X} = (2\pi)^d \delta^{(d)}(p_1 - p_2 - q) \tag{8.48}$$

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 2). The convergence factor

$$e^{i\omega O^+} \tag{8.49}$$

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

$$X_{cm} = \frac{X_1 + X_2 + \ldots X_n}{n} \tag{8.50}$$

and the relative co-ordinates

$$\tilde{X}_r = X_r - X_1, \qquad (r > 1), \tag{8.51}$$

as follows

$$\prod_{r=1,n} d^d X_r = d^d X_{cm} \prod_{r=2,n} d^d \tilde{X}_r \tag{8.52}$$

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

$$\int d^d X_{cm} = (2\pi)^d \delta^{(d)}(0) \equiv VT \tag{8.53}$$

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

$$\ln S = VT \sum \text{ linked cluster diagrams in momentum space}\}. \tag{8.54}$$

In other words, the phase-factor associated with the S-matrix grows extensively with the volume and the time over which the interactions act.

8.0.7 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 $-i\Delta ET$:

$$S[T] = \langle -\infty | \hat{U}(T/2) U^\dagger(-T/2) | \infty \rangle \propto e^{-i\Delta ET} \tag{8.55}$$

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,

$$\ln S[T] = -i\Delta ET + \text{constant} \tag{8.56}$$

But from the linked cluster theorem, we know that

$$\mathrm{S} = VT \sum \{\text{linked clusters in momentum space}\} \tag{8.57}$$

which then means that the change in the ground-state energy due to interactions is given by

$$\Delta E = iV \sum \{\text{linked clusters in momentum space}\} \tag{8.58}$$

To show this result, let us turn on the interaction for a period of time T, writing the ground-state S-matrix as

$$S[T] = \langle -\infty | \hat{U}(T/2) U^\dagger(-T/2) | \infty \rangle \tag{8.59}$$

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

$$S[T] = \sum_\lambda \langle -\infty|\hat{U}(T/2)|\lambda\rangle\langle\lambda|U^\dagger(-T/2)|\infty\rangle \tag{8.60}$$

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

$$S(T) \to \mathcal{U}(T/2)\mathcal{U}^\dagger(-T/2)\langle\phi|^\dagger(-T/2)|\infty\rangle \tag{8.61}$$

where $\mathcal{U}(\tau) = \langle -\infty|\hat{U}(\tau/2)|\phi\rangle$. Now differentiating the first term in this product, we obtain

$$\begin{aligned}\frac{\partial}{\partial\tau}\mathcal{U}(\tau) &= \frac{\partial}{\partial T}\langle\psi_o|e^{iH_o\tau/2}e^{-iH\tau/2}|\psi_g\rangle \\ &= \frac{i}{2}\langle\psi_o|\{H_oU(\tau/2) - U(\tau/2)H\}|\psi_g\rangle \\ &= -\frac{i\Delta E}{2}\mathcal{U}(\tau)\end{aligned} \tag{8.62}$$

Similarly, $\frac{\partial}{\partial\tau}\mathcal{U}^\dagger(-\tau) = -\frac{i\Delta E}{2}\mathcal{U}^\dagger(-\tau)$, so that

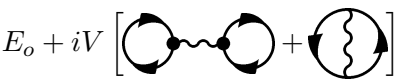
$$\frac{\partial S(T)}{\partial T} = -i\Delta E S(T) \tag{8.63}$$

which proves the original claim.

8.1 Examples

8.1.1 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

$E_g = E_o + iV$  (8.64)

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

$$\int \frac{d\omega}{2\pi}G(\mathbf{k},\omega) = if_{\mathbf{k}} = i\theta(\mathbf{k}_F - |\mathbf{k}|) \tag{8.65}$$

so that the shift in the ground-state energy is given by

$$\Delta E_{HF} = \frac{V}{2}\int \frac{d^3k d^3k'}{(2\pi)^6}\left[+(2S+1)^2(V_{\mathbf{q}=\mathbf{0}}) - (2S+1)(V_{\mathbf{k}-\mathbf{k}'})\right] f_{\mathbf{k}} f_{\mathbf{k}'} \tag{8.66}$$

We could have obtained this result by directly evaluating the ground-state expectation value of the interaction part of the Hamiltonian. 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. 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 lowering the Coulomb interaction between them. The interaction per unit volume is given by

$$\frac{\Delta E_{HF}}{V} = \frac{\rho^2}{2} V_{\mathbf{q}=\mathbf{0}} - \text{Exchange energy} \tag{8.67}$$

Note that for the Coulomb interaction, without screening, the Hartree interaction becomes infinite!

8.1.2 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,

$$H(t) = H_o + H_s(t) \tag{8.68}$$

where

$$H_s(t) = -A(t)f(t) \tag{8.69}$$

involves the coupling of an external force to a variable of the system. Examples would include

$$\begin{aligned} H_s(t) &= -\mu_B \int d^3x \mathbf{S}(x)\cdot\mathbf{B}(x,t), \qquad \text{External magnetic field} \\ H_s(t) &= -\int d^3x \rho(\mathbf{x})\Phi(x,t) \qquad \text{External potential} \end{aligned} \tag{8.70}$$

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

$$A_H(t) = U^\dagger(t) A_I(t) U(t) \tag{8.71}$$

where, from chapter 7,

$$U(t) = T\exp\left[-i\int_{-\infty}^{t} H_s(t')dt'\right] \tag{8.72}$$

We shall now drop the subscript I, because $A_I(t) = A(t)$ also corresponds to the Heisenberg representation of H_o. Expanding (8.71) to linear order in H_s, we obtain

$$A_H(t) = A(t) - i\int_{-\infty}^{t}[A(t), H_s(t')]dt' + O(H_s^2) \tag{8.73}$$

Finally, taking expectation values, we obtain

$$\langle A_H(t)\rangle = \langle\phi|A(t)|\phi\rangle - i\int_{-\infty}^{t}\langle\phi|[A(t), H_s(t')]|\phi\rangle dt' \tag{8.74}$$

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

$$\langle A_H(t)\rangle = \int_{-\infty}^{\infty} dt'\mathcal{G}(t-t')f(t')dt' \tag{8.75}$$

where

$$\mathcal{R}(t-t') = i\langle\phi|[A(t), A(t')]|\phi\rangle\theta(t-t') \tag{8.76}$$

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

$$G(1-2) = i\langle\phi|TA(1)A(2)|\phi\rangle \tag{8.77}$$

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,

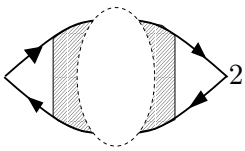
$$\begin{aligned}\mathcal{R}(\omega) &= \sum_\lambda \frac{|M_\lambda|^2}{\omega_\lambda - \omega - i\delta} \\ G(\omega) &= \sum_\lambda \frac{|M_\lambda|^2}{\omega_\lambda - \omega - i\delta\mathrm{sgn}(\omega_\lambda)}\end{aligned} \tag{8.78}$$

so that the response function can be simply related to the time-ordered response at a small imaginary frequency:

$$\mathcal{R}(\omega) = G(\omega + i\delta) \tag{8.79}$$

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,

$$-i\frac{\delta^2}{\delta f(1)\delta f(2)}\ln S[f] = i\langle\phi|T[A(1)A(2)]|\phi\rangle = -i1$$



$$2 \tag{8.80}$$

Diagramatically, the time-ordered correlation function for the quantity A, is given by

$$G(\omega) = -i\sum\{\text{diagrams formed by connecting two "A" vertices together.}\} \tag{8.81}$$

as summarized in Table 3.

8.1.3 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

$$H = \sum_{\mathbf{k}} \epsilon_{\mathbf{k}} c^\dagger{}_{\mathbf{k}} c_{\mathbf{k}} + H_{sc} \tag{8.82}$$

where $\epsilon_{\mathbf{k}} = k^2/2m - \mu$ and the scattering potential is given by

$$H_{sc} = \int d^3x \psi^\dagger(x)\psi(x)U(x) \tag{8.83}$$

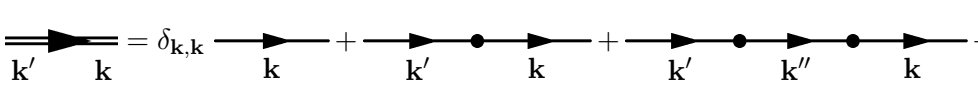
If we Fourier transform the scattering potential, writing

$$U(x) = \int_{\mathbf{q}} U(\mathbf{q}) e^{i\mathbf{q}\cdot\mathbf{x}} \tag{8.84}$$

then the scattering potential becomes

$$H_{sc} = \int_{\mathbf{k},\mathbf{k}'} \underbrace{U_{\mathbf{k}-\mathbf{k}'}}_{\text{amplitude to transfer momentum } \mathbf{k}-\mathbf{k}'} c^\dagger{}_{\mathbf{k}} c_{\mathbf{k}'} \tag{8.85}$$

The Feynman diagrams for the one-electron Green's function are then



(8.86)

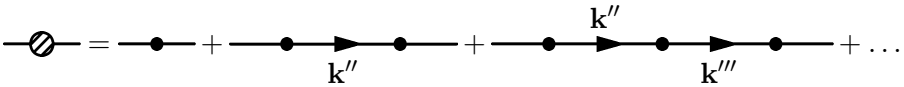
where

$$\underset{\mathbf{k}}{\longrightarrow} = G^o(\mathbf{k},\omega) = \frac{1}{\omega - \epsilon_{\mathbf{k}} - i\delta_{\mathbf{k}}} \tag{8.87}$$

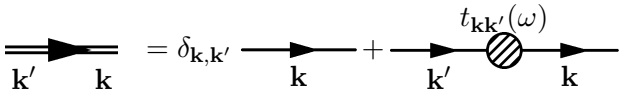
denotes the propagator in the absence of potential scattering and

$$\underset{\mathbf{k}'\ \ \mathbf{k}}{\text{—●—}} = U_{\mathbf{k}-\mathbf{k}'} \tag{8.88}$$

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

$t_{\mathbf{k},\mathbf{k}'}(\omega) =$  (8.89)

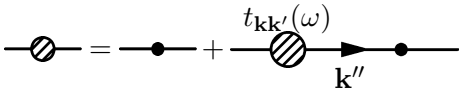
With this short-hand notation, the diagrams for the electron propagator become

 (8.90)

Written out as an equation, this is

$$G(\mathbf{k},\mathbf{k}',\omega) = \delta_{\mathbf{k},\mathbf{k}'}G^o(\mathbf{k},\omega) + G^o(\mathbf{k},\omega)t_{\mathbf{k},\mathbf{k}'}(\omega)G^o(\mathbf{k}',\omega) \tag{8.91}$$

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

 (8.92)

Written out explicitly, this is

$$t_{\mathbf{k}\mathbf{k}'}(\omega) = U_{\mathbf{k}-\mathbf{k}'} + \sum_{\mathbf{k}''} U_{\mathbf{k}-\mathbf{k}''}G_o(\mathbf{k}'',\omega)t_{\mathbf{k}''\mathbf{k}'}(\omega) \tag{8.93}$$

Equations (8.91) and (8.93) 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:

$$U(\mathbf{x}) = U\delta^{(d)}(\mathbf{x}) \tag{8.94}$$

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

$$t(\omega) = U + U\sum_{\mathbf{k}''} G^o(\mathbf{k}'',\omega)t(\omega) \tag{8.95}$$

or

$$t(\omega) = \frac{U}{1 - UF(\omega)} \tag{8.96}$$

where

$$\begin{aligned} F(\omega) &= \int \frac{d^d p}{(2\pi)^d} \frac{1}{\omega - \epsilon_{\mathbf{k}} + i\delta_{\mathbf{k}}} \\ &= \int_0^\Lambda N(\epsilon) \frac{1}{\omega - \epsilon + i\delta \text{sign}(\epsilon)} \end{aligned} \tag{8.97}$$

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

$$\epsilon_{\mathbf{k}} = \frac{k^2}{2m} \tag{8.98}$$

In d-dimensions, the density of states is given by

$$N(\epsilon) \propto k^{d-1} \frac{dk}{d\epsilon} \propto \epsilon^{\frac{d}{2}-1} \tag{8.99}$$

The low energy behavior of $F(\omega)$ is then given by

$$F(\omega) \propto -\omega^{d/2-1} \tag{8.100}$$

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 $U = -|U|$,

$$t(\omega) = -\frac{|U|}{1 - |U|N(0)\ln\frac{\Lambda}{-\omega}} = \frac{1}{N(0)\ln\left(\frac{\omega_o}{-\omega}\right)} \tag{8.101}$$

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.

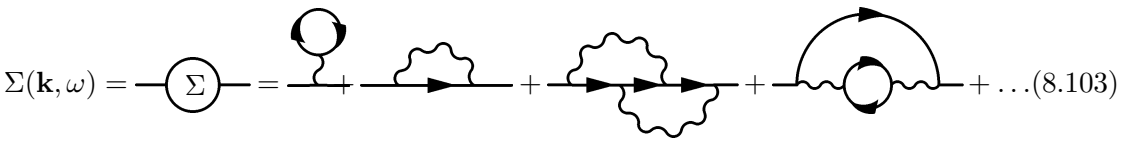
8.1.4 The self-energy

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

(8.102)

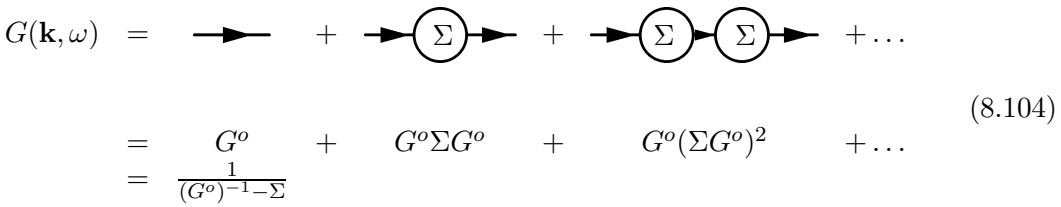
where



(8.103)

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



(8.104)

So that

$$G(\mathbf{k},\omega) = \frac{1}{\omega - \epsilon_{\mathbf{k}} - \Sigma(\mathbf{k},\omega)} \tag{8.105}$$

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.

$$\Sigma(\mathbf{k},\omega - i\delta) = \Sigma'(\mathbf{k},\omega) + i\Gamma(\mathbf{k},\omega) \tag{8.106}$$

If we use this expression to evaluate the one-particle spectral function, we obtain

$$A(\mathbf{k},\omega) = \frac{1}{\pi}\mathrm{Im}G(\mathbf{k},\omega - i\delta) = \frac{\Gamma(\mathbf{k},\omega)}{[\omega - \epsilon_{\mathbf{k}} - \Sigma'(\mathbf{k},\omega)]^2 + \Gamma(\mathbf{k},\omega)^2} \tag{8.107}$$

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,

$$G(\mathbf{k}, \omega - i\delta) = \frac{Z_{\mathbf{k}}}{\omega - \epsilon^*_{\mathbf{k}} - i\Gamma^*_{\mathbf{k}}} \tag{8.108}$$

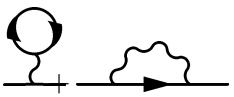
corresponding to a "quasiparticle" excitation with a finite lifetime. The finite width reflects the fact that an electron can now decay into combinations of electrons, plus electron-hole pairs. The reduced weight reflects the finite overlap between the bare electron, and the renormalized excitation:

$$\begin{aligned} \epsilon^*_{\mathbf{k}} &= \epsilon_{\mathbf{k}} + \Sigma'(\mathbf{k}, \epsilon^*_{\mathbf{k}}), && \text{renormalized energy} \\ \tau^{-1} &= Z_{\mathbf{k}}\Gamma(\mathbf{k}, \epsilon^*_{\mathbf{k}}), && \text{Lifetime} \\ Z_{\mathbf{k}} &= |\langle \text{q.ptcle } \mathbf{k}\sigma | c^\dagger{}_{\mathbf{k}\sigma} | \phi \rangle|^2 && \text{"Wavefunction renormalization"} \end{aligned} \tag{8.109}$$

8.1.5 Hartree-Fock Self-energy

The simplest example of the self-energy is the Hartree-Fock self energy, given by the two diagrams

$\Sigma_{HF}(\mathbf{p}, \omega)$ =



$$= i\int_{\mathbf{p}'} \{-(2S+1)V_{\mathbf{q}=0} + V_{\mathbf{p}-\mathbf{p}'}\} \int \frac{d\omega}{2\pi} G^o(k) e^{i\omega 0^+} \tag{8.110}$$

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

$$\Sigma_{HF}(\mathbf{p}) = \int_{|\mathbf{p}'|<k_F} \frac{d^3k'}{(2\pi)^3} \Big[(2S+1)V_{\mathbf{q}=0} - V_{\mathbf{p}-\mathbf{p}'} \Big] \tag{8.111}$$

In the Hartree-Fock approximation, the electron acquires a renormalized energy

$$\epsilon^*_{\mathbf{p}} = \epsilon_{\mathbf{p}} + \Sigma_{HF}(\mathbf{p}) \tag{8.112}$$

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

$$\frac{\mathbf{p}}{m^*} = \nabla_{\mathbf{p}} \epsilon^*_{\mathbf{p}} = \Big[\frac{\mathbf{p}}{m} + \nabla_{\mathbf{p}} \Sigma_{HF}(\mathbf{p}) \Big] \tag{8.113}$$

then integrating by parts,

$$\nabla_{\mathbf{p}}\Sigma_{HF}(\mathbf{p}) = -\int_{\mathbf{p}'} V_{\mathbf{p}-\mathbf{p}'}\nabla_{\mathbf{p}'}f_{\mathbf{p}'} \tag{8.114}$$

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

$$\nabla_{\mathbf{p}}\Sigma_{HF}(\mathbf{p}) = \frac{\mathbf{p}}{3m^*}F_1^s \tag{8.115}$$

where, by analogy with Fermi liquid theory, we have written,

$$F_1^s = -N(0)\int \frac{d\Omega_{\hat{\mathbf{p}}'}}{4\pi}V_{\mathbf{p}-\mathbf{p}'}\cos(\hat{\mathbf{p}}\cdot\hat{\mathbf{p}}'). \tag{8.116}$$

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

$$\frac{m^*}{m} = 1 + \frac{1}{3}F_1^s \tag{8.117}$$

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.

8.1.6 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 $\hbar$

$$\frac{1}{N} \sim \hbar \tag{8.118}$$

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

$$H = \sum_{\mathbf{k},\sigma} \epsilon_{\mathbf{k}} c^\dagger{}_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} + \frac{1}{2} \sum V_{\mathbf{q}} c^\dagger{}_{\mathbf{k}+\mathbf{q}\sigma} c^\dagger{}_{\mathbf{k}'-\mathbf{q}\sigma'} c_{\mathbf{k}'\sigma'} c_{\mathbf{k}\sigma} \tag{8.119}$$

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

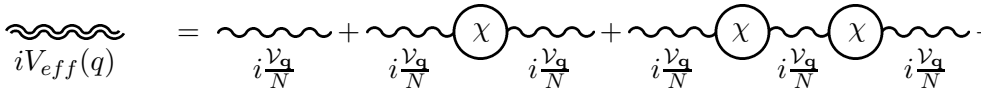
$$V_{\mathbf{q}} = \frac{1}{N} \mathcal{V}_{\mathbf{q}} \tag{8.120}$$

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

$$V_{\mathbf{q}} = \frac{1}{N} \frac{4\pi\tilde{e}^2}{q^2} \tag{8.121}$$

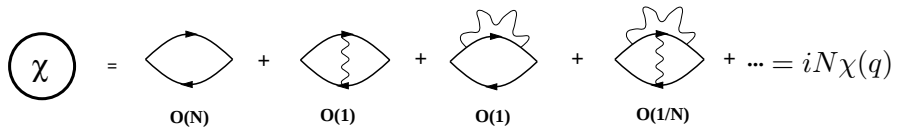
and $\tilde{e}^2 = 2e^2$. At the end, we set $N = 2$, hoping that the key features of the solution around $N = 2$ will be shared by the entire family of models.

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



(8.122)

The "self-energy" diagram for the interaction line is called a "polarization bubble", and has the following diagramatic expansion.



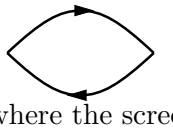
(8.123)

By summing the geometric series that appears in (8.122) we obtain

$$V_{eff} = \frac{1}{N}\frac{\mathcal{V}(q)}{1+\mathcal{V}(q)\chi(q)} \tag{8.124}$$

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

$$i\chi_0(q)N = \tag{8.125}$$



In the case of a Coulomb interaction, where the screened interaction becomes

$$V_{eff}(\mathbf{q},\omega) = \frac{1}{N}\frac{4\pi\tilde{e}^2}{q^2\epsilon(\mathbf{q},\omega)} \tag{8.126}$$

where we have identified

$$\epsilon(\mathbf{q},\omega) = 1+\mathcal{V}(q)\chi(q) = 1+\frac{4\pi\tilde{e}^2}{q^2}\chi_o(q) \tag{8.127}$$

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

$$iN\chi_o(q) = (-N)\int \frac{d^4k}{(2\pi)^4}G_o(k+q)G_o(k) \tag{8.128}$$

where the factor $-N$ comes from the fermion loop, and the sum over the N spin indices. Written out explicitly, this is

$$\chi_o(\mathbf{q},\nu) = i\int_{\mathbf{k}}\int_{-\infty}^{\infty}\frac{d\omega}{(2\pi)}\frac{1}{\omega+\nu-\epsilon_{\mathbf{k+q}}+i\delta_{\mathbf{k+q}}}\frac{1}{\omega-\epsilon_{\mathbf{k}}+i\delta_{\mathbf{k}}} \tag{8.129}$$

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 $if_{\mathbf{k+q}}$ for the poles in the two Green's functions. The result of this calculation is then

$$\chi_o(\mathbf{q},\nu) = \int_{\mathbf{k}}\frac{f_{\mathbf{k+q}}-f_{\mathbf{k}}}{\nu-(\epsilon_{\mathbf{k+q}}-\epsilon_{\mathbf{k}})+i\delta_{\mathbf{k},\mathbf{q}}} \tag{8.130}$$

where $\delta_{\mathbf{k},\mathbf{q}} = \delta\text{sign}(\epsilon_{\mathbf{k+q}}-\epsilon_{\mathbf{k}})$ 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

$$\chi''(\mathbf{q},\nu)=\int_{\mathbf{k}}\pi\delta[\nu-(\epsilon_{\mathbf{k}+\mathbf{q}}-\epsilon_{\mathbf{k}})](f_{\mathbf{k}}-f_{\mathbf{k}+\mathbf{q}}), \tag{8.131}$$

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

$$\chi_o(\mathbf{q})=N(0)F(\frac{q}{2k_F}) \tag{8.132}$$

where $N(0)$ is the density of states per spin at the Fermi surface and

$$F(x)=\frac{1}{2x}(1-x^2)\ln\left|\frac{1+x}{1-x}\right| \tag{8.133}$$

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

$$V_{eff}(\mathbf{q},\nu)=\frac{1}{N}\frac{4\pi\tilde{e}^2}{q^2+\kappa^2} \tag{8.134}$$

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

$$V_{eff}(r)\propto\frac{\cos 2k_Fr}{r^3} \tag{8.135}$$

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

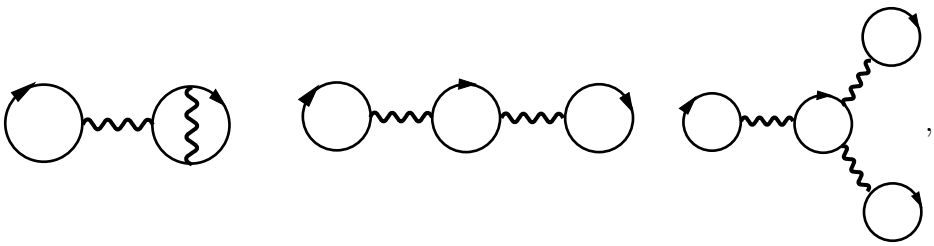
$$\epsilon_o(\mathbf{q},\nu)=1-\frac{\omega_p^2}{\nu^2} \tag{8.136}$$

where

$$\omega^2=\frac{4\pi\tilde{e}^2\tilde{n}}{m} \tag{8.137}$$

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

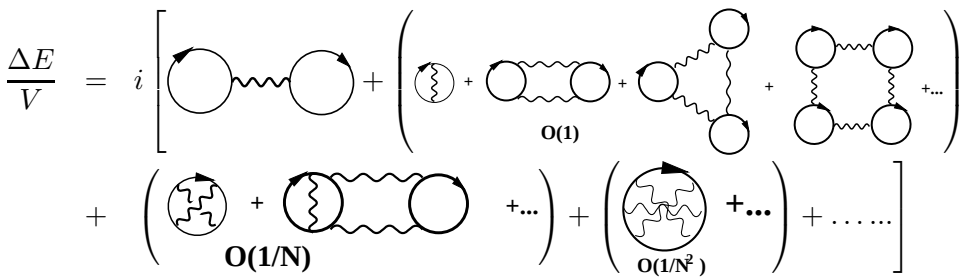


, (8.138)

identically vanish. This is because, these diagrams involve a power of the propagator higher than one, inside integrals of the form

$$\int d\omega G(\mathbf{k},\omega)^n = o, \qquad (n > 1) \tag{8.139}$$

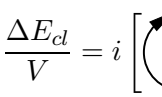
which are zero, because there is no other ω dependent function inside the integral. The only nonzero diagrams are then:



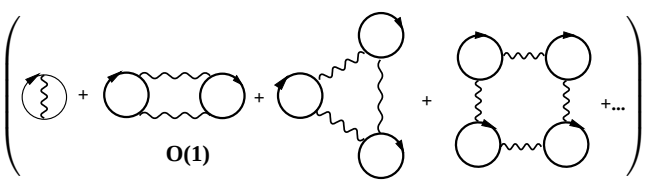
(8.140)

We shall select the two leading contributions,

$$\frac{\Delta E_{cl}}{V} = i\left[\quad\right], \qquad \text{(O(N))} \tag{8.141}$$



which corresponds to the classical repulsive energy between particles, and the sum



(8.142)

These diagrams are derived from the zero the zero-point fluctuations in charge density, which modify the ground-state energy $E \to E_o + E_{zp}$. 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

$$E_{zp} = i\sum_{n=1}^{\infty}\frac{1}{2n}\int\frac{d^4q}{(2\pi)^4}(-\chi_o(q)\mathcal{V}(q))^n. \tag{8.143}$$

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

$$\begin{aligned} E_{zp} &= -\frac{i}{2}\int_{\mathbf{q}}\int_0^{\infty}\frac{d\omega}{2\pi}\left[\ln[1+\chi_o(\mathbf{q},\nu+i\delta)\mathcal{V}_{\mathbf{q}}] - \ln[1+\chi_o(\mathbf{q},\nu-i\delta)\mathcal{V}_{\mathbf{q}}]\right] \\ &= \frac{1}{2}\int_{\mathbf{q}}\int_0^{\infty}\frac{d\omega}{\pi}\arctan\left(\frac{\mathcal{V}_{\mathbf{q}}\chi''(\mathbf{q},\nu)}{[1+\mathcal{V}_{\mathbf{q}}\chi'(\mathbf{q},\nu)]}\right) \end{aligned} \tag{8.144}$$

If we associate a "phase shift"

$$\delta(\mathbf{q},\omega) = \arctan\left(\frac{\mathcal{V}_{\mathbf{q}}\chi''(\mathbf{q},\nu)}{[1+\mathcal{V}_{\mathbf{q}}\chi'(\mathbf{q},\nu)]}\right) \tag{8.145}$$

then we can the zero-point fluctuation energy can also be written in the form

$$\Delta E_{zp} = \int\frac{d^3q}{(2\pi)^3}\int_0^{\infty}d\omega\Lambda(\omega)\left[\frac{\omega}{2}\right] \tag{8.146}$$

where

$$\Lambda(\omega) = \frac{1}{\pi}\frac{\partial\delta(\mathbf{q},\omega)}{\partial\omega}. \tag{8.147}$$

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: Derive the Lindhard function for the zero-frequency susceptibility of the non-interacting electron gas.

Example: Show that the dynamical charge susceptibility of an interacting electron gas in the large N limit, defined by

$$\chi(\mathbf{q}, \nu + i\delta) = \int d^x \int_0^\infty i\langle\phi|[\rho(\mathbf{x}, t), \rho(0, 0)]|\phi\rangle e^{-i(\mathbf{q}\cdot\mathbf{x}-\omega t)} \tag{8.148}$$

contains a pole at frequencies

$$\omega_q = \omega_p(1 + \frac{3}{10}qv_F) \tag{8.149}$$

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.

Table. 8.1 Real Space Feynman Rules .

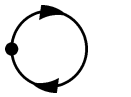
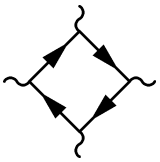
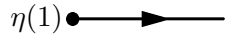
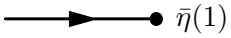
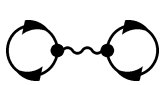
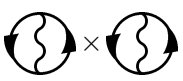
	$G(\mathbf{2}-\mathbf{1})$
	$U(x_1)$
	$iV(\mathbf{1}-\mathbf{2})$
$\prod_i \int d^3x_i dt_i$	Integrate over all intermediate times and positions.
	$-(2S+1)G(\vec{0},0^-)$
	$[-(2S+1)]^F$, $F=$ no. Fermion loops.
	$\eta(1)$
	$i\bar{\eta}(1)$
 $p=2$	$\frac{1}{p}$
 $p=8$	$p=$ order of symmetry group.

Table. 8.2 Momentum Space Feynman Rules .

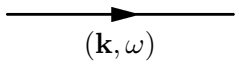
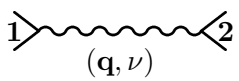
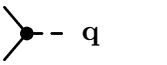
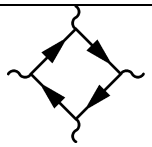
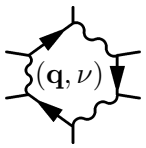
	$G_o(\mathbf{k},\omega)$	Fermion propagator
	$iV(q)$ $ig_q^2 D_o(q)$	Interaction Exchange Boson.
	$U(\mathbf{q})$	Scattering potential
	$[-(2S+1)]^F$,	F= no. Fermion loops
	$\int \frac{d^d q d\nu}{(2\pi)^{d+1}} e^{i\omega 0^+}$	Integrate over internal loop momenta and frequency.
$p=2$ $p=8$	$\frac{1}{p}$	p = order of symmetry group.

Table. 8.3 Relationship With Physical Quantities.

ΔE	$iV\sum\{\text{linked clusters}\}$	$iV\left[\quad+\quad+\ldots\right]$
$\ln S$	$VT\sum\{\text{linked clusters}\}$	$VT\left[\quad+\quad+\ldots\right]$
1 ⟶ 2 $-i\langle T\psi(2)\psi^\dagger(1)\rangle$	$\sum\{\text{Two leg diagrams}\}$	$+\quad+\quad+$
$(-i)^n\langle T\psi(1)\ldots\psi^\dagger(2n)\rangle$ G $n=2$	$\sum\{\text{2n- leg diagrams}\}$	$-\quad+\quad+$
Response Functions $(-i)^2\langle\psi\vert T[A(2)B(1)]\vert\psi\rangle=\chi^T_{AB}$ $B(1)$ $A(2)$ $i\langle[A(2),B(1)]\rangle\theta(t_1-t_2)=\chi_{AB}$	$\chi_{AB}=-i\chi^T_{AB}(\omega-i\delta)$	$+\quad+\ldots$

Chapter 9

Finite Temperature and the Fluctuation-Dissipation Theorem

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

$$p_\lambda = \frac{e^{-\beta E_\lambda}}{Z} \tag{9.1}$$

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. In fact, in many ways, the formulation is easier to handle. The essential step that makes this possible was first carried out by the Japanese physicist Matsubara in the early fifties, who noticed that the quantum-mechanical partition function can be regarded as a time-evolution operator in imaginary time:

$$\hat{\rho} \propto e^{-\beta \hat{H}} \sim e^{-\frac{it\hat{H}}{\hbar}}\Big|_{t=-i\frac{\hbar}{k_B T}}, \tag{9.2}$$

suggesting that a finite temperature many body physics is equivalent to zero-temperature physics at an imaginary time

$$\frac{it}{\hbar} \longrightarrow \tau. \tag{9.3}$$

For example, the partition function of a quantum system is simply the trace of the time-evolution operator, evaluated at imaginary time:

$$Z = \mathrm{Tr} e^{-\beta H} = \mathrm{Tr} U(t)|_{t=-i\frac{\hbar}{k_B T}}. \tag{9.4}$$

9.1 Quantum Mechanical Response Functions.

If we couple a force $f(t)$ to variable A according to

$$H = H_o - f(t)A,$$

then 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 $f(t)$,

$$\begin{aligned} U(t) &= 1 + i \int_{-\infty}^{t} dt' A(t') f(t'), \\ U^\dagger(t) &= 1 - i \int_{-\infty}^{t} dt' A(t') f(t') \end{aligned}$$

so that

$$A_H(t) = A(t) + i \int_{-\infty}^{t} dt' [A(t), A(t')]\, f(t'),$$

In thermal equilibrium if $\langle A \rangle = 0$, the response to the applied force is given by

$$\langle A_H(t) \rangle = \int_{-\infty}^{+\infty} dt' \ \chi(t-t')\, f(t'),$$

where

$$\chi(t-t') = i \langle [A(t), A(t')] \rangle \theta(t-t')$$

is the "dynamical susceptibility": the quantum mechanical response function.

9.2 Fluctuation Dissipation Theorem

In a system in thermal equilibrium, we expect there to be a link between the thermal and quantum fluctuations about equilibrium, and the response to external stimulii. Intuitively, if the susceptibility of the system to external change is large, then the fluctuations about equilibrium will be large. It turns out that fluctuations and response are intimately related. We will see that if

$$i \langle [A(1), A(2)] \rangle \theta(t-t') = \chi(t-t') = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} e^{-i\omega(t-t')} \chi(\omega)$$

is the response function to a force $f(t)$ whcih couples to $A(t)$, i.e.

$$\langle A(t)\rangle = \int_{-\infty}^{\infty} dt' \chi(t-t') f(t'), \quad \langle A(\omega)\rangle = \chi(\omega) f(\omega),$$

then the fluctuations about equilibrium, defined by

$$C(t-t') = \frac{1}{2}\langle\{A(t),\, A(t')\}\rangle = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} e^{-i\omega(t-t')} C(\omega),$$

are related to the response function via the fluctuation dissipation relation

$$\overbrace{C(\omega)}^{\text{Fluctuations}} = \hbar[\underbrace{1}_{\text{Quantum}} + \overbrace{2n_B(\omega)}^{\text{Thermal}}] \underbrace{\chi''(\omega)}_{\text{Dissipation}}$$

where $\chi''(\omega) = \text{Im}\ \chi(\omega)$ describes the dissipative part of the response function. In the limit, $\omega << \mathrm{k}_B T$, when $n(\omega) \sim \mathrm{k}_B T/\hbar\omega$, this result reverts to the classical fluctuation-dissipation theorem,

$$C(\omega) = \frac{2\mathrm{k}_B T}{\omega}\chi''(\omega)$$

Thus in principle, if we know the correlation functions in thermal equilibrium, we can compute the response function of the system. In practice, the theorist takes advantage of a completely parallel fluctuation-dissipation theorem which exists in imaginary time. The imaginary time correlation function is given by

$$\chi(\tau) = \langle A(\tau)A(0)\rangle = \frac{1}{\beta}\sum_n e^{-i\nu_n\tau}\chi(i\nu_n)$$

The relation between this function and the physical response function is given by

$$\chi(i\nu_n) = \chi(z = i\nu_n),$$

where

$$\chi(z) = \int \frac{d\omega}{\pi}\frac{1}{\omega - z}\chi''(\omega)$$

is the analytic extension of $\chi(\omega)$ into the complex plane. This relation permits us to compute the physical response function by analytically continuing the imaginary-time correlation functions onto the real axis.

To develop the fluctuation dissipation theorem, we carry out a spectral decomposition of the various response and correlation functions. The procedure is basically the same for each function, but for completeness, we now carry out the complete procedure.

9.2.1 Spectral decomposition of $\chi(t-t')$

We begin by expanding the response function in terms of a complete set of energy eigenstates which satisfy

$$\begin{aligned} H\,|\lambda\rangle &= E_\lambda\,|\lambda\rangle\,, \\ \sum_\lambda |\lambda\rangle\,\langle\lambda| &= 1, \\ \langle\lambda\,|A(t)|\,\zeta\rangle &= \left\langle \lambda \left| e^{iHt} A\, e^{-iHt} \right| \zeta \right\rangle = e^{-i(E_\zeta - E_\lambda)(t-t')}\,\langle\lambda\,|A|\,\zeta\rangle\,. \end{aligned}$$

Using these key results, we make the expansion as follows,

$$\begin{aligned} \chi(t-t') &= i\sum_{\lambda,\zeta} e^{-\beta(E_\lambda - F)}\left\{\langle\lambda\,|A(t)|\,\zeta\rangle\,\langle\zeta\,|A(t')|\,\lambda\rangle - \langle\lambda\,|A(t')|\,\zeta\rangle\,\langle\zeta\,|A(t)|\,\lambda\rangle\right\}\theta(t-t') \\ &= i\sum_{\lambda,\zeta} e^{\beta F}(e^{-\beta E_\lambda} - e^{-\beta E_\zeta})\,|\langle\zeta\,|A|\,\lambda\rangle|^2\, e^{-i(E_\zeta - E_\lambda)(t-t')}\theta(t-t'). \end{aligned}$$

So introducing the spectral function

$$\chi''(\omega) = \pi(1-e^{-\beta\omega})\sum_{\lambda,\zeta} |\langle\zeta\,|A|\,\lambda\rangle|^2\,\delta[\omega - (E_\zeta - E_\lambda)]e^{-\beta(E_\lambda - F)},$$

we see that the response function can be written,

$$\chi(t) = i\int d\omega\, e^{-i\omega t}\theta(t)\,\chi''(\omega).$$

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

$$\chi(\omega) = \int \frac{d\omega'}{\pi}\,\frac{1}{\omega'-\omega-i\delta}\chi''(\omega').$$

This "Kramers-Krönig" relation can be used to extend the response function into the complex plane. Notice that because the response function is *causal*, the poles of $\chi(\omega)$ all lie just below the real axis, at $z = \omega' - i\delta$.

9.2.2 Spectral decomposition of $C(t-t')$

Following the same procedure as used for the response function, the correlation function is written,

$$
\begin{aligned}
C(t-t') &= \frac{1}{2}\sum_{\lambda,\zeta} e^{-\beta(E_\lambda - F)} \left\{ \langle \lambda \left| A(t) \right| \zeta \rangle \langle \zeta \left| A(t') \right| \lambda \rangle + \langle \lambda \left| A(t') \right| \zeta \rangle \langle \zeta \left| A(t) \right| \lambda \rangle \right\} \\
&= \frac{1}{2}\sum_{\lambda,\zeta} e^{\beta F}(e^{-\beta E_\lambda} + e^{-\beta E_\zeta}) \left| \langle \zeta \left| A \right| \lambda \rangle \right|^2 e^{-i(E_\zeta - E_\lambda)(t-t')} \\
&= \frac{1}{2}\sum_{\lambda,\zeta} e^{-\beta(E_\lambda - F)}(1 + e^{-\beta(E_\zeta - E_\lambda)}) \left| \langle \zeta \left| A \right| \lambda \rangle \right|^2 e^{-i(E_\zeta - E_\lambda)(t-t')}
\end{aligned}
$$

Using the spectral function defined above, we can write this in the form,

$$C(t) = \frac{1}{2\pi}\int d\omega\, e^{-i\omega t}\, \frac{1+e^{-\beta\omega}}{1-e^{-\beta\omega}} \chi''(\omega),$$

where the factor $\frac{1+e^{-\beta\omega}}{1-e^{-\beta\omega}}$ is required to convert the factor $(1-e^{-\beta(E_\zeta - E_\lambda)})$ appearing inside $\chi(t)$ to the factor $(1+e^{-\beta(E_\zeta - E_\lambda)})$ appearing inside $C(t)$. We can rewrite this expression as

$$
\begin{aligned}
C(\omega) &= \int \frac{d\omega}{\pi}\, e^{-i\omega t}\, \left[\frac{1}{2} + \frac{1}{e^{\beta\omega}-1} \right] \chi''(\omega) \\
&= \int \frac{d\omega}{2\pi}\, e^{-i\omega t}\, \left[1 + 2n_B(\omega) \right] \chi''(\omega).
\end{aligned}
$$

If we now Fourier transform this expression, we obtain

$$C(\omega) = 2\left[\frac{1}{2} + n_B(\omega) \right] \chi''(\omega).$$

If we restore $\hbar$, this becomes

$$C(\omega) = 2\hbar\left[\frac{1}{2} + n_B(\omega) \right] \chi''(\omega),$$

where

$$\chi''(\omega) = \pi(1 - e^{-\beta\hbar\omega}) \sum_{\lambda,\zeta} \left| \langle \zeta \left| A \right| \lambda \rangle \right|^2 \delta[\hbar\omega - (E_\zeta - E_\lambda)] e^{-\beta(E_\lambda - F)},$$

thus proving the fluctuation-dissipation theorem.

9.2.3 Spectral decomposition of $\chi(\tau)$

This is the easiest decomposition of the three to carry out. We write, for $\tau - \tau' > 0$,

$$
\begin{aligned}
\chi(\tau - \tau') &= \sum_{\lambda,\zeta} e^{-\beta(E_\lambda - F)} \left\{ \langle \lambda \left| A(\tau) \right| \zeta \rangle \langle \zeta \left| A(\tau') \right| \lambda \rangle \right\} \\
&= \sum_{\lambda,\zeta} e^{-\beta(E_\lambda - F)} e^{-(E_\lambda - E_\zeta)(\tau - \tau')} \left| \langle \zeta \left| A \right| \lambda \rangle \right|^2 .
\end{aligned}
$$

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

$$\begin{aligned}\chi(i\nu_n) &= \int_0^\beta d\tau\, e^{i\nu_n\tau}\chi(\tau) \\ &= \sum_{\lambda,\zeta} e^{-\beta(E_\lambda - F)}(1 - e^{-\beta(E_\zeta - E_\lambda)})\,|\langle\zeta\,|A|\,\lambda\rangle|^2\,\frac{1}{(E_\zeta - E_\lambda - i\nu_n)},\end{aligned}$$

which enables us to write

$$\chi(i\nu_n) = \int \frac{d\omega}{\pi}\frac{1}{\omega - i\nu_n}\chi''(\omega) \tag{9.5}$$

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 9.5, and to use this to read off $\chi''(\omega)$.

Table. 9.1 Real Space Feynman Rules: Finite Temperature .

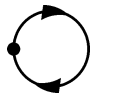
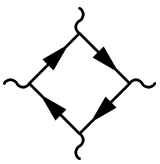
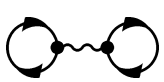
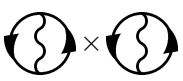
	$G(\mathbf{2}-\mathbf{1})$
	$U(x_1)$
	$-V(\mathbf{1}-\mathbf{2})$
$\prod_i \int d^3x_i \int_0^\beta d\tau$	Integrate over all intermediate times and positions.
	$-(2S+1)G(\vec{0},0^-)$
	$[-(2S+1)]^F$, $F=$ no. Fermion loops.
	$\eta(1)$
	$i\bar{\eta}(1)$
 $p=2$	$\frac{1}{p}$
 $p=8$	$p=$ order of symmetry group.

Table. 9.2 Momentum Space Feynman Rules: Finite Temperature .

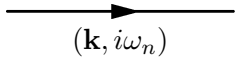
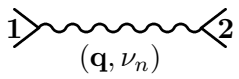
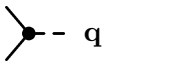
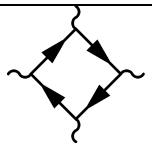
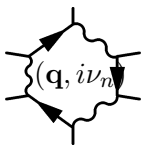
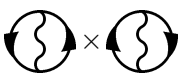
	$G_o(\mathbf{k}, i\omega_n)$	Fermion propagator
	$-V(q)$ $-g_q^2 D_o(\mathbf{q}, i\nu_n)$ $= -g_{\mathbf{q}}^2 \left[\frac{2\omega_q}{(i\nu_n)^2 - \omega_{\mathbf{q}}^2} \right]$	Interaction Exchange Boson.
	$U(\mathbf{q})$	Scattering potential
	$[-(2S+1)]^F$,	F= no. Fermion loops
	$T \sum_n \int \frac{d^d q}{(2\pi)^d}$	Sum over internal loop frequency and momenta.
$p = 2$  $p = 8$	$\frac{1}{p}$	p = order of symmetry group.

Table. 9.3 Relationship With Physical Quantities: Finite Temperature

ΔF	$-V\sum\{\text{linked clusters}\}$	$-V\left[\quad+\quad+\ldots\right]$
$\ln Z/Z_o$	$V\beta\sum\{\text{linked clusters}\}$	$VT\left[\quad+\quad+\ldots\right]$
1 2 $-\langle T\psi(2)\psi^\dagger(1)\rangle$	$\sum\{\text{Two leg diagrams}\}$	$+\quad+\quad+$
$(-1)^n\langle T\psi(1)\ldots\psi^\dagger(2n)\rangle$ G $n=2$	$\sum\{\text{2n- leg diagrams}\}$	$-\quad+\quad+$
Response Functions $\langle\psi\vert T[A(2)B(1)]\vert\psi\rangle=\chi^T_{AB}$ $B(1)$ $A(2)$ $i\langle[A(2),B(1)]\rangle\theta(t_1-t_2)=\chi_{AB}$	$\chi_{AB}=\chi^T_{AB}(\omega-i\delta)$	$+\quad+\ldots$

Chapter 10

Path Integrals and Phase transitions

10.1 Introduction

There are two key ideas behind the functional integration technique: (i) the Feynman concept of summing over quantum histories,

$$Z = \sum_{\text{path}} \exp\Big[-S_{\text{path}}\Big] \tag{10.1}$$

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

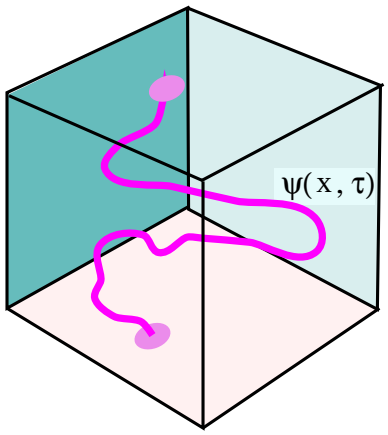
$$|\psi(x)\rangle = \exp\Big[-\int d^3x \psi(x)\hat{\psi}^\dagger(x)\Big]|0\rangle \tag{10.2}$$

to be the coherent state of the field ψ. This state is the eigenvector of the microscopic quantum field, in that

$$\hat{\psi}(x)|\psi\rangle = \psi(x)|\psi\rangle \tag{10.3}$$

where $\psi(x)$ is a "c-number", not an operator. These 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

$$S_{PATH} = \int_0^\beta d\tau \mathcal{L}[\bar{\psi}, \psi] \tag{10.4}$$



where

$$\mathcal{L}[\bar{\psi},\psi] = \int d^3x[\bar{\psi}(x,\tau)\partial_\tau\psi(x,\tau)] + H[\bar{\psi},\psi] \tag{10.5}$$

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.

$$Z_{\text{interacting}} \longrightarrow \sum_{\{\Delta\}} \Big[\text{path integral of fermions moving in field } \Delta\Big] \tag{10.6}$$

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.

10.2 Coherent states and Grassman numbers

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

$$|c\rangle = e^{-c\hat{c}^\dagger}|0\rangle$$

and its conjugate is given by

$$\langle\bar{c}| = \langle 0|e^{-\hat{c}\bar{c}}$$

We use $\bar{c}$, rather than a dagger, because we shall need to consider c and $\bar{c}$ to be independent variables.

10.2.1 Grassman Mathematics

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 numbers $\hat{O}$

$$c\hat{O} = \hat{O}c$$

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

$$c\bar{c} + \bar{c}c = 0, \tag{10.7}$$
$$c\hat{\psi} + \hat{\psi}c = 0, \tag{10.8}$$

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	$f[\bar{c}, c] = f_o + f_1\bar{c} + \tilde{f}_1 c + f_{12}c\bar{c}$	Since $c^2 = 0$, truncate at linear order in each variable.
Calculus	$\partial f = \tilde{f}_1 + f_{12}\bar{c}$	Differentiation
	$\bar{\partial} f = f_1 - f_{12}\bar{c}$	
	$\int dc \equiv \partial_c$	$\int dc1 = \partial_c 1 = 0$
		$\int dcc = \partial_c c = 1$
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, $f(\bar{c}, c)$

$$f[\bar{c}, c] = f_o + f_1\bar{c} + \tilde{f}_1 c + f_{12}c\bar{c}$$

only has four terms! The coherent state (10.2) also truncates, so that

$$|c\rangle = |0\rangle - c\hat{c}^\dagger|0\rangle,$$

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.

10.2.2 Completeness and matrix elements

Coherent states are over-complete: you can see that

$$\langle \bar{c}|c\rangle = \langle 0|(1-\hat{c}\bar{c})(1-c\hat{c}^\dagger)|0\rangle = 1+\bar{c}c = e^{\bar{c}c} \tag{10.9}$$

and for this reason, the completeness relation contains a normalization term. It is straightforward to verify that

$$\int d\bar{c}dc|c\rangle\langle\bar{c}|e^{-\bar{c}c} = |0\rangle\langle 0| + |1\rangle\langle 1| \equiv \underline{1} \tag{10.10}$$

is the identity operator, where $|1\rangle = \hat{c}^\dagger|0\rangle$ is the state with one particle in it. Note that the exponential may be loosely regarded as a normalizing factor which takes account of the over-completeness:

$$e^{-\bar{c}c}|c\rangle\langle\bar{c}| = \frac{|c\rangle\langle\bar{c}|}{\langle\bar{c}|c\rangle}.$$

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

$$\langle\bar{c}|\hat{A}|c\rangle = \langle\bar{c}|c\rangle A[\bar{c},c] = e^{\bar{c}c}A[\bar{c},c], \tag{10.11}$$

i.e

$$\langle\bar{c}|\hat{A}|c\rangle = e^{\bar{c}c}\times \text{ c-number formed by replacing } (\hat{c},\hat{c}^\dagger)\to(c,\bar{c}).$$

The direct expansion of this matrix element is given by

$$\begin{aligned}\langle\bar{c}|\hat{A}|c\rangle &= (\langle 0| + \bar{c}\langle 1|)\hat{A}(|0\rangle + |1\rangle c) \\ &= \langle 0|\hat{A}|0\rangle - \bar{c}\langle 1|\hat{A}|0\rangle - c\langle 0|\hat{A}|1\rangle + \bar{c}c\langle 1|\hat{A}|1\rangle\end{aligned} \tag{10.12}$$

By integrating this with $e^{\bar{c}c}$, we find

$$\mathrm{Tr}[\hat{A}] = \langle 0|\hat{A}|0\rangle + \langle 1|\hat{A}|1\rangle = -\int d\bar{c}dce^{\bar{c}c}\langle\bar{c}|\hat{A}|c\rangle \tag{10.13}$$

We shall make extensive use of the completeness and trace formulae (10.10) and (10.13) 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,

$$\begin{aligned}d\bar{c}dc &\equiv \prod_j d\bar{c}_j dc_j, \\ \bar{c}c &= \sum_j \bar{c}_j c_j.\end{aligned} \tag{10.14}$$

10.3 Path integral for the partition function

To begin with, we consider a single fermion, with Hamiltonian

$$H = \epsilon \hat{c}^\dagger \hat{c} \tag{10.15}$$

Using the trace formula (10.13), the partition function

$$Z = \mathrm{Tr} e^{-\beta H}$$

can be re-written in terms of coherent states:

$$Z = -\int d\bar{c}_N dc_1 e^{\bar{c}_N c_1} \langle \bar{c}_N | e^{-\beta H} | c_1 \rangle, \tag{10.16}$$

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

$$Z = \int \prod_{j=1}^{N} d\bar{c}_j dc_{j+1} e^{-\bar{c}_j c_{j+1}} \langle \bar{c}_j | e^{-H\Delta\tau} | c_j \rangle \tag{10.17}$$

where, in order to take care of the minus sign which appears in the trace (10.16) we must define

$$c_{N+1} = -c_1, \qquad \bar{c}_{N+1} = -\bar{c}_1. \tag{10.18}$$

This innocuous looking boundary condition plays a central role in the Fermi-Dirac statistics of the these fields.

Provided each time-slice is of sufficiently brief duration, we can replace $e^{-\Delta\tau H}$ by its normal ordered form, so that

$$\langle \bar{c}_j | e^{-H\Delta\tau} | c_j \rangle = e^{\bar{c}_j \bar{c}_j} e^{-H[\bar{c}_j c_j]\Delta\tau},$$

where $H[\bar{c}, c] = \epsilon \bar{c} c$ is the normal-ordered Hamiltonian, with Grassman numbers replacing operators.

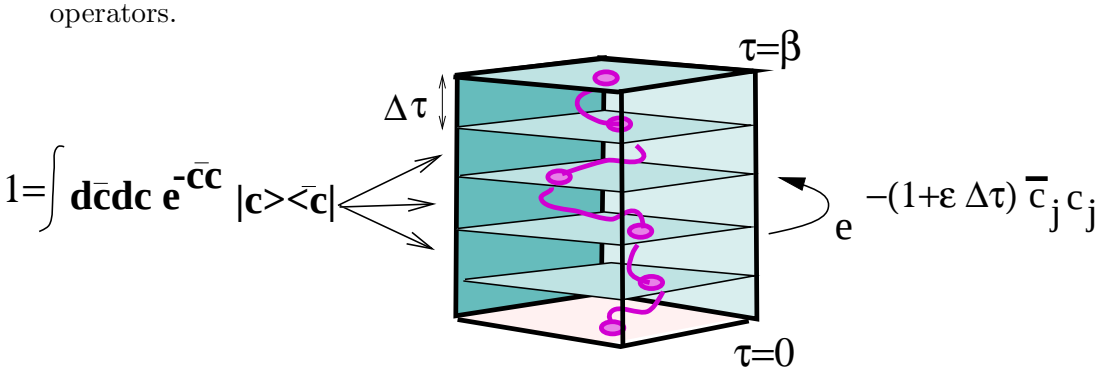


Fig. 2 Division of time evolution into "time-slices".

Combining (10.16) and (10.17) we can write

$$\begin{aligned} Z_N &= \int \prod_{j=1}^{N} d\bar{c}_j dc_j \exp\Big[-S\Big] \\ S &= \sum_{j=1}^{N} \Big[\bar{c}_j(c_{j+1}-c_j)/\Delta\tau + \epsilon\bar{c}_j, c_j\Big]\Delta\tau, \end{aligned} \tag{10.19}$$

Let us pause to reflect on what this means. This path integral represents a sum over all possible values "histories" of the fields:

$$c(\tau_j) \equiv \{c_1, c_2 \ldots c_N\}, \tag{10.20}$$

$$\bar{c}(\tau_j) \equiv \{\bar{c}_1, \bar{c}_2 \ldots \bar{c}_N\} \tag{10.21}$$

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 elevated to the status of continuous functions. The boundary condition (10.18) 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

$$\begin{aligned} \bar{c}_j(c_j - c_{j-1})/\Delta\tau &\to \bar{c}\partial_\tau c, \\ \sum_j \Delta\tau &\to \int_0^\beta d\tau. \end{aligned} \tag{10.22}$$

These cavalier replacements require some thought, for we are not, in general dealing with smooth functions. The sense in which c_j becomes "close" to c_{j+1} needs to be carefully understood. In practice, path-integral is dominated by functions c_j with a maximum characteristic temporal frequency $\omega_{max} \sim \epsilon$, so that the functions $c(\tau)$ which dominate the path integral are not arbitrarily jagged: once $\omega_{\max}\Delta\tau << 1$, the discrete and continuous differentials are essentially identical. With these provisos, the continuum limit of the action and path integral are then

$$\begin{aligned} S &= \int_0^\infty d\tau \Big[\bar{c}(\partial_\tau + \epsilon)c\Big], \\ Z &= \int \mathcal{D}[\bar{c}, c] \exp\Big[-S\Big] \end{aligned} \tag{10.23}$$

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 $\partial_\tau \to -i\omega_n$ 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

$$Z = \int \prod_n d\bar{c}_n dc_n \exp\Big[\sum_n \bar{c}_n(-i\omega_n + \epsilon)c_n\Big] = \prod_n (-i\omega_n + \epsilon)$$

so that the Free energy is given by

$$F = -T \ln Z = -T \sum_n \ln(\epsilon - i\omega_n)$$

We can show that this reverts to the standard expression for one-particle free energy by replacing the Matsubara sum with a contour integral:

$$F = T \oint \frac{dz}{2\pi i} f(z) \ln[\epsilon_\lambda - z] \tag{10.24}$$

where the contour integral passes counter-clockwise around the poles of the Fermi function at $z = i\omega_n$. 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

$$\begin{aligned} F &= -\int_\epsilon^\infty \frac{d\omega}{2\pi i} f(\omega) \Big[\ln(\epsilon - \omega - i\delta) - (\text{c.c.})\Big] \\ &= \int_\epsilon^\infty d\omega f(\omega) \\ &= -T \ln[1 + e^{-\beta\epsilon}] \end{aligned} \tag{10.25}$$

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:

- 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.

$$: H[c^\dagger, c] :\rightarrow H[\bar{c}, c]$$

- 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

$$\mathcal{D}[\bar{c}, c] = \prod_{\tau_l, r} d\bar{c}_r(\tau_l) dc_r(\tau_l)$$

- 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,

$$\begin{aligned} c_{\mathbf{k}} &= \frac{1}{\sqrt{\beta}} \sum_n c_{\mathbf{k}n} e^{i\omega_n \tau}, \\ \partial_\tau &\rightarrow -i\omega_n \\ \mathcal{D}[\bar{c}, c] &\rightarrow \prod_{\mathbf{k},n} d\bar{c}_{\mathbf{k}n} dc_{\mathbf{k}n}. \end{aligned} \tag{10.26}$$

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

$$\begin{aligned} c_{\mathbf{k}} &= \frac{1}{\sqrt{V}} \int d^3x \psi(\mathbf{x}) e^{-i\mathbf{k}\cdot\mathbf{x}}, \\ \epsilon_{\mathbf{k}} &\rightarrow -\frac{\nabla^2}{2m} - \mu \\ \mathcal{D}[\bar{c}, c] &\rightarrow \mathcal{D}[\bar{\psi}, \psi]. \end{aligned} \tag{10.27}$$

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, (10.26) and (10.27) 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 $c_{\mathbf{k}n}$.

10.4 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,

$$\frac{\delta \ln Z[\bar{j}, j]}{\delta \bar{j}(1)} = \langle c(1)\rangle \tag{10.28}$$

$$\frac{\delta^2 \ln Z[\bar{j}, j]}{\delta \bar{j}(2)\delta j(1)} = \langle T[c(1)c^\dagger(2)]\rangle - \langle c(2)\rangle\langle c^\dagger(1)\rangle \tag{10.29}$$

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

$$Z[\bar{j},j] = \int \mathcal{D}[\bar{c},c]e^{-S} \tag{10.30}$$

$$S = \int d\tau \Big[\bar{c}(\tau)(\partial_\tau + \underline{h})c(\tau) - \bar{j}(\tau)c(\tau) - \bar{c}(\tau)j(\tau)\Big] \tag{10.31}$$

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

$$\langle c(1)\rangle = \frac{1}{Z[\bar{j},j]}\int \mathcal{D}[\bar{c},c]c(1)e^{-S} \tag{10.32}$$

$$\langle T[c(1)c^\dagger(2)]\rangle = \frac{1}{Z[\bar{j},j]}\int \mathcal{D}[\bar{c},c]c(1)\bar{c}(2)e^{-S} \tag{10.33}$$

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

$$F = -T\ln Z = -T\,\mathrm{lndet}[\partial_\tau + \underline{h}] = -T\,\mathrm{Trln}[\partial_\tau + \underline{h}] = T\,\mathrm{Trln}[-G^{-1}]$$

where we have used the result $\mathrm{lndet}[A] = \mathrm{Trln}[\partial_\tau + \underline{h}]$.

To explicitly compute the Free energy it is useful to transform to Fourier components,

$$c_\lambda(\tau) = \frac{1}{\sqrt{\beta}}\sum_n c_{\lambda n}e^{-i\omega_n\tau},$$

$$j_\lambda(\tau) = \frac{1}{\sqrt{\beta}}\sum_n j_{\lambda n}e^{-i\omega_n\tau}, \tag{10.34}$$

In this basis,

$$\begin{aligned}(\partial_\tau + \epsilon_\lambda) &\longrightarrow (-i\omega_n + \epsilon_\lambda)\\ \underline{G} = -(\partial_\tau + \epsilon_\lambda)^{-1} &\longrightarrow (i\omega_n - \epsilon_\lambda)^{-1}\end{aligned} \tag{10.35}$$

so that

$$S = \sum_{\lambda,n}\Big[[-i\omega_n + \epsilon_\lambda]\bar{c}_{\lambda n}c_{\lambda n} - \bar{j}_{\lambda n}c_{\lambda n} - \bar{c}_{\lambda n}j_{\lambda n}\Big] \tag{10.36}$$

whereupon,

$$\begin{aligned}\det[\partial_\tau + \underline{h}] &= \prod_{\lambda,n}(-i\omega_n + \epsilon_\lambda) \\ Z[\bar{j}, j] &= \prod_{\lambda,n}(-i\omega_n + \epsilon_\lambda)\exp\Big[\sum_{\lambda,n}(-i\omega_n + \epsilon_\lambda)^{-1}\bar{j}_{\lambda n} j_{\lambda n}\Big] \qquad (10.37)\end{aligned}$$

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

$$\begin{aligned}F &= T\sum_\lambda \oint \frac{dz}{2\pi i} f(z)\ln[\epsilon_\lambda - z] \qquad (10.38)\\ &= -T\sum_\lambda \ln[1 + e^{-\beta\epsilon_\lambda}] \qquad (10.39)\end{aligned}$$

If we differentiate Z with respect to its source terms, we obtain the Green's function:

$$-\frac{\delta^2 \ln Z}{\delta\bar{j}_{\lambda n}\delta j_{\lambda' n'}} = [\underline{G}]_{\lambda n,\lambda' n'} = \delta_{\lambda\lambda'}\delta_{nn'}\frac{1}{i\omega_n - \epsilon_\lambda}$$

10.5 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 $-gA(x) \to \Delta(x)$, in the following way

$$-gA^\dagger(x)A(x) \to A^\dagger(x)\Delta(x) + \bar{\Delta}(x)A(x) + \frac{\bar{\Delta}(x)\Delta(x)}{g}$$

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

$$\int \frac{d\Delta d\bar{\Delta}}{2\pi i g} e^{-\bar{\Delta}\Delta/g} = 1. \tag{10.40}$$

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 (10.40) as follows

$$\int \mathcal{D}[\bar{\Delta},\Delta] \exp\Big[\int d^3x \int_0^\beta d\tau \frac{\bar{\Delta}(x)\Delta(x)}{g}\Big] = 1, \tag{10.41}$$

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, $(\delta x, \Delta\tau) \to 0$, 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

$$Z = \int \mathcal{D}[\bar{c},c] e^{-\int_0^\beta d\tau \Big[\bar{c}(\partial_\tau + \underline{h})c + H_I\Big]}$$

By introducing the unit identity (10.41) into the fermionic path integral, we obtain

$$Z = \int \mathcal{D}[\bar{c},c] \int \mathcal{D}[\bar{\Delta},\Delta] e^{-\int_0^\beta d\tau \Big[\bar{c}(\partial_\tau + \underline{h})c + H_I'\Big]} \tag{10.42}$$

where

$$H_I' = \int d^3x \Big\{ \frac{\bar{\Delta}(x)\Delta(x)}{g} - g\bar{A}(x)A(x) \Big\} \tag{10.43}$$

Now if we shift the Δ field as follows

$$\begin{aligned}\Delta(x) &\rightarrow \Delta(x) - gA(x),\\ \bar{\Delta}(x) &\rightarrow \bar{\Delta}(x) - g\bar{A}(x),\end{aligned}$$

the measure is unchanged. Making this substitution in (10.43), we obtain

$$H_I' = \int d^3x \Big\{ \bar{A}(x)\Delta(x) + \bar{\Delta}(x)A(x) + \frac{\bar{\Delta}(x)\Delta(x)}{g} \Big\}. \tag{10.44}$$

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 (10.42), we now obtain

$$\begin{aligned} Z &= \int \mathcal{D}[\bar{\Delta},\Delta] e^{-\int d^3 d\tau \frac{\bar{\Delta}(x)\Delta(x)}{g}} \int \mathcal{D}[\bar{c},c] e^{-\tilde{S}} \\ \tilde{S} &= \int_0^\beta d\tau \bar{c}\partial_\tau c + H_{eff}[\bar{\Delta},\Delta] \end{aligned} \tag{10.45}$$

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,

$$Z = \sum_{\{\Delta\}} e^{-\int d^4x \frac{|\Delta|^2}{g}} [\text{ Path integral of fermions moving in field } \Delta\ ]$$

[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

$$\frac{\partial^2 \ln\Lambda[j,\bar{j}]}{\partial\bar{j}(x)\partial j(x')}\Big|_{j,\bar{j}=0} = \langle \Delta(x\bar{\Delta}(x') \rangle = gd^{(4)}(x-x')$$

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

$$e^{-S_\psi[\bar{\Delta},\Delta]} = \int \mathcal{D}[\bar{c},c]e^{-\tilde{S}} = \det[\partial_\tau + \underline{h}_{eff}[\bar{\Delta},\Delta]] \tag{10.46}$$

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

$$\begin{aligned} S_{eff}[\bar{\Delta},\Delta] &= \int d^3x d\tau \frac{\bar{\Delta}(x)\Delta(x)}{g} - \ln\det[\partial_\tau + \underline{h}_{eff}[\bar{\Delta},\Delta]] \\ &= \int d^3x d\tau \frac{\bar{\Delta}(x)\Delta(x)}{g} - \mathrm{Trln}[\partial_\tau + \underline{h}_{eff}[\bar{\Delta},\Delta]] \end{aligned} \tag{10.47}$$

where we have made the replacement $\ln\det \to \mathrm{Tr}\det$. 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.

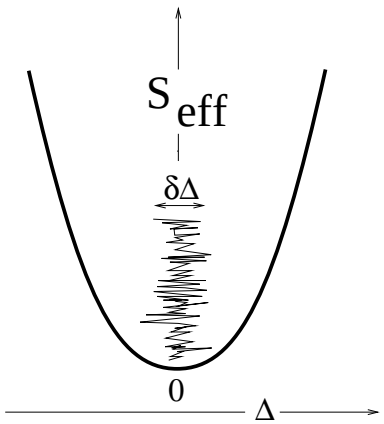
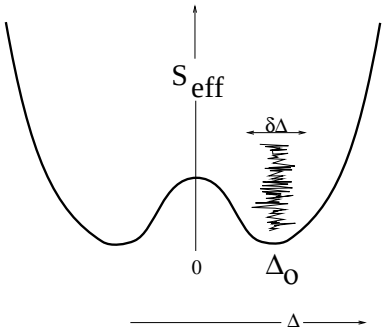
(i) Decoupled from Fermions **white noise**	 $S = \int d^4x \frac{\|\Delta\|^2}{g}$
(ii) Coupled to Fermions: $\Delta_o \neq 0$	 $S_{eff} = \int d^4x \frac{\|\Delta\|^2}{g} - \mathrm{Trln}(\partial_\tau + h_{eff}[\bar{\Delta}, \Delta])$

Fig. 3 Effective action for auxilliary field.

10.6 BCS theory using path integrals

As a specific illustration of the above approach, we re-derive BCS theory using the path integral method. We start with the BCS Hamiltonian

$$H = \sum_{\mathbf{k}\sigma} \epsilon_{\mathbf{k}\sigma} c^\dagger{}_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} - \frac{g}{V} A^\dagger A$$

where

$$A = \sum_{\mathbf{k}} c_{-\mathbf{k}\downarrow} c_{\mathbf{k}\uparrow}, \qquad A^\dagger = \sum_{\mathbf{k}} c^\dagger{}_{\mathbf{k}\uparrow} c^\dagger{}_{-\mathbf{k}\downarrow},$$

are the operators that annihilate or create a uniform pair density. This "simplified" pairing Hamiltonian is actually the one originally used by BCS. Notice how the interaction

$$H_I = -\frac{g}{V}\sum_{\mathbf{k},\mathbf{k}'} c^\dagger{}_{\mathbf{k}\uparrow} c^\dagger{}_{-\mathbf{k}\downarrow} c_{-\mathbf{k}'\downarrow} c_{\mathbf{k}'\uparrow},$$

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.

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

$$S = \int_0^\beta \sum_{\mathbf{k}\sigma} \bar{c}_{\mathbf{k}\sigma}(\partial_\tau + \epsilon_{\mathbf{k}}) c_{\mathbf{k}\sigma} - \frac{g}{V}\bar{A}A$$

Next we introduce the identity

$$\int \mathcal{D}[\bar{\Delta}, \Delta] \exp\Big[\frac{V}{g}\int_0^\beta d\tau \bar{\Delta}(\tau)\Delta(\tau)\Big] = 1 \tag{10.48}$$

into the path integral. By shifting the variables $\Delta \to \Delta - \frac{g}{V}A$, $\bar{\Delta} \to \bar{\Delta} - \frac{g}{V}\bar{A}$, we obtain

$$\begin{aligned} Z &= \int \mathcal{D}[\bar{\Delta}, \Delta, \bar{c}, c] e^{-S} \\ S &= \int_0^\beta d\tau \left\{ \sum_{\mathbf{k}\sigma} \bar{c}_{\mathbf{k}\sigma}(\partial_\tau + \epsilon_{\mathbf{k}}) c_{\mathbf{k}\sigma} + \Delta A + \bar{A}\Delta + \frac{V}{g}\bar{\Delta}\Delta \right\} \end{aligned} \tag{10.49}$$

where $\Delta(\tau)$ is a function of time only. In a Nambu notation, this can be re-written

$$S = \int_0^\beta d\tau \left\{ \sum_{\mathbf{k}} \bar{\psi}_{\mathbf{k}}(\partial_\tau + \underline{h}_{\mathbf{k}})\psi_{\mathbf{k}} + \frac{V}{g}\bar{\Delta}\Delta \right\}$$

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 $\rightarrow$ 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 $V \rightarrow \infty$. 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 $V \rightarrow \infty$, 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,

$$\partial_\tau + h \rightarrow [-i\omega_n + \underline{h}_{\mathbf{k}}]$$

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

$$F_{eff} = \frac{S_{eff}}{\beta} = -T \sum_{\mathbf{kn}} \ln[\omega_n^2 + \epsilon_{\mathbf{k}}^2 + |\Delta|^2] + V\frac{|\Delta|^2}{g}$$

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

$$\frac{\partial F_{eff}}{\partial \bar{\Delta}} = -\sum_{\mathbf{k}n} \frac{\Delta}{\omega_n^2 + E_{\mathbf{k}}^2} + V\frac{\Delta}{g} = 0 \tag{10.50}$$

$$\Rightarrow \frac{1}{g} = \frac{1}{\beta V}\sum_{\mathbf{k}n} \frac{1}{\omega_n^2 + E_{\mathbf{k}}^2} \tag{10.51}$$

where

$$E_{\mathbf{k}} = \sqrt{\epsilon_{\mathbf{k}}^2 + |\Delta|^2}$$

is the quasiparticle energy.

We could have carried out the Matsubara sum at any stage in the above manipulation. Using the contour integration method,

$$F_{eff} = -\sum_{\mathbf{k}} \oint \frac{dz}{2\pi i} f(z)\ln[E_{\mathbf{k}}^2 - z^2] + V\frac{|\Delta|^2}{g}$$

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

$$\int \frac{dx}{2\pi i} f(x)\{\ln[E_{\mathbf{k}}^2 - (x+i\delta)^2] - \ln[E_{\mathbf{k}}^2 - (x-i\delta)^2]\} = -\int_{-E_{\mathbf{k}}}^{E_{\mathbf{k}}} dx f(x) = -2T\ln\Big[2\cosh(\beta E_{\mathbf{k}}/2)\Big] \tag{10.52}$$

The Free energy then becomes

$$F_{eff} = -2TV\int \frac{d^3k}{(2\pi)^3}\ln\Big[2\cosh(\beta E_{\mathbf{k}}/2)\Big] + V\frac{|\Delta|^2}{g}.$$

Differentiating w.r.t. $\bar{\Delta}$ then gives

$$\frac{1}{g} = \int \frac{d^3k}{(2\pi)^3}\left[\frac{\tanh(\beta E_{\mathbf{k}}/2)}{2E_{\mathbf{k}}}\right]$$

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.

A Appendix: Grassman Calculus

A.1 Differentiation and Integration

Differentiation is defined to have the normal linear properties of the differential operator. We define

$$\partial \equiv \frac{\partial}{\partial c}, \quad \bar{\partial} \equiv \frac{\partial}{\partial \bar{c}} \tag{10.53}$$

so that

$$\partial c = \bar{\partial}\bar{c} = 1, \tag{10.54}$$

and thus if $f(\bar{c}, c)$ is defined as above, then

$$\begin{aligned} \partial f &= \tilde{f}_1 + f_{12}\bar{c} \\ \bar{\partial} f &= f_1 - f_{12}\bar{c} \end{aligned} \tag{10.55}$$

where the minus sign in the second 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 :

$$\int dc \equiv \partial, \qquad \int d\bar{c} \equiv \bar{\partial} \tag{10.56}$$

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 $\xi\to\xi-A^{-1}j$, 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 $A\to-G^{-1}$ becomes the inverse propagator for the fermions, and $\xi_n\to\psi(i\omega_n)$ 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.