9 Fluctuation–dissipation theorem and linear response theory

9.1 Introduction

In this chapter we will discuss the deep link between fluctuations about equilibrium and the response of a system to external forces. If the susceptibility of a system to external change is large, then the fluctuations about equilibrium are expected to be large. The mathematical relationship that quantifies this connection is called the *fluctuation–dissipation theorem* [1–3]. We shall discuss and derive this relationship in this chapter. It turns out that the link between fluctuations and dissipation also extends to imaginary time, enabling us to relate equilibrium correlation functions and response functions to the imaginary-time Green's function of the corresponding variables.

To describe the fluctuations and response at a finite temperature, we will introduce related types of Green's function: the correlation function $S(t)$ [4],

$$S(t-t') = \langle A(t)\, A(t')\rangle = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} e^{-i\omega(t-t')} S(\omega); \tag{9.1}$$

the dynamical susceptibility $\chi(t)$,

$$\chi(t-t') = i\langle [A(t), A(t')]\rangle \theta(t-t'), \tag{9.2}$$

which determines the retarded response

$$\langle A(t)\rangle = \int_{-\infty}^{\infty} dt' \chi(t-t') f(t'), \quad \langle A(\omega)\rangle = \chi(\omega) f(\omega), \tag{9.3}$$

to a force term $f(t)$ coupled to A inside the Hamiltonian $H_I = -f(t)A(t)$; and, lastly, the imaginary-time response function $\chi(\tau)$,

$$\chi(\tau-\tau') = \langle TA(\tau)A(\tau')\rangle. \tag{9.4}$$

The fluctuation–dissipation theorem [1–3] relates the Fourier transforms of these quantities, according to

$$\underbrace{S(\omega)}_{\text{fluctuations}} = 2\hbar[\overbrace{1}^{\text{quantum}} + \overbrace{n_B(\omega)}^{\text{thermal}}] \underbrace{\chi''(\omega)}_{\text{dissipation}}, \tag{9.5}$$

where $\chi''(\omega)$ = 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,

$$S(\omega) = \frac{2k_B T}{\omega}\chi''(\omega). \tag{9.6}$$

Thus, in principle, if we know the correlation functions in thermal equilibrium, we can compute the response function of the system.

The dissipative response of the system also enters into the Kramers–Kronig expansion of the response function,

$$\chi(z) = \int \frac{d\omega}{\pi}\frac{1}{\omega - z}\chi''(\omega). \tag{9.7}$$

This allows us to interpret

$$-\frac{1}{\pi}\chi''(\omega)d\omega = \text{residue of poles between } \omega \text{ and } \omega + d\omega, \tag{9.8}$$

so that $\chi''(\omega)$ is a kind of spectral density for excitations, weighted by the matrix element of the corresponding operator. Using this expression, the dynamical susceptibility can be analytically extended into the complex plane. We will see that above the real axis $\chi(z)$ describes causal, retarded responses to an applied force, where as below the real axis, it describes a time-reversed "advanced" response to changes in the future.

In practice, the theorist takes advantage of a completely parallel fluctuation–dissipation theorem which exists in imaginary time. The imaginary-time correlation function $\chi(\tau)$ is periodic in time $\chi(\tau+\beta) = \chi(\tau)$, and has a discrete Matsubara Fourier expansion, given by

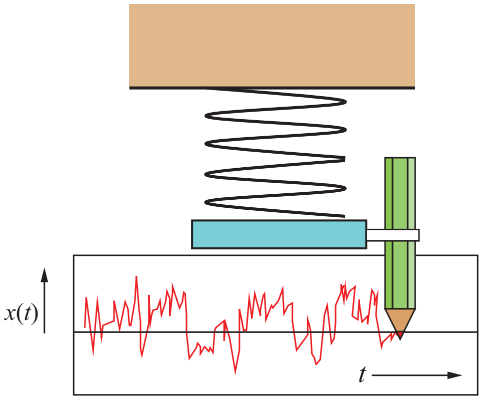
$$\chi(\tau) = \langle TA(\tau)A(0)\rangle = \frac{1}{\beta}\sum_n e^{-i\nu_n\tau}\chi_M(i\nu_n). \tag{9.9}$$

The key relation between this function and the physical response function is that

$$\chi_M(i\nu_n) = \chi(z)|_{z=i\nu_n}. \tag{9.10}$$

This relation permits us to compute the physical response function by analytically continuing the Fourier components of the imaginary-time correlation functions onto the real axis.

To understand these relations, we first need to understand the nature of the quantum mechanical response functions. We shall then carry out a *spectral decomposition* of each of the above functions, deriving the fluctuation–dissipation theorem by showing that the same underlying matrix elements enter into each expression. A heuristic understanding of the relationship between fluctuations and dissipation is obtained by examining a classical example. The main difference between the classical and quantum fluctuation–dissipation theorems is that in classical mechanics we are obliged to explicitly include the external sources of noise, whereas in the quantum case the noise is intrinsic and we can analyze the fluctuations without any specific reference to external sources of noise. Nevertheless, the classical case is highly pedagogical, and it is this limit that we shall consider first.



$$\overbrace{\langle x(t)x(0)\rangle}^{\text{fluctuations}} = 2k_BT \int \frac{d\omega}{2\pi} \underbrace{\frac{\chi''(\omega)}{\omega}}_{\text{dissipation}} e^{-i\omega t}$$

Fig. 9.1 Fluctuations in a classical harmonic oscillator are directly related to the dissipative response function via the fluctuation–dissipation theorem.

9.2 Fluctuation–dissipation theorem for a classical harmonic oscillator

In a classical system, to examine correlation functions we need to include an explicit source of external noise. To illustrate the procedure, consider a harmonic oscillator in thermal equilibrium inside a viscous medium. Suppose that thermal fluctuations give rise to a random force, acting on the oscillator according to the equation of motion

$$m(\ddot{x} + \omega_0^2 x) + \eta \dot{x} = f(t). \tag{9.11}$$

If we Fourier transform this relationship, we obtain

$$\begin{aligned} x(\omega) &= \chi(\omega) f(\omega) \\ \chi(\omega) &= [m(\omega_0^2 - \omega^2) - i\omega\eta]^{-1}. \end{aligned} \tag{9.12}$$

Here $\chi(\omega)$ is the response function or susceptibility to the external force. The imaginary part of the susceptibility governs the dissipation and is given by

$$\chi''(\omega) = \frac{\omega\eta}{m(\omega_0^2 - \omega^2) + \omega^2\eta^2} = |\chi(\omega)|^2 \omega\eta. \tag{9.13}$$

Now let us consider the fluctuations in thermal equilibrium. Over long time periods, we expect the two-point correlation function to be purely a function of the time difference:

$$\langle x(t)x(t')\rangle = \langle x(t - t')x(0)\rangle. \tag{9.14}$$

The power spectrum of fluctuations is defined as

$$\langle |x(\omega)|^2 \rangle = \int dt \langle x(t)x(0) \rangle e^{i\omega t} \tag{9.15}$$

and the inverse relation gives

$$\langle x(t)x(t') \rangle = \int \frac{d\omega}{2\pi} e^{-i\omega(t-t')} \langle |x(\omega)|^2 \rangle. \tag{9.16}$$

Now in thermal equilibrium the equipartition theorem tells us that

$$\frac{m\omega_0^2}{2} \langle x^2 \rangle = \frac{k_B T}{2} \tag{9.17}$$

or

$$\langle x^2 \rangle = \int \frac{d\omega}{2\pi} \langle |x(\omega)|^2 \rangle = \int \frac{d\omega}{2\pi} |\chi(\omega)|^2 \langle |f(\omega)|^2 \rangle = \frac{k_B T}{m\omega_0^2}. \tag{9.18}$$

Since the integrand is very sharply peaked around $|\omega| = \omega_0$, we replace $\langle |f(\omega)|^2 \rangle \to \langle |f(\omega_0)|^2 \rangle$ in the above expression. Replacing $|\chi(\omega)|^2 \to \frac{1}{\omega\eta}\chi''(\omega)$, we then obtain

$$\frac{k_B T}{m\omega_0^2} = \frac{\langle |f(\omega_0)|^2 \rangle}{2\eta} \int \frac{d\omega}{\pi} \frac{\chi''(\omega)}{\omega} = \frac{|f(\omega_0)|^2}{2\eta m\omega_0^2}, \tag{9.19}$$

so that the spectrum of force fluctuations is determined by the viscosity η:

$$\langle |f(\omega_0)|^2 \rangle = 2\eta k_B T. \tag{9.20}$$

Now if we assume that the noise spectrum depends only on the properties of the viscous medium in which the oscillator is embedded, and not on the properties of the oscillator, then we expect this expression to hold for any frequency ω_0, and since it is *independent* of the frequency, we conclude that the power spectrum of the force is a flat function of frequency, enabling us to replace $\omega_0 \to \omega$ in the above expression. This implies that, in thermal equilibrium, the force coupling the system to the environment is a source of white noise of an amplitude which depends on the viscosity of the medium:

$$\langle f(t)f(t') \rangle = \int \frac{d\omega}{2\pi} e^{-i\omega(t-t')} \overbrace{\langle |f(\omega)|^2 \rangle}^{2\eta k_B T} = 2\eta k_B T \delta(t-t'). \tag{9.21}$$

We can now compute the noise spectrum of fluctuations, which is given by

$$S(\omega) = \langle |x(\omega)|^2 \rangle = |\chi(\omega)|^2 \langle |f(\omega)|^2 \rangle = \langle |f(\omega)|^2 \rangle \frac{\chi''(\omega)}{\omega\eta} = \frac{2k_B T}{\omega} \chi''(\omega). \tag{9.22}$$

This expression relates the thermal fluctuations of a classical system to the dissipation, as described by the imaginary part of the response function, $\chi''(\omega)$.

9.3 Quantum mechanical response functions

Suppose we couple a force f to variable A. For later generality, it suits our needs to consider a force in both real and imaginary time, with Hamiltonian

$$H = H_0 - f(t)A \tag{9.23}$$

$$H = H_0 - f(\tau)A. \tag{9.24}$$

We shall now show that the response to these forces is given by

$$\begin{aligned} \langle A(t)\rangle &= \langle A\rangle + \int_{-\infty}^{\infty} \chi(t-t')f(t')dt' \\ \langle A(\tau)\rangle &= \langle A\rangle + \int_{0}^{\beta} \tilde{\chi}(\tau-\tau')f(\tau')d\tau' \end{aligned} \tag{9.25}$$

$$\begin{aligned} \chi(t-t') &= i\langle[A(t),\ A(t')]\rangle\theta(t-t') \\ \tilde{\chi}(\tau-\tau') &= \langle TA(\tau)A(\tau')]\rangle - \langle A\rangle^2, \end{aligned} \tag{9.26}$$

where $\langle A\rangle$ is the value of A in thermal equilibrium.

Let us begin in real time. Suppose we want to look at the future response to a force $f(t)$ applied in the past. Using the interaction representation, we know that

$$A_H(t) = U^\dagger(t)A_I(t)\,U(t), \tag{9.27}$$

where

$$U(t) = T\exp\left[i\int_{-\infty}^{t} dt' A_I(t')f(t')\right]. \tag{9.28}$$

Remembering that the interaction representation corresponds to the Heisenberg representation for H_0, we can drop the subscript on $A_I(t) \equiv A(t)$, so that, to linear order in $f(t)$,

$$\begin{aligned} U(t) &= 1 + i\int_{-\infty}^{t} dt' A(t')f(t') \\ U^\dagger(t) &= 1 - i\int_{-\infty}^{t} dt' A(t')f(t'), \end{aligned} \tag{9.29}$$

so that

$$A_H(t) = A(t) + i\int_{-\infty}^{t} dt'[A(t),A(t')]f(t'). \tag{9.30}$$

In thermal equilibrium $\langle A(t)\rangle = \langle A\rangle$, so the response to the applied force is given by

$$\langle A_H(t)\rangle = \langle A\rangle + \int_{-\infty}^{+\infty} dt'\ \chi(t-t')f(t'), \tag{9.31}$$

where

$$\chi_R(t-t') = i\langle [A(t), A(t')]\,\rangle \theta(t-t') \tag{9.32}$$

retarded response function

is the *retarded response function*. The above equation is particularly interesting, for it relates a response to a quantum mechanical correlation function. For completeness, we note that the corresponding backwards-time quantity

$$\chi_A(t-t') = -i\langle [A(t), A(t')]\,\rangle \theta(t'-t) \tag{9.33}$$

advanced response function

is known as the *advanced response function*, corresponding to a fictional time-reversed world in which we propagate the effects of a disturbance backwards in time!

Let us now switch to consider imaginary time. In this case, the partition function in the presence of a perturbation is

$$Z = Z_0 \langle T \exp \int_0^\beta d\tau f(\tau) A_I(\tau)\rangle_0. \tag{9.34}$$

The expectation value of $A(\tau)$ is then given by

$$\begin{aligned}\langle A(\tau)\rangle = \frac{\delta \ln Z}{\delta f(\tau)} &= \frac{\langle T A(\tau) \exp \int_0^\beta d\tau' f(\tau') A_I(\tau')\rangle}{\langle T \exp \int_0^\beta d\tau' f(\tau') A_I(\tau')\rangle} \\ &= \langle A\rangle + \int_0^\beta d\tau' \overbrace{\Big[\langle T A(\tau) A(\tau')\rangle - \langle A\rangle^2\Big]}^{\tilde{\chi}(\tau-\tau')} f(\tau') + O(f^2),\end{aligned} \tag{9.35}$$

so that the thermal response to the applied force is given by a Green's function that is time-ordered in imaginary time:

$$\begin{aligned}\tilde{\chi}(\tau-\tau') &= \langle T A(\tau) A(\tau')\rangle - \langle A\rangle^2 \\ &= \langle T (A(\tau) - \langle A\rangle)(A(\tau') - \langle A\rangle)\rangle,\end{aligned} \tag{9.36}$$

where expectation values are to be taken at thermal equilibrium for H_0. $\chi(\tau-\tau')$ describes the thermal and quantum fluctuations of the quantity $\hat{A}$ in imaginary time.

9.4 Fluctuations and dissipation in a quantum world

The quantum Boltzmann formulation of many-body physics is naturally tailored to a discussion of the statistics of fluctuations and dissipation. Quantum systems are naturally noisy, and there is no need for us to add any additional noise source to examine the deep link between fluctuations and dissipation in a quantum many-body system. Indeed, the quantum fluctuation–dissipation theorem can be derived in rather mechanistic fashion by carrying out a spectral decomposition of the various response and correlation functions. The procedure is formally more direct than its classical analogue, but the algebra tends to hide the fact that the underlying physics holds precisely the same link between fluctuations – now both thermal and quantum in character – and dissipation.

To derive the quantum fluctuation–dissipation theorem, we must first spectrally decompose the correlation function $S(t-t')$ and the retarded response function $\chi_R(t-t')$.

9.4.1 Spectral decomposition I: the correlation function $S(t-t')$

This is the easiest decomposition of the three to carry out. We begin by expanding the response function in terms of a complete set of energy eigenstates which satisfy

$$\begin{aligned} H\left|\lambda\right\rangle &= E_\lambda \left|\lambda\right\rangle \\ \sum_\lambda \left|\lambda\right\rangle\left\langle\lambda\right| &= 1 \\ \left\langle\lambda\left|A(t)\right|\zeta\right\rangle &= \left\langle\lambda\left|e^{iHt}A\,e^{-iHt}\right|\zeta\right\rangle = e^{-i(E_\zeta-E_\lambda)(t-t')}\left\langle\lambda\left|A\right|\zeta\right\rangle . \end{aligned} \tag{9.37}$$

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

$$\begin{aligned} S(t-t') &= \langle A(t)A(t')\rangle \\ &= \sum_{\lambda,\zeta} e^{-\beta(E_\lambda-F)}\left\langle\lambda\left|A(t)\right|\zeta\right\rangle\left\langle\zeta\left|A(t')\right|\lambda\right\rangle \\ &= \sum_{\lambda,\zeta} e^{-\beta(E_\lambda-F)}\left|\left\langle\zeta\left|A\right|\lambda\right\rangle\right|^2 e^{-i(E_\zeta-E_\lambda)(t-t')}. \end{aligned} \tag{9.38}$$

If we now Fourier transform this expression, the frequency-dependent correlation function can be written

$$\begin{aligned} S(\omega) &= \int_{-\infty}^{\infty} dt e^{i\omega t} S(t) \\ &= \sum_{\lambda,\zeta} e^{-\beta(E_\lambda-F)}\left|\left\langle\zeta\left|A\right|\lambda\right\rangle\right|^2 2\pi\,\delta(E_\zeta-E_\lambda-\omega). \end{aligned} \tag{9.39}$$

This is the frequency spectrum of the correlations.

9.4.2 Spectral decomposition II: the retarded response function $\chi_R(t-t')$

We now use the same spectral decomposition approach for the retarded response function. In this case, we need to take care of two operator orderings inside the commutator, which yield

$$\begin{aligned} \chi_R(t-t') &= i\langle[A(t),A(t')]\,\rangle\theta(t-t') \\ &= i\sum_{\lambda,\zeta} e^{-\beta(E_\lambda-F)}\left\{\left\langle\lambda\left|A(t)\right|\zeta\right\rangle\left\langle\zeta\left|A(t')\right|\lambda\right\rangle - \left\langle\lambda\left|A(t')\right|\zeta\right\rangle\left\langle\zeta\left|A(t)\right|\lambda\right\rangle\right\}\theta(t-t') \\ &= i\sum_{\lambda,\zeta} e^{\beta F}(e^{-\beta E_\lambda}-e^{-\beta E_\zeta})\left|\left\langle\zeta\left|A\right|\lambda\right\rangle\right|^2 e^{-i(E_\zeta-E_\lambda)(t-t')}\theta(t-t'). \end{aligned} \tag{9.40}$$

By introducing the spectral function

$$\chi''(\omega) = \pi(1 - e^{-\beta\omega}) \sum_{\lambda,\zeta} p_\lambda \, |\langle\zeta\, |A|\, \lambda\rangle|^2 \, \delta[\omega - (E_\zeta - E_\lambda)], \tag{9.41}$$

where $p_\lambda = e^{-\beta(E_\lambda - F)}$ is the probability of being in the initial state $|\lambda\rangle$, we see that the retarded response function can be written

$$\chi_R(t) = i \int \frac{d\omega}{\pi} \, e^{-i\omega t} \theta(t) \, \chi''(\omega). \tag{9.42}$$

Fourier transforming this result, using

$$i \int_0^\infty dt \, e^{i(\omega - \omega' + i\delta)\, t} = \frac{1}{\omega' - \omega - i\delta}, \tag{9.43}$$

we can read off the Fourier transform of the retarded response function as

$$\chi_R(\omega) = \int \frac{d\omega'}{\pi} \frac{1}{\omega' - \omega - i\delta} \chi''(\omega'). \tag{9.44}$$

This is known as a *Kramers–Kronig relation*. The Kramers–Kronig relation can be used to extend the response function into the complex plane by writing

$$\chi(z) = \int \frac{d\omega'}{\pi} \frac{1}{\omega' - z} \chi''(\omega'). \tag{9.45}$$

dynamical susceptibility

This is the *dynamical susceptibility*. When we evaluate $\chi(z)$ just above the real axis, we get the retarded response function $\chi_R(\omega) = \chi(\omega + i\delta)$. The upper half-plane is thus the analytic extension of $\chi_R(\omega)$. But what about the lower half-plane? Remarkably, this gives the advanced response function, such that $\chi_A(\omega) = \chi(\omega - i\delta)$. From the definition of $\chi(z)$, we see that its poles are located exclusively along the real axis at $z = \omega'$, so that $\chi(z)$ is analytic everywhere *except* the real axis. Substituting the Cauchy–Dirac relation

$$\frac{1}{\omega' - \omega \mp i\delta} = \mathrm{P}\frac{1}{\omega' - \omega} \pm i\pi\delta(\omega' - \omega), \tag{9.46}$$

where P denotes the principal part, into (9.45), we see that above and below the real axis at $z = \omega \pm i\delta$ the dynamical susceptibility is given by

$$\chi(\omega \pm i\delta) = \int \frac{d\omega'}{\pi} \mathrm{P}\left(\frac{1}{\omega' - \omega}\right) \chi''(\omega') \pm i\chi''(\omega) = \chi'(\omega) \pm i\chi''(\omega), \tag{9.47}$$

so that the real part of $\chi(z)$ is continuous across the real axis, but the dissipative imaginary part has a *discontinuity* given by

$$\chi''(\omega) = \mathrm{Im}\, \chi(\omega + i\delta) = \frac{\chi(\omega + i\delta) - \chi(\omega - i\delta)}{2i}. \tag{9.48}$$

This branch cut along the imaginary axis is a universal property of the dynamical response function.

Example 9.1 (a) By carrying out a spectral decomposition of the advanced response function $\chi_R(t-t') = -i\langle[A(t), A(t')]\rangle\theta(t'-t)$, show that its Fourier transform is determined by the same spectral function as the retarded reponse, namely

$$\chi_A(t) = -i\theta(t)\int \frac{d\omega}{\pi} e^{-i\omega t}\chi''(\omega). \tag{9.49}$$

(b) By Fourier transforming this expression, show that

$$\chi_A(\omega) = \int \frac{d\omega'}{\pi}\frac{1}{\omega'-\omega+i\delta}\chi''(\omega') = \chi(\omega - i\delta) = [\chi_R(\omega)]^*. \tag{9.50}$$

Solution

(a) To prove the first part, we carry out a spectral decomposition as follows:

$$\begin{aligned}
\chi_A(t-t') &= -i\langle[A(t), A(t')]\,\rangle\theta(t'-t)\\
&= -i\sum_{\lambda,\zeta} e^{-\beta(E_\lambda - F)}\left\{\langle\lambda\,|A(t)|\,\zeta\rangle\left\langle\zeta\,\left|A(t')\right|\,\lambda\right\rangle - \left\langle\lambda\,\left|A(t')\right|\,\zeta\right\rangle\langle\zeta\,|A(t)|\,\lambda\rangle\right\}\theta(t'-t)\\
&= -i\sum_{\lambda,\zeta} e^{\beta F}(e^{-\beta E_\lambda} - e^{-\beta E_\zeta})\,|\langle\zeta\,|A|\,\lambda\rangle|^2\, e^{-i(E_\zeta - E_\lambda)(t-t')}\theta(t'-t)\\
&= -i\theta(t'-t)\int d\omega\, e^{-i\omega(t-t')}\overbrace{\sum_{\lambda,\zeta} p_\lambda(1-e^{-\beta\omega})\,|\langle\zeta\,|A|\,\lambda\rangle|^2\,\delta(\omega - (E_\zeta - E_\lambda))}^{\chi''(\omega)/\pi}\\
&= -i\theta(t'-t)\int\frac{d\omega}{\pi}e^{-i\omega t}\chi''(\omega).
\end{aligned} \tag{9.51}$$

(b) Next, we Fourier transform the result of the last part, to obtain

$$\begin{aligned}
\chi_A(\omega) &= \int_{-\infty}^{0} dt\, e^{i\omega t + \delta t}\chi_A(t)\\
&= -i\int_{-\infty}^{0} dt\, e^{i\omega t+\delta t}\int_{-\infty}^{\infty}\frac{d\omega'}{\pi}\chi''(\omega')e^{-i\omega' t}.
\end{aligned} \tag{9.52}$$

Inverting the order of integration gives

$$\begin{aligned}
\chi_A(\omega) &= \int_{-\infty}^{\infty}\frac{d\omega'}{\pi}\chi''(\omega')\left(-i\int_{-\infty}^{0} dt e^{i(\omega-\omega'-i\delta)t}\right)\\
&= \int_{-\infty}^{\infty}\frac{d\omega'}{\pi}\chi''(\omega')\left(\frac{1}{\omega'-\omega+i\delta}\right).
\end{aligned} \tag{9.53}$$

9.4.3 Quantum fluctuation–dissipation theorem

If we compare the relations (9.41) and (9.39), we see that

$$S(\omega) = \frac{2}{1-e^{-\beta\omega}}\chi''(\omega). \tag{9.54}$$

If we restore $\hbar$, this becomes

$$S(\omega) = \frac{2\hbar}{1 - e^{-\beta\hbar\omega}}\chi''(\omega) = 2\hbar\,[1 + n_B(\hbar\omega)]\,\chi''(\omega). \tag{9.55}$$

quantum fluctuation–dissipation theorem

Thus, by carrying out a spectral analysis we have been able to directly link the correlation function $S(\omega)$ with the dissipative part of the retarded response function $\chi(\omega)$.

9.4.4 Spectral decomposition III: fluctuations in imaginary time

For the final of our three decompositions, we move to imaginary time and write, for $\tau - \tau' > 0$,

$$\begin{aligned}\chi(\tau - \tau') &= \sum_{\lambda,\zeta} e^{-\beta(E_\lambda - F)} \left\{\langle\lambda \left|A(\tau)\right| \zeta\rangle\langle\zeta \left|A(\tau')\right| \lambda\rangle\right\} \\ &= \sum_{\lambda,\zeta} p_\lambda e^{-(E_\lambda - E_\zeta)(\tau-\tau')} \left|\langle\zeta \left|A\right| \lambda\rangle\right|^2,\end{aligned} \tag{9.56}$$

where, as before, $p_\lambda = e^{-\beta(E_\lambda - F)}$ is the Boltzmann probability of being in state $|\lambda\rangle$. Now

$$\int_0^\beta d\tau\, e^{i\nu_n\tau} e^{-(E_\lambda - E_\zeta)\tau} = \frac{1}{(E_\zeta - E_\lambda - i\nu_n)}(1 - e^{-(E_\lambda - E_\zeta)\beta}), \tag{9.57}$$

so

$$\begin{aligned}\chi(i\nu_n) &= \int_0^\beta d\tau\, e^{i\nu_n\tau}\chi(\tau) \\ &= \sum_{\lambda,\zeta} p_\lambda (1 - e^{-\beta(E_\zeta - E_\lambda)}) \left|\langle\zeta \left|A\right| \lambda\rangle\right|^2 \frac{1}{(E_\zeta - E_\lambda - i\nu_n)}.\end{aligned} \tag{9.58}$$

Using (9.41), we can write this as

$$\chi(i\nu_n) = \int \frac{d\omega}{\pi} \frac{1}{\omega - i\nu_n} \chi''(\omega). \tag{9.59}$$

But this is nothing more than the dynamical susceptibility $\chi(z)$, evaluated at $z = i\nu_n$. In other words, $\chi(i\nu_n)$ is the unique analytic extension of the dynamical susceptibility $\chi(\omega)$ into the complex plane. Our procedure to calculate response functions will be to write $\chi(i\nu_n)$ in the form (9.29), and to use this to then read off the spectral function $\chi''(\omega)$, which in turn determines the dynamical response function.

9.5 Calculation of response functions

Having made the link between the imaginary-time and real-time response functions, we are ready to discuss how we can calculate response functions from Feynman diagrams. Our procedure is to compute the imaginary-time response function and then analytically

Table 9.1 Selected operators and corresponding response functions.

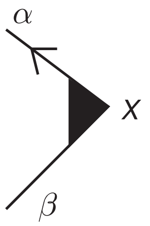
Quantity	Operator $\hat{A}^{a}$	$A(\mathbf{k})$	Response function
Density	$\hat{\rho}(x) = \psi^\dagger(x)\psi(x)$	$\rho_{\alpha\beta} = \delta_{\alpha\beta}$	Charge susceptibility
Spin density	$\vec{S}(x) = \psi^\dagger_\alpha(x)\left(\frac{\vec{\sigma}}{2}\right)_{\alpha\beta}\psi_\beta(x)$	$\vec{M}_{\alpha\beta} = \mu_B\vec{\sigma}_{\alpha\beta}$	Spin susceptibility
Current density[a]	$\frac{e}{m}\psi^\dagger(x)\left(-i\hbar\overleftrightarrow{\nabla} - e\vec{A}\right)\psi(x)$	$\vec{j} = e\vec{v}_{\mathbf{k}} = e\vec{\nabla}\epsilon_{\mathbf{k}}$	Conductivity
Thermal current[a]	$\frac{\hbar^2}{2m}\psi^\dagger(x)\overleftrightarrow{\nabla}\overleftrightarrow{\partial}_t\psi(x)$	$\vec{j}_T = i\omega_n\vec{v}_{\mathbf{k}} = i\omega_n\vec{\nabla}\epsilon_{\mathbf{k}}$	Thermal conductivity

[a] $\overleftrightarrow{\nabla} \equiv \frac{1}{2}\left(\overrightarrow{\nabla} - \overleftarrow{\nabla}\right)$, $\overleftrightarrow{\partial}_t \equiv \frac{1}{2}\left(\overrightarrow{\partial}_t - \overleftarrow{\partial}_t\right)$.

continue to real frequencies. Suppose we are interested in the response function for $\hat{A}$, where

$$\hat{A}(x) = \psi^\dagger_\alpha(x)A_{\alpha\beta}\psi_\beta(x) \tag{9.60}$$

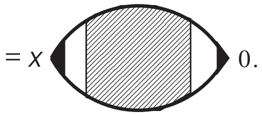
(see table 9.1). The corresponding operator generates the vertex



$$= A_{\alpha\beta}. \tag{9.61}$$

where the spin variables $\alpha\beta$ are to be contracted with the internal spin variables of the Feynman diagram. This inevitably means that the variable $A_{\alpha\beta}$ becomes part of an internal trace over spin variables. If we expand the corresponding response function $\chi(x) = \langle\hat{A}(x)\hat{A}(0)\rangle$ using Feynman diagrams, we obtain

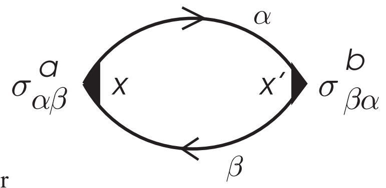
$$\chi(\tau) = \langle\hat{A}(x)\hat{A}(0)\rangle = \sum\{\text{closed linked two-vertex diagrams}\} \tag{9.62}$$



(9.63)

For example, in a non-interacting electron system, the imaginary-time spin response function involves $A(x) = \mu_B\psi^\dagger_\alpha(x)\sigma_{\alpha\beta}\psi_\beta(x)$, so the corresponding response function is

$$\chi^{ab}(x-x') = \mu_B^2 \times$$



Trace over spin variables

$$= \overbrace{-\mathrm{Tr}}^{\text{Trace over spin variables}}\left[\sigma^a\mathcal{G}(x-x')\sigma^b\mathcal{G}(x'-x)\right]$$
$$= -\delta^{ab}2\mu_B^2\mathcal{G}(x-x')\mathcal{G}(x'-x). \tag{9.64}$$

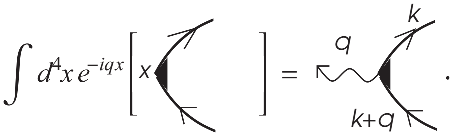
Now to analytically continue to real frequencies, we need to transform to Fourier space, writing

$$\chi(q) = \int d^4x\, e^{-iqx} \chi(x), \tag{9.65}$$

where the integral over time τ runs from 0 to β. This procedure converts the Feynman diagram from a real-space to a momentum-space Feynman diagram. At the measurement vertex at position x, the incoming and outgoing momenta of the fermion line give the following integral:

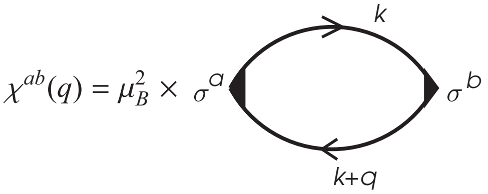
$$\int d^4x\, e^{-iqx} e^{i(k_{in}-k_{out})x} = \beta V \delta^4(k_{out} - k_{in} + q). \tag{9.66}$$

As in the case of the free energy, the βV term cancels with the $1/(\beta V)\sum_k$ terms associated with each propagator, leaving behind one factor of $1/(\beta V) = T/V$ per internal momentum loop. Schematically, the effect of the Fourier transform on the measurement vertex at position x is then



(9.67)

For example, the momentum-dependent spin response function of the free electron gas is given by



$$= -\frac{1}{\beta V}\sum_k \mathrm{Tr}\left[\sigma^a \mathcal{G}(k+q)\sigma^b \mathcal{G}(k)\right] = \delta^{ab}\chi(q) \tag{9.68}$$

where

$$\chi(\mathbf{q}, i\nu_r) = -2\mu_B^2 \int_{\mathbf{k}} T \sum_{i\omega_n} \mathcal{G}(\mathbf{k}+\mathbf{q}, i\omega_n + i\nu_r)\mathcal{G}(\mathbf{k}, i\omega_n). \tag{9.69}$$

When we carry out the Matsubara summation in the above expression by a contour integral (see Chapter 8), we obtain

$$\begin{aligned} -T\sum_{i\omega_n} \mathcal{G}(\mathbf{k}+\mathbf{q}, i\omega_n + i\nu_r)\mathcal{G}(\mathbf{k}, i\omega_n) &= -\int_{C'} \frac{dz}{2\pi i} f(z)\mathcal{G}(\mathbf{k}+\mathbf{q}, z + i\nu_r)\mathcal{G}(\mathbf{k}, z) \\ &= \left(\frac{f_{\mathbf{k}} - f_{\mathbf{k}+\mathbf{q}}}{(\epsilon_{\mathbf{k}+\mathbf{q}} - \epsilon_{\mathbf{k}}) - i\nu_r}\right), \end{aligned} \tag{9.70}$$

where C' encloses the poles of the Green's functions. Inserting this into (9.69), we obtain $\chi(\mathbf{q}, i\nu_r) = \chi(\mathbf{q}, z)|_{z=i\nu_r}$, where

$$\chi(\mathbf{q}, z) = 2\mu_B^2 \int_{\mathbf{k}} \left(\frac{f_{\mathbf{k}} - f_{\mathbf{k}+\mathbf{q}}}{(\epsilon_{\mathbf{k}+\mathbf{q}} - \epsilon_{\mathbf{k}}) - i\nu_r}\right). \tag{9.71}$$

From this we can also read off the power spectrum of spin fluctuations:

$$\chi''(\mathbf{q},\omega) = \mathrm{Im}\,\chi(\mathbf{q},\omega+i\delta) = 2\mu_B^2 \int_{\mathbf{q}} \pi\,\delta(\epsilon_{\mathbf{q+k}} - \epsilon_{\mathbf{k}} - \omega)\left[f_{\mathbf{k}} - f_{\mathbf{k+q}}\right]. \tag{9.72}$$

When we come to consider conductivities, which involve the response function of current operators, we need to know how to deal with an operator that involves spatial or temporal derivatives. To do this, it is convenient to examine the Fourier transform of the operator $A(x)$:

$$\int d^4x\, e^{-iqx}\psi^\dagger(x)A\psi(x) = \sum_k \psi^\dagger(k-q/2)A\psi(k+q/2). \tag{9.73}$$

In current operators, A is a function of gradient terms such as $\overleftrightarrow{\nabla}$ and $\overleftrightarrow{\partial}_t$. In this case, the use of the symmetrized gradient terms ensures that, when we Fourier transform, the derivative terms are replaced by the midpoint momentum and frequency of the incoming or outgoing electron:

$$\int d^4x\, e^{-iqx}\psi^\dagger(x)A[-i\overleftrightarrow{\nabla}, i\overleftrightarrow{\partial}_t]\psi(x) = \sum_k \psi^\dagger(k-q/2)A(\mathbf{k}, i\omega_n)\psi(k+q/2). \tag{9.74}$$

For example, the current operator $\vec{J}(x) = \frac{e\hbar}{m}\left(-i\overleftrightarrow{\nabla}\right)$ becomes

$$J(q) = \sum_k e\vec{v}_{\mathbf{k}}\psi^\dagger(k-q/2)\psi(k+q/2), \tag{9.75}$$

where $\vec{v}_{\mathbf{k}} = \frac{\hbar\vec{k}}{m}$ is the electron velocity. For the thermal current operator $\vec{J}_t(\vec{x}) = \frac{\hbar^2}{m}\left(\overleftrightarrow{\nabla}\overleftrightarrow{\partial}_t\right)$,

$$\vec{J}_t(q) = \sum_k i\omega_n \frac{\hbar^2\vec{k}}{m}\psi^\dagger(k-q/2)\psi(k+q/2). \tag{9.76}$$

Example 9.2 Calculate the imaginary part of the dynamical susceptibility for non-interacting electrons and show that at low energies, $\omega << \epsilon_F$,

$$\frac{\chi''(\mathbf{q},\omega)}{\omega} = \begin{cases} \mu_B^2\frac{N(0)}{v_F q} & (q < 2k_F) \\ 0 & (q > 2k_F), \end{cases} \tag{9.77}$$

where $v_F = \hbar k_F/m$ is the Fermi velocity.

Solution

Starting with (9.72) in the low-energy limit, we can write

$$\begin{aligned} \lim_{\omega\to 0}\frac{\chi''(\mathbf{q},\omega)}{\omega} &= 2\mu_B^2\int_{\mathbf{q}}\delta(\epsilon_{\mathbf{q+k}} - \epsilon_{\mathbf{k}})\frac{f_{\mathbf{k+q}} - f_{\mathbf{k}}}{\epsilon_{\mathbf{k}} - \epsilon_{\mathbf{k+q}}} \\ &= 2\mu_B^2\int_{\mathbf{q}}\delta(\epsilon_{\mathbf{q+k}} - \epsilon_{\mathbf{k}})\left(-\frac{df}{d\epsilon_{\mathbf{k}}}\right). \end{aligned} \tag{9.78}$$

Replacing

$$\int_{\mathbf{q}} \to \int d\epsilon N(\epsilon)\int_{-1}^{1}\frac{d\cos\theta}{2}, \tag{9.79}$$

we obtain

$$\lim_{\omega\to 0}\frac{\chi''(\mathbf{q},\omega)}{\omega} = 2\mu_B^2 N(0)\int_{-1}^{1}\frac{d\cos\theta}{2}\delta\left(\frac{q^2}{2m}+\frac{qk_F}{m}\cos\theta\right)$$

$$= 2\mu_B^2 N(0)\frac{m}{2qk_F} = \mu_B^2\left(\frac{N(0)}{v_F q}\right) \qquad (q < 2k_F). \tag{9.80}$$

9.6 Spectroscopy: linking measurement and correlation

The spectroscopies of condensed matter (Table 9.2) provide an essential window on the underlying excitation spectrum, the collective modes, and ultimately the ground-state correlations of the medium. Research in condensed matter depends critically on the creative new interpretations given to measurements. It is from these interpretations that new models can be built and new insights discovered, leading ultimately to quantitative theories of matter.

Understanding the link between experiment and the microscopic world is essential for theorist and experimentalist. At the start of a career, the student is often flung into a seminar room, where it is difficult to absorb the content of the talk because the true meaning of the spectroscopy or measurements is obscure to all but the expert, so it is important to get a rough idea of how and what each measurement technique probes – to know some of the pitfalls of interpretation – and to have an idea about how one begins to calculate the corresponding quantities from simple theoretical models.

Fundamentally, each measurement is related to a given correlation function. This is seen most explicity in scattering experiments. Here, one is sending in a beam of particles and measuring the flux of outgoing particles at a given energy transfer E and momentum transfer $\mathbf{q}$. The ratio of outgoing to incoming particle flux determines the differential scattering cross-section:

$$\frac{d^2\sigma}{d\Omega d\omega} = \frac{\text{outward particle flux}}{\text{inward particle flux}}. \tag{9.81}$$

When the particles scatter, they couple to some microscopic variable $A(x)$ within the matter, such as the spin density in neutron scattering or the particle field $\psi(x)$ itself in photoemission spectroscopy. The differential scattering cross-section this gives rise to is, in essence, a measure of the autocorrelation function of $A(x)$ at the wavevector $\mathbf{q}$ and frequency $\omega = E/\hbar$ inside the material:

$$\frac{d^2\sigma}{d\Omega d\omega} \sim \int d^4x\,\langle A(\mathbf{x},t)A(0)\rangle e^{-i(\mathbf{q}\cdot\mathbf{x}-\omega t)} = S(\mathbf{q},\omega). \tag{9.82}$$

Remarkably, scattering probes matter at two points in space! How can this be? To understand this, recall that the differential scattering rate is actually an (imaginary) part of the forward scattering amplitude of the incoming particle. The amplitude for the incoming

Table 9.2 Selected spectroscopies.

Type	Name	Spectrum	A	Notes and common measurement issues
ELECTRON	STM[a]	$\frac{dI}{dV}(\mathbf{x}) \propto A(\mathbf{x},\omega)\vert_{\omega=eV}$	$\psi(x)$	Surface probe. $T\sim 0$ measurement. Does the surface characterize the bulk?
	ARPES[b]	$I(\mathbf{k},\omega) \propto f(-\omega)A(\mathbf{k},-\omega)$	$c_{\mathbf{k}\sigma}(t)$	$p_\perp$ unresolved. Surface probe; no magnetic field possible.
	IPES[c]	$I(\omega) \propto \sum_{\mathbf{k}}[1-f(\omega)]A(\mathbf{k},\omega)$	$c^\dagger_{\mathbf{k}\sigma}(t)$	**p** unresolved. Surface probe.
SPIN	Magnetic susceptibility	$\chi_{DC} = \int \frac{d\omega}{\pi\omega}\chi''(\mathbf{q}=0,\omega)$	M	$\chi \sim \frac{1}{T+\theta}$, Curielaw: local moments. $\chi \sim$ constant paramagnet.
	Inelastic neutron scattering	$S(\mathbf{q},\omega) = \frac{1}{1-e^{-\beta\omega}}\chi''(\mathbf{q},\omega)$	$S(\mathbf{q},t)$	What is the background? Quality of crystal?
	NMR[d]			
	Knight shift	$K_{contact} \propto \chi_{\text{local}}$	$S(\mathbf{x},t)$	How is the orbital part subtracted?
	Nuclear relaxation rate	$\frac{1}{T_1} = T\int_q F(\mathbf{q})\frac{\chi''(\mathbf{q},\omega)}{\omega}\Big\vert_{\omega=\omega_N}$		How does powdering affect sample?
CHARGE	Resistivity	$\rho = \frac{1}{\sigma(0)}$	$\vec{j}(\omega=0)$	How big is the resistance ratio $R(T=300\,\text{K})/R(T=0\,\text{K})$ of the sample?
	Optical conductivity	$\sigma(\omega) = \frac{1}{-i\omega}\left[\langle j(\omega')j(-\omega')\rangle\right]_0^\omega$	$\vec{j}(\omega)$	For optical reflectivity measurements: how was the Kramers–Kronig analysis done? Spectral weight transfer.

[a] Scanning tunneling spectroscopy.

[b] Angle resolved photoemission spectroscopy.

[c] Inverse photoemission spectroscopy.

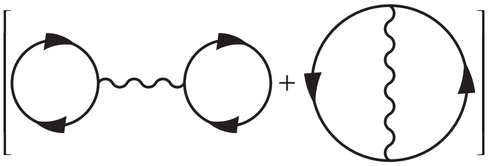
[d] Nuclear magnetic resonance.

particle to scatter in a forward direction contains the Feynman process where it omits a fluctuation of the quantity A at position x', traveling for a brief period of time as a scattered particle before reabsorbing the fluctuation at x. The amplitude for the intermediate process is nothing more than electron potential that arise in a disordered medium behave like a highly retarded potential, and the scattering created by these fluctuations is responsible for the Drude lifetime in a disordered medium. As our third introductory example, we will examine an electron moving under the retarded interaction effects produced by the exchange of phonons, examining for the first time how inelastic scattering generates an electron lifetime.

8.6.1 Hartree–Fock at a finite temperature

As a first example, consider the Hartree–Fock correction to the free energy,

$$\frac{\Delta F_{HF}}{V} = -$$



$$.\qquad (8.75)$$

These diagrams are precisely the same as those encountered in Chapter 7, but now to evaluate them we implement the finite-temperature rules, which give

$$\frac{\Delta F_{HF}}{V} = \frac{1}{2}\sum_k \mathcal{G}(k)\sum_{k'}\mathcal{G}(k')\left\{[-(2S+1)]^2\, V(k-k') - (2S+1)V(q=0)\right\}, \qquad (8.76)$$

where the prefactor is the $p = 2$ symmetry factor for these diagrams and

$$\sum_k \mathcal{G}(k) \equiv \int_{\mathbf{k}} T\sum \frac{1}{i\omega_n - \epsilon_{\mathbf{k}}} e^{i\omega_n 0^+}.$$

Using the contour integration method introduced in Section (8.3), following (8.47), we have

$$T\sum \frac{1}{i\omega_n - \epsilon_{\mathbf{k}}} e^{i\omega_n 0^+} = \int_C \frac{dz}{2\pi i}\frac{1}{z-\epsilon_{\mathbf{k}}} e^{z0^+} f(z) = f(\epsilon_{\mathbf{k}}),$$

where the contour C runs counterclockwise around the pole at $z = \epsilon_{\mathbf{k}}$, so that the first-order shift in the free energy is

$$\Delta F_{HF} = \frac{1}{2}\int_{\mathbf{k},\mathbf{k}'}\left[(2S+1)^2(V_{\mathbf{q}=0}) - (2S+1)(V_{\mathbf{k}-\mathbf{k}'})\right] f_{\mathbf{k}} f_{\mathbf{k}'}.$$

This is formally exactly the same as at zero temperature, except that now $f_{\mathbf{k}}$ refers to the finite-temperature Fermi–Dirac function. Notice that we could have applied exactly the same method to bosons, the main result being a change in sign of the second Fock term.

8.6.2 Electron in a disordered potential

As a second example of the application of finite-temperature methods, we shall consider the propagator for an electron in a disordered potential. This will introduce the concept of an *impurity average*.

Our interest in this problem is driven ultimately by a desire to understand the bulk properties of a disordered metal. The problem of electron transport is almost as old as our knowledge of the electron itself. The term "electron" was coined to describe the fundamental unit of charge (already measured from electrolysis) by the Irish physicist George Johnstone Stoney in 1891 [3]. Heinrich Lorentz derived his famous force law for charged ions in 1895 [4], but did not use the term "electron" until 1899. In 1897 J. J. Thomson [5] made the crucial discovery of the electron by correctly interpreting his measurement of the m/e ratio for cathode rays in terms of a new state of particulate matter "from which all chemical elements are built up." Within three years of this discovery, Paul Drude [6] had synthesized these ideas and had argued, based on the idea of a classical gas of charged electrons, that electrons would exhibit a mean free path $l = v_{electron}\tau$, where τ is the scattering rate and l the average distance between scattering events. In Drude's theory, electrons were envisioned as diffusing through the metal, and he was able to derive his famous formula for the conductivity σ:

$$\sigma = \frac{ne^2\tau}{m}.$$

Missing from Drude's pioneering picture was any notion of the Fermi–Dirac statistics of the electron fluid. He had, for example, no notion that the characteristic velocity of the electrons was given by the Fermi velocity, $v_{electron} \sim v_F$, a vastly greater velocity at low temperatures than could ever be expected on the grounds of a Maxwell–Boltzmann fluid of particles. This raises the question: how, in a fully quantum mechanical picture of the electron fluid, can we rederive Drude's basic model?

A real metal contains both disorder and electron–electron interactions; in this book we shall only touch on the simpler problem of disorder in an otherwise free electron gas. We shall actually return to this problem in earnest in the next chapter; our task here is to examine the electron propagator in a disordered medium of elastically scattering impurities. We shall consider an electron in a disordered potential:

$$\begin{aligned} H &= \sum_{\mathbf{k}} \epsilon_{\mathbf{k}} c^{\dagger}_{\mathbf{k}} c_{\mathbf{k}} + V_{disorder} \\ V_{disorder} &= \int d^3x U(\vec{x})\psi^{\dagger}(\mathbf{x})\psi^{\dagger}(\mathbf{x}), \end{aligned} \tag{8.77}$$

where $U(\mathbf{x})$ represents the scattering potential generated by a random array of N_i impurities located at positions $\mathbf{R}_j$, each with atomic potential $\mathcal{U}(\mathbf{x} - \mathbf{R}_j)$,

$$U(\mathbf{x}) = \sum_j \mathcal{U}(\mathbf{x} - \mathbf{R}_j).$$

An important aspect of this Hamiltonian is that it contains no interactions between electrons, and as such the energy of each individual electron is conserved: all interactions are elastic.

We shall not be interested in calculating the value of a physical quantity for a *specific* location of impurities, but rather the value of that quantity after we have averaged over the locations of the impurities, i.e.

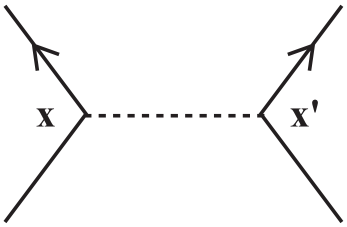
$$\overline{\langle A\rangle} = \int \prod_j \frac{1}{V}\, d^3R_j \langle \hat{A}[\{\mathbf{R}_j\}]\rangle.$$

This is an elementary example of a *quenched average*, in which the *impurity average* takes place *after* the thermodynamic average. Here we'll calculate the impurity-averaged Green's function. To do this we need to know something about the fluctuations of the impurity scattering potential about its average. It is these fluctuations that scatter the electrons.

Electrons will in general scatter off the fluctuations in the potential. The average impurity potential $\overline{U(\mathbf{x})}$ plays the roll of a kind of shifted chemical potential. Indeed, if we shift the chemical potential by an amount $\Delta\mu$, the scattering potential becomes $\tilde{U}(\mathbf{x}) = U(\mathbf{x}) - \Delta\mu$, and we can always choose $\Delta\mu = \overline{U(\mathbf{x})}$ so that $\overline{\tilde{U}(\mathbf{x})} = 0$. The residual potential describes the fluctuations in the scattering potential: $\delta U(\mathbf{x}) = U(\mathbf{x}) - \overline{U(\mathbf{x})}$. We shall now drop the tilde. The fluctuations in the impurity potential are spatially correlated, and we shall shortly show that

$$\overline{\delta U(\mathbf{x})\delta U(\mathbf{x}')} = \int_{\mathbf{q}} e^{i\mathbf{q}\cdot(\mathbf{x}-\mathbf{x}')} n_i \, |u(\mathbf{q})|^2 \,, \tag{8.78}$$

where $u(\mathbf{q}) = \int d^3x \mathcal{U}(\mathbf{x}) e^{-i\mathbf{q}\cdot\mathbf{x}}$ is the Fourier transform of the scattering potential and $n_i = N_i/V$ is the concentration of impurities. It is these fluctuations that scatter the electrons, and when we come to consider the impurity-averaged Feynman diagrams, we'll see that the spatial correlations in the potential fluctuations induce a sort of attractive interaction, denoted by the diagram



$$\int_{\mathbf{q}} n_i |u(\mathbf{q})|^2 e^{i\mathbf{q}\cdot(\mathbf{x}-\mathbf{x}')} = -V_{eff}(\mathbf{x}-\mathbf{x}'). \tag{8.79}$$

Although in principle we should keep all higher moments of the impurity scattering potential in practice the leading-order moments are enough to extract a lot of the basic physics in weakly disordered metals. Notice that the fluctuations in the scattering potential are short-range – they only extend over the range of the scattering potential. Indeed, if we neglect the momentum dependence of $u(\mathbf{q})$, assuming that the impurity scattering is dominated by low-energy s-wave scattering, then we can write $u(\mathbf{q}) = u_0$. In this situation, the fluctuations in the impurity scattering potential are entirely local:

$$\overline{\delta U(\mathbf{x})\delta U(\mathbf{x}')} = n_i u_0^2 \delta(\mathbf{x}-\mathbf{x}'). \qquad \text{white-noise potential}$$

In our discussion here, we will neglect the higher-order moments of the scattering potential, effectively assuming that it is purely Gaussian.

To prove (8.78), we first Fourier transform the potential

$$U(\mathbf{q}) = \sum_j e^{-i\mathbf{q}\cdot\mathbf{R}_j} \int d^3x\, \mathcal{U}(\mathbf{x}-\mathbf{R}_j) e^{-i\mathbf{q}\cdot(\mathbf{x}-\mathbf{R}_j)} = u(\mathbf{q}) \sum_j e^{-i\mathbf{q}\cdot\mathbf{R}_j}, \tag{8.80}$$

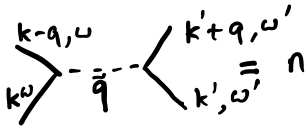
Path Integral

$$Z = \int \mathcal{D}[u]\, e^{-S} = \overline{Z}$$

"quenched disorder

$$\langle u(x,\tau)\, u(x',\tau') \rangle = u_0^2$$

$$S = \int d\tau\, d^3x \left[\bar{\psi} \left(\partial_\tau + h_0 + u(x) \right) \psi \right] + \int \frac{u^2(\vec{x})}{2 n_i u_0^2}\, d^3x\, d\tau$$



$= n_i u_0^2$

$n_i u_0^2$

We really want

$$\overline{\ln Z} = \int \mathcal{D}[u]\, e^{-\int d^4x \frac{u(x)^2}{2 u_0^2 n_i}} \ln Z[u]$$

$$\lim_{n \to 0} \frac{(Z^n - 1)}{n} = \lim_{n \to 0} \left(\frac{e^{n \ln Z} - 1}{n} \right) = \ln Z \, .$$

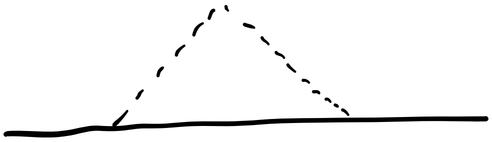
$$\overline{\ln Z} = \lim_{n \to 0} \int \mathcal{D}[u]\, e^{-S[u]} \left(\frac{Z^n - 1}{n} \right)$$

$$\psi \to \psi_\lambda \qquad \lambda = (1, \dots n)$$

Diagrams that dominate

$O(n)$

one loop only



$$n_i u_0^2 \sum_k \frac{1}{(i\omega_n - \epsilon_k)}$$

so that the locations of the impurities are encoded in the phase shifts which multiply $u(\mathbf{q})$. If we now carry out the average,

$$\begin{aligned}\overline{\delta U(\mathbf{x})\delta U(\mathbf{x}')} &= \int_{\mathbf{q},\mathbf{q}'} e^{i(\mathbf{q}\cdot\mathbf{x}-\mathbf{q}\cdot\mathbf{x}')}\left(\overline{U(\mathbf{q})U(-\mathbf{q}')} - \overline{U(\mathbf{q})}\ \overline{U(-\mathbf{q}')}\right)\\ &= \int_{\mathbf{q},\mathbf{q}'} e^{i(\mathbf{q}\cdot\mathbf{x}-\mathbf{q}\cdot\mathbf{x}')} u(\mathbf{q})u(-\mathbf{q}')\sum_{i,j}\left(\overline{e^{-i\mathbf{q}\cdot\mathbf{R}_i}e^{i\mathbf{q}'\cdot\mathbf{R}_j}} - \overline{e^{-i\mathbf{q}\cdot\mathbf{R}_i}}\ \overline{e^{i\mathbf{q}'\cdot\mathbf{R}_j}}\right). \end{aligned} \quad (8.81)$$

Now since the phase terms are independent at different sites, the variance of the random phase term in the above expression vanishes unless $i = j$, so

$$\begin{aligned}\sum_{i,j}\left(\overline{e^{-i\mathbf{q}\cdot\mathbf{R}_i}e^{i\mathbf{q}'\cdot\mathbf{R}_j}} - \overline{e^{-i\mathbf{q}\cdot\mathbf{R}_i}}\ \overline{e^{i\mathbf{q}'\cdot\mathbf{R}_j}}\right) &= N_i\int \frac{1}{V} d^3R_j e^{-i(\mathbf{q}-\mathbf{q}')\cdot\mathbf{R}_j}\\ &= n_i(2\pi)^3\delta^{(3)}(\mathbf{q}-\mathbf{q}'), \end{aligned}\quad (8.82)$$

from which

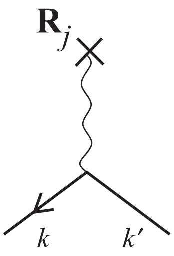
$$\overline{U(\mathbf{q})U(-\mathbf{q}')} - \overline{U(\mathbf{q})}\ \overline{U(-\mathbf{q}')} = n_i|u(\mathbf{q})|^2(2\pi)^3\delta^{(3)}(\mathbf{q}-\mathbf{q}'),$$

and (8.78) follows.

Now let us examine how electrons scatter off these fluctuations. If we substitute $\psi^\dagger(\mathbf{x}) = \int_{\mathbf{k}} c^\dagger_k e^{-i\mathbf{k}\cdot\mathbf{x}}$ into $\hat{V}_{disorder}$, we obtain

$$\hat{V} = \int_{\mathbf{k},\mathbf{k}'} c^\dagger_{\mathbf{k}} c_{\mathbf{k}'}\delta U(\mathbf{k}-\mathbf{k}').$$

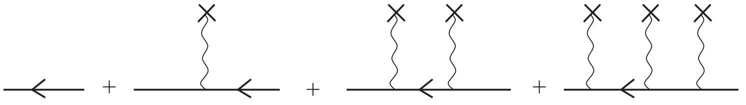
We shall represent the scattering amplitude for scattering once by



$$\delta U(\mathbf{k}-\mathbf{k}') = \left(u(\mathbf{k}-\mathbf{k}')\textstyle\sum_j e^{i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{R_j}}\right) - \Delta\mu\delta_{\mathbf{k}-\mathbf{k}'}, \quad (8.83)$$

where we have subtracted the scattering off the average potential. The potential transfers momentum, but does not impart any energy to the electron, and for this reason frequency is conserved along the electron propagator. Let us now write down in momentum space the Green's function of the electron:

$$\mathcal{G}(\mathbf{k},\mathbf{k}', i\omega_n) =$$



$$+\cdots,$$

$$\begin{aligned}&= \mathcal{G}^0(\mathbf{k}, i\omega_n)\delta_{\mathbf{k},\mathbf{k}'} + \mathcal{G}^0(\mathbf{k}, i\omega_n)\delta U(\mathbf{k}-\mathbf{k}')\mathcal{G}^0(\mathbf{k}', i\omega_n)\\ &\quad + \int_{\mathbf{k}_1}\mathcal{G}^0(\mathbf{k}, i\omega_n)\delta U(\mathbf{k}-\mathbf{k}_1)\mathcal{G}^0(\mathbf{k}_1, i\omega_n)\delta U(\mathbf{k}_1-\mathbf{k}')\mathcal{G}^0(\mathbf{k}', i\omega_n) + \cdots ,\end{aligned}\quad (8.84)$$

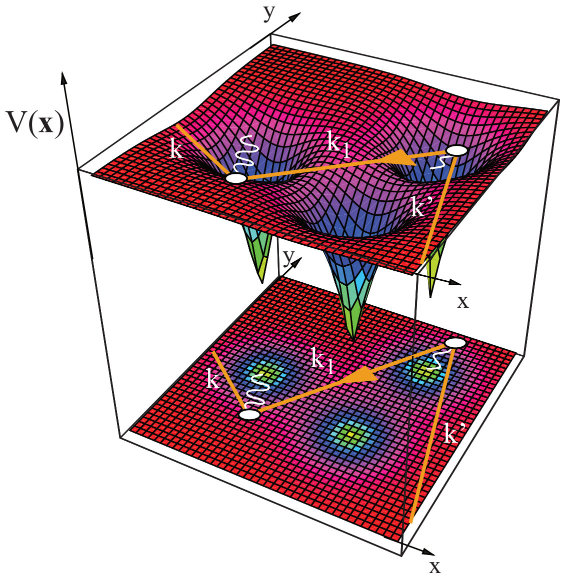


Fig. 8.5 Double scattering event in the random impurity potential.

where the frequency $i\omega_n$ is constant along the electron line. Notice that $\mathcal{G}$ is actually a function of each impurity position! Figure 8.5 illustrates one of the scattering events contributing to the third diagram in this sum. We want to calculate the quenched average $\overline{\mathcal{G}(\mathbf{k},\mathbf{k}',i\omega_n)}$, and to do this we need to average each Feynman diagram in the above series.

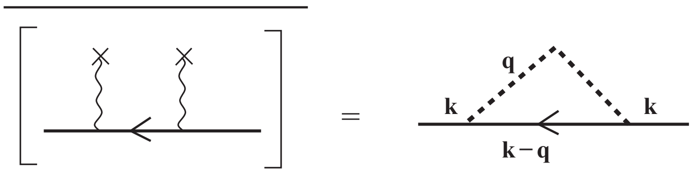
When we impurity-average the single scattering event, it vanishes:

$$\overline{\mathcal{G}^0(\mathbf{k},i\omega_n)\delta U(\mathbf{k}-\mathbf{k}')\mathcal{G}^0(\mathbf{k}',i\omega_n)} = \mathcal{G}^0(\mathbf{k},i\omega_n)\overbrace{\overline{\delta U(\mathbf{k}-\mathbf{k}')}}^{=0}\mathcal{G}^0(\mathbf{k}',i\omega_n),$$

but the average of a double scattering event is

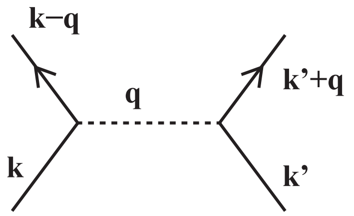
$$\begin{aligned}&\sum_{\mathbf{k}_1}\mathcal{G}^0(\mathbf{k},i\omega_n)\mathcal{G}^0(\mathbf{k}_1,i\omega_n)\mathcal{G}^0(\mathbf{k}',i\omega_n)\times\overbrace{\overline{\delta U(\mathbf{k}-\mathbf{k}_1)\delta U(\mathbf{k}_1-\mathbf{k}')}}^{n_i|u_{\mathbf{k}-\mathbf{k}'}|^2\delta_{\mathbf{k}-\mathbf{k}'}}\\&\qquad=\delta_{\mathbf{k}-\mathbf{k}'}\times\mathcal{G}^0(\mathbf{k},i\omega_n)^2 n_i\sum_{\mathbf{k}_1}u(\mathbf{k}-\mathbf{k}_1)^2\mathcal{G}^0(\mathbf{k}_1,i\omega_n)\mathcal{G}^0(\mathbf{k},i\omega_n).\end{aligned}\tag{8.85}$$

Notice something fascinating: after impurity averaging, momentum is now conserved. We can denote the impurity-averaged double scattering event Feynman diagram by



(8.86)

where we have introduced the Feynman diagram



$$n_i|u(\mathbf{q})|^2 = -V_{eff}(\mathbf{q}) \tag{8.87}$$

to denote the momentum transfer produced by the quenched fluctuations in the random potential. In writing the diagram this way, we bring out the notion that quenched disorder can be very loosely thought of as an interaction with an effective potential

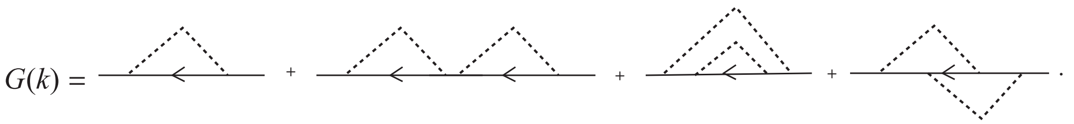
$$V_{eff}(\mathbf{q}, i\nu_n) = \int_0^\beta d\tau e^{i\nu_n\tau} \overbrace{V_{eff}(\mathbf{q},\tau)}^{-n_i|u(\mathbf{q})|^2} = -\beta\delta_{n0} n_i |u(\mathbf{q})|^2,$$

where the $\beta\delta_{n0} \equiv \int d\tau e^{i\nu_n\tau}$, derived from the fact that the interaction $V_{eff}(\mathbf{q},\tau)$ does not depend on the time difference, guarantees that there is no energy transfered by the quenched scattering events. In other words, quenched disorder induces a sort of *infinitely retarded attractive potential* between electrons.[2] The notion that disorder induces interactions is an interesting one, for it motivates the idea that disorder can lead to new kinds of collective behavior.

After the impurity averaging, we notice that momentum is now conserved, so that the impurity-averaged Green's function is now diagonal in momentum space:

$$\overline{\mathcal{G}(\mathbf{k}, \mathbf{k}', i\nu_n)} = \delta_{\mathbf{k}-\mathbf{k}'}\mathcal{G}(\mathbf{k}, i\nu_n).$$

If we now carry out the impurity averaging on multiple scattering events, only repeated scattering events at the same sites will give rise to non-vanishing contributions. If we take account of all scattering events induced by the Gaussian fluctuations in the scattering potential, then we generate a series of diagrams of the form



In the Feynman diagrams, we can group all scatterings into connected self-energy diagrams, as follows:

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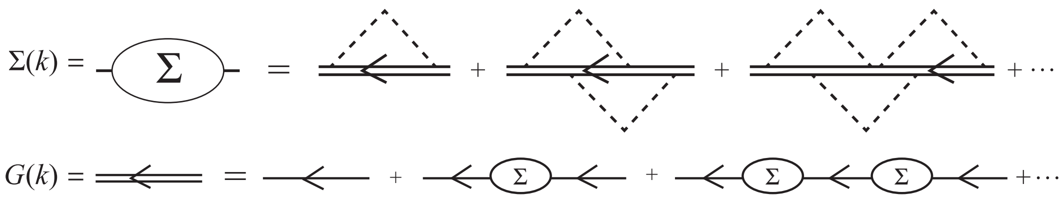
[2] Our statement can be made formally correct in the language of replicas: this interaction takes place between electrons of the same or different replica index. In the $N \to 0$ limit, the residual interaction only acts on one electron in the same replica.



$$= [i\omega_n - \epsilon_{\mathbf{k}} - \Sigma(k)]^{-1}. \tag{8.88}$$

In the case of s-wave scattering, all momentum dependence of the scattering processes is lost, so that in this case $\Sigma(k) = \Sigma(i\omega_n)$ only depends on the frequency. In the above diagram, the double line on the electron propagator indicates that all self-energy corrections have been included. From the above, you can see that the self-energy corrections calculated from the first expression are fed into the electron propagator, which in turn is used in a self-consistent way inside the self-energy.

We shall begin by trying to calculate the above first-order diagrams for the self-energy without imposing any self-consistency. This diagram is given by

$\Sigma(i\omega_n) =$

$$= n_i \sum_{\mathbf{k}'} |u(\mathbf{k}-\mathbf{k}')|^2 G(\mathbf{k}', i\omega_n)$$
$$= n_i \sum_{\mathbf{k}'} |u(\mathbf{k}-\mathbf{k}')|^2 \frac{1}{i\omega_n - \epsilon_{\mathbf{k}'}}. \tag{8.89}$$

Now we can replace the summation over momentum inside this self-energy by an integration over solid angle and energy, as follows:

$$\sum_{\mathbf{k}'} \rightarrow \int \frac{d\Omega_{\mathbf{k}'}}{4\pi} d\epsilon' N(\epsilon'),$$

where $N(\epsilon)$ is the density of states. With this replacement,

$$\Sigma(i\omega_n) = n_i u_0^2 \int d\epsilon N(\epsilon) \frac{1}{i\omega_n - \epsilon},$$

where

$$u_0^2 = \int \frac{d\Omega_{\mathbf{k}'}}{4\pi} |u(\mathbf{k}-\mathbf{k}')|^2 = \frac{1}{2}\int_{-1}^{1} d\cos\theta\, |u(\theta)|^2$$

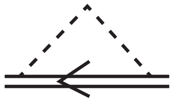
is the angular average of the squared scattering amplitude. To a good approximation, this expression can be calculated by replacing the energy-dependent density of states by its value at the Fermi energy. In so doing, we neglect a small real part of the self-energy, which can in any case be absorbed by the chemical potential. This kind of approximation is extremely common in many-body physics, in cases where the key physics is dominated by electrons close to the Fermi energy. The deviations from constancy in $N(\epsilon)$ will in practice affect the real part of $\Sigma(i\omega_n)$, and these small changes can be accomodated by a shift in the chemical potential. The resulting expression for $\Sigma(i\omega_n)$ is then

$$\Sigma(i\omega_n) = n_i u_0^2 N(0) \int_{-\infty}^{\infty} d\epsilon \frac{1}{i\omega_n - \epsilon} = -i\frac{1}{2\tau}\mathrm{sgn}(\omega_n), \tag{8.90}$$

where we have identified $\frac{1}{\tau} = 2\pi n_i u_0^2$ as the electron elastic scattering rate. We notice that this expression is entirely imaginary, and it only depends on the sign of the Matsubara frequency. Notice that in deriving this result we have extended the limits of integration to infinity, an approximation that involves neglecting terms of order $1/(\epsilon_F \tau)$.

We can now attempt to recompute $\Sigma(i\omega_n)$ with self-consistency. In this case,

$$\Sigma(i\omega_n) =$$



$$= n_i u_0^2 \sum_{\mathbf{k}'} \frac{1}{i\omega_n - \epsilon_{\mathbf{k}'} - \Sigma(i\omega_n)}. \tag{8.91}$$

If we carry out the energy integration again, we see that the imposition of self-consistency has no effect on the scattering rate:

$$\begin{aligned}\Sigma(i\omega_n) &= n_i u_0^2 N(0) \int_{-\infty}^{\infty} d\epsilon \frac{1}{i\omega_n - \epsilon - \Sigma(i\omega_n)} \\ &= -i\frac{1}{2\tau}\mathrm{sgn}(\omega_n).\end{aligned} \tag{8.92}$$

Our result for the electron propagator, ignoring the *vertex corrections* to the scattering self-energy, is given by

$$G(\mathbf{k}, z) = \frac{1}{z - \epsilon_{\mathbf{k}} + i\frac{1}{2\tau}\mathrm{sgn}\,\mathrm{Im}\,z},$$

where we have boldly extended the Green's function into the complex plane. We may now make a few remarks:

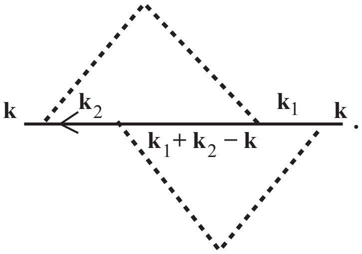
- The original pole of the Green's function has been broadened. The electron *spectral function*,

  $$A(\mathbf{k}, \omega) = \frac{1}{\pi}\mathrm{Im}\,G(\mathbf{k}, \omega - i\delta) = \frac{1}{\pi}\frac{(2\tau)^{-1}}{(\omega - \epsilon_{\mathbf{k}})^2 + (2\tau)^{-2}},$$

  is a Lorentzian of width $1/\tau$. The electron of momentum $\mathbf{k}$ now has a lifetime τ due to elastic scattering effects.
- Although the electron has a mean free path $l = v_F\tau$, its propagator displays no features of diffusion. The main effect of the finite scattering rate is to introduce a decay length into the electron propagation. The electron propagator does not bear any resemblance to the "diffusion propagator" $\chi = 1/(i\nu - Dq^2)$ – that is, the Green's function for the diffusion equation $(\partial_t - D\nabla^2)\chi = -\delta(x, t)$. The physics of diffusion and Ohm's law do not appear until we are able to examine the charge and spin response functions, and for this we have to learn how to compute the density and current fluctuations in thermal equilibrium (Chapter 9).
- The scattering rate that we have computed is often called the "classical" electron scattering rate. The neglected higher-order diagrams with vertex corrections are actually smaller than the leading-order contribution by an amount of order

  $$\frac{1}{\epsilon_F\tau} = \frac{1}{k_F l}.$$

This parameter defines the size of “quantum corrections” to the Drude scattering physics, which are the origin of the physics of electron localization. To understand how this small number arises in the self-energy, consider the first vertex correction to the impurity scattering:



(8.93)

This diagram is given by

$$\begin{aligned}\Sigma_2 &= \overbrace{N(0)\int\frac{d\epsilon_1}{i\omega_n-\epsilon_1}}^{-i\frac{1}{2\tau}}\overbrace{N(0)\int\frac{d\epsilon_2}{i\omega_n-\epsilon_2}}^{-i\frac{1}{2\tau}}\overbrace{\int\frac{d\Omega_1 d\Omega_2}{(4\pi)^2}\frac{1}{i\omega_n-\epsilon_{\mathbf{k}_1+\mathbf{k}_2-\mathbf{k}}}}^{\sim\frac{-i}{k_F v_F}}\\ &\sim i\frac{1}{\tau}\times\frac{1}{k_F l},\end{aligned} \qquad (8.94)$$

where the last term in the integral derives from the central propagator in the self-energy. In this self-energy, the momentum of the central propagator is entirely determined by the momentum of the two other internal legs, so that the energy associated with this propagator is $\epsilon_{-\mathbf{k}+\mathbf{k}_1+\mathbf{k}_2}$. This energy is only close to the Fermi energy when $\mathbf{k}_1 \sim -\mathbf{k}_2$, so that only a small fraction $1/(k_F l)$ of the possible directions of k_2 give a large contribution to the scattering processes.

8.7 Interacting electrons and phonons

The electron–phonon interaction is one of the earliest successes of many-body physics in condensed matter. In many ways, it is the condensed-matter analogue of quantum electrodynamics – and the early work on the electron–phonon problem was carried out by physicists who had their early training in the area of quantum electrodynamics.

When an electron passes through a crystal, it attracts the nearby ions, causing a local build-up of positive charge. Perhaps a better analogy is with a supersonic aircraft, for an electron moves at about Mach 100. We can confirm this with a back-of-the envelope calculation. First notice that the ratio of the sound velocity v_s to the Fermi velocity v_F is determined by the ratio of the Debye frequency to the Fermi energy:

$$\frac{v_s}{v_F}\sim\frac{\nabla_k\omega_k}{\nabla_k\epsilon_k}\sim\frac{\omega_D/a}{\epsilon_F/a}=\frac{\omega_D}{\epsilon_F},$$

where a is the size of the unit cell. Now an approximate estimate for the Debye frequency is given by $\omega_D^2 \sim k/M$, where M is the mass of an atomic nucleus and $k \sim \epsilon_F/a^2$ is the “spring constant” associated with atomic motions.

Thus,

$$\omega_D^2 \sim \left(\frac{\epsilon_F}{a^2}\right)\frac{1}{M}$$

and

$$\frac{\omega_D^2}{\epsilon_F^2} \sim \underbrace{\frac{1}{(\epsilon_F a^2)}}_{\sim 1/m}\frac{1}{M} \sim \frac{m}{M},$$

so that

$$\frac{v_s}{v_F} \sim \sqrt{\frac{m}{M}} \sim \frac{1}{100},$$

confirming the supersonic nature of electrons at the Fermi surface. As it moves through the crystal, an electron leaves behind a narrow wake of positive charge caused by the distortion in the crystal lattice in response to its momentary presence. This distortion attracts other electrons, long after the original disturbance has passed by. This is the origin of the weak attractive interaction induced by the exchange of virtual phonons. This attraction is highly retarded, quite unlike the repulsive Coulomb interaction which is almost instantaneous in time (the ratio of characteristic time scales being $\sim \frac{\epsilon_F}{\omega_D} \sim \sqrt{\frac{M}{m}} \sim 100$). Thus, whereas two electrons at the same place and time feel a strong mutual Coulomb repulsion, two electrons which arrive at the same place but at different times are generally subject to an attractive electron–phonon interaction. It is this attraction that is responsible for the development of superconductivity in many conventional metals.

In an electron fluid, we must take into account the quantum nature of the sound vibrations. An electron cannot continuously interact with the surrounding atomic lattice – it must do so by the emission and absorption of sound quanta or *phonons*. The basic Hamiltonian to describe the electron–phonon problem is the Fröhlich Hamiltonian, derived by Herbert Fröhlich, a German emigré to Britain, who worked in Liverpool shortly after the Second World War [7, 8]. He recognized that the electron–phonon interaction is closely analogous to the electron-photon interaction of quantum electrodynamics. Fröhlich appreciated that this interaction would give rise to an effective attraction between electrons and, together with Bardeen, was the first to identify the electron–phonon interaction as the driving force behind conventional superconductivity.

To introduce the Fröhlich Hamiltonian, we will imagine we have three phonon modes, labeled by the index $\lambda = (1, 2, 3)$, with frequencies $\omega_{\mathbf{q}\lambda}$. For the moment, we shall ignore the Coulomb interaction between electrons. The Fröhlich Hamiltonian is then

$$\begin{aligned} H_e &= \sum_{\mathbf{k}\sigma} \epsilon_{\mathbf{k}} c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} \\ H_p &= \sum_{\mathbf{q},\lambda} \omega_{\mathbf{q}\lambda}(a^\dagger_{\mathbf{q}\lambda} a_{\mathbf{q}\lambda} + \frac{1}{2}) \\ H_I &= \sum_{\mathbf{k},\mathbf{q},\lambda} g_{\mathbf{q}\lambda} c^\dagger_{\mathbf{k}+\mathbf{q}\sigma} c_{\mathbf{k}\sigma}\left[a_{\mathbf{q}\lambda} + a^\dagger_{-\mathbf{q}\lambda}\right]. \end{aligned} \tag{8.95}$$

To understand the electron–phonon coupling, let us consider how long-wavelength fluctuations of the lattice couple to the electron energies. Let $\vec{\Phi}(\mathbf{x})$ be the displacement of the lattice at a given point $\mathbf{x}$, so that the strain tensor in the lattice is given by

$$u_{\mu\nu}(\mathbf{x}) = \frac{1}{2}\left(\nabla_\mu \Phi_\nu(\mathbf{x}) + \nabla_\nu \Phi_\mu(\mathbf{x})\right).$$

In general, we expect a small change in the strain to modify the background potential of the lattice, modifying the energies of the electrons so that, locally,

$$\epsilon(\mathbf{k}) = \epsilon_0(\mathbf{k}) + C_{\mu\nu} u_{\mu\nu}(\mathbf{x}) + \cdots .$$

Consider the following very simple model. In a free electron gas, the Fermi energy is related to the density of the electrons N/V by

$$\epsilon_F = \frac{1}{2m}\left(\frac{3\pi^2 N}{V}\right)^{\frac{2}{3}}. \tag{8.96}$$

When a portion of the lattice expands from $V \to V + dV$, the positive charge of the background lattice is unchanged, and preservation of overall charge neutrality guarantees that the number of electrons N remains constant, so the change in the Fermi energy is given by

$$\frac{\delta\epsilon_F}{\epsilon_F} = -\frac{2}{3}\frac{dV}{V} \sim -\frac{2}{3}\vec{\nabla}\cdot\vec{\Phi}.$$

On the basis of this simple model, we expect the following coupling between the displacement vector and the electron field:

$$H_I = C\int d^3x \psi^\dagger_\sigma(\mathbf{x})\psi_\sigma(\mathbf{x})\vec{\nabla}\cdot\vec{\Phi}, \qquad C = -\frac{2}{3}\epsilon_F. \tag{8.97}$$

The quantity C is often called the *deformation potential*. Now the displacement of the the phonons was studied in Chapter 3. In a general model, it is given by

$$\Phi(\mathbf{x}) = -i\sum_{\mathbf{q}\lambda} \mathbf{e}^\lambda_{\mathbf{q}}\, \Delta x_{\mathbf{q}\lambda}\left[a_{\mathbf{q}\lambda} + a^\dagger_{-\mathbf{q}\lambda}\right] e^{i\mathbf{q}\cdot\mathbf{x}},$$

where we've introduced the shorthand

$$\Delta x_{\mathbf{q}\lambda} = \left(\frac{\hbar}{2MN_s\omega_{\mathbf{q}\lambda}}\right)^{\frac{1}{2}}$$

to denote the characteristic zero-point fluctuation associated with a given mode. (N_s is the number of sites in the lattice.) The body of this expression is essentially identical to the displacement of a one-dimensional harmonic lattice (see (2.88)), dressed up with additional polarization indices. The unfamiliar quantity $\mathbf{e}^\lambda_{\mathbf{q}}$ is the *polarization vector* of the mode. For longitudinal phonons, for instance, $\mathbf{e}^L_{\mathbf{q}} = \hat{q}$. The $-i$ in front of the expression has been introduced into the definition of the phonon creation and annihilation operators so that the requirement that the Hamiltonian be Hermitian (which implies $(\mathbf{e}^\lambda_{\mathbf{q}})^* = -(\mathbf{e}^\lambda_{-\mathbf{q}})$)

10 Electron transport theory

10.1 Introduction

Resistivity is one of the most basic properties of conductors. Surprisingly, Ohm's law,

$$V = IR, \tag{10.1}$$

requires quite a sophisticated understanding of quantum many-body physics. In a classical electron gas, the electron current density

$$\vec{j}(x) = ne\vec{v}(x) \tag{10.2}$$

is a simple c-number related to the average drift velocity $\vec{v}(x)$ of the negatively charged electron fluid. This is the basis of the Drude model of electricity, which Paul Drude introduced shortly after the discovery of the electron [1]. Fortunately, many of the key concepts evolved in the Drude model extend to the a quantum description of electrons, where $\vec{j}(x)$ is an operator. To derive the current operator, we may appeal to the continuity equation, or alternatively we can take the derivative of the Hamiltonian with respect to the vector potential:

$$\vec{j}(x) = -\frac{\delta H}{\delta \vec{A}(x)}, \tag{10.3}$$

where

$$H = \int d^3x \left[\frac{1}{2m} \psi^\dagger(x) \left(-i\hbar\vec{\nabla} - e\vec{A}(x) \right)^2 \psi(x) - e\phi(x)\psi^\dagger(x)\psi(x) \right] + V_{INT}, \tag{10.4}$$

where the Hamiltonian is written out for electrons of charge $q = e = -|e|$. Now only the kinetic energy term depends on $\vec{A}$, so that

$$\vec{j}(x) = -\frac{ie\hbar}{m} \psi^\dagger(x) \overset{\leftrightarrow}{\nabla} \psi(x) - \left(\frac{e^2}{m} \right) \vec{A}(x)\rho(x), \tag{10.5}$$

where $\overset{\leftrightarrow}{\nabla} = \frac{1}{2}\left(\overset{\rightarrow}{\nabla} - \overset{\leftarrow}{\nabla} \right)$ is the symmetrized derivative.

The discussion we shall follow dates back to pioneering work by Fritz London [2, 3]. London noticed, in connection with his research on superconductivity, that the current operator splits up into components, which he identified with the paramagnetic and diamagnetic responses of the electron fluid:

$$\vec{j}(x) = \vec{j}_P(x) + \vec{j}_D(x), \tag{10.6}$$

where

$$\vec{j}_P(x) = -\frac{ie\hbar}{m}\psi^\dagger(x)\overleftrightarrow{\nabla}\psi(x) \tag{10.7}$$

and

$$\vec{j}_D(x) = -\left(\frac{e^2}{m}\right)\vec{A}(x)\rho(x). \tag{10.8}$$

Although the complete expression for the current density is invariant under gauge transformations, $\psi(x) \to e^{i\phi(x)}\psi(x), \vec{A}(x) \to \vec{A} - \frac{\hbar}{e}\vec{\nabla}\phi(x)$, the separate parts are not. However, in a *specific* gauge such as the London or Coulomb gauge, where $\vec{\nabla} \cdot A = 0$, they do have physical meaning. We shall identify this last term as the term responsible for the diamagnetic response of a conductor, while the first term, the paramagnetic current, is responsible for the decay of the current in a metal.

In a non-interacting system, the current operator commutes with the kinetic energy operator H_0 and is formally a constant of the motion. In a periodic crystal, electron momentum is replaced by the lattice momentum **k**, which is, in the absence of lattice vibrations, a constant of the motion, with the result that the electron current still does not decay. What is the origin of electrical resistance?

There are then two basic sources of current decay inside a conductor:

- disorder, which destroys the translational invariance of the crystal
- interactions, between the electrons and phonons and between the electrons themselves, which cause the electron momenta and currents to decay.

The key response function which determines electron current is the conductivity, relating the Fourier component of current density at frequency ω to the corresponding frequency-dependent electric field:

$$\vec{j}(\omega) = \sigma(\omega)\vec{E}(\omega). \tag{10.9}$$

We would like to understand how to calculate this response function in terms of microscopic correlation functions.

The classical picture of electron conductivity was developed by Paul Drude in 1900, while working at the University of Leipzig [1]. Although his model was introduced before the advent of quantum mechanics, many of his basic concepts carry over to the quantum theory of conductivity. Drude introduced the the concept of the *electron mean free path l*, the mean distance between scattering events. The characteristic time scale between scattering events is called the *transport scattering time* τ_{tr}. (We use the “tr” subscript to distinguish this quantity from the quasiparticle scattering time τ, because not all scattering events cause the electric current to decay.) In a Fermi gas, the characteristic velocity of electrons is the Fermi velocity and the mean free path and transport scattering time are related by the simple relation

$$l = v_F\tau_{tr}. \tag{10.10}$$

The ratio of the mean free path to the electron wavelength is determined by the product of the Fermi wavevector and the mean free path. This quantity is the same order of magnitude as the ratio of the scattering time to the characteristic time scale $\hbar/\epsilon_F$ associated with the Fermi energy, so that

$$\frac{l}{\lambda_F} = \frac{k_F l}{2\pi} \sim \frac{\tau_{tr}}{\hbar/\epsilon_F} = \frac{\epsilon\tau_{tr}}{\hbar}. \tag{10.11}$$

In very pure metals, the mean free path l of Bloch wave electrons can be tens or even hundreds of microns, $l \sim 10^{-6}$ m, so this ratio can become as large as 10^4 or even 10^6. From this perspective, the rate at which current decays in a good metal is very slow on atomic time scales.

There are two important aspects to the Drude model (see Figure 10.1):

- the diffusive nature of density fluctuations
- the Lorentzian lineshape of the optical conductivity,

$$\sigma(\omega) = \frac{ne^2}{m}\frac{1}{\tau_{tr}^{-1} - i\omega}. \tag{10.12}$$

Drude recognized that, on length scales much larger than the mean free path, multiple scattering events induce diffusion in the electron motion. On large length scales, the current and density will be related by he diffusion equation,

$$\vec{j}(x) = -D\vec{\nabla}\rho(x), \tag{10.13}$$

where $D = \frac{1}{3}\frac{l^2}{\tau_{tr}} = \frac{1}{3}v_F^2\tau_{tr}$, which together with the continuity equation

$$\vec{\nabla}\cdot\vec{j} = -\frac{\partial\rho}{\partial t} \tag{10.14}$$

gives rise to the diffusion equation,

$$\left[-\frac{\partial}{\partial t} + D\nabla^2\right]\rho = 0. \tag{10.15}$$

The response function $\chi(q,\nu)$ of the density to small changes in potential must be the Green's function for this equation, so that in Fourier space

$$[i\nu - Dq^2]\chi(q,\nu) = 1, \tag{10.16}$$

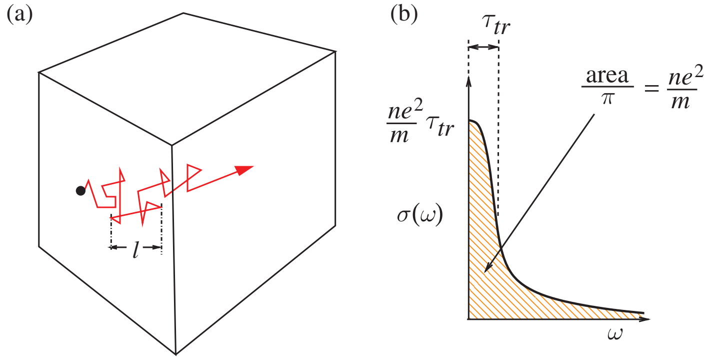


Fig. 10.1 Illustrating (a) the diffusion of electrons on length scales large compared with the mean free path l; (b) The Drude frequency-dependent conductivity. The short-time behavior of the current is determined by Newton's law, which constrains the area under the curve to equal $\int d\omega\sigma(\omega) = \pi\frac{ne^2}{m}$, a relation known as the f-sum rule.

from which we expect the response function and density–density correlation functions to contain a diffusive pole,

$$\langle \delta\rho(q,\nu)\delta\rho(-q,-\nu)\rangle \sim \frac{1}{i\nu - Dq^2}. \tag{10.17}$$

The second aspect of the Drude theory concerns the slow decay of current on the typical time scale τ_{tr}, so that, in response to an electric field pulse $E = E_0\delta(t)$, the current decays as

$$j(t) = e^{-\frac{t}{\tau_{tr}}}. \tag{10.18}$$

In the previous chapter, we discussed how, from a quantum perspective, this current is made up of two components, a diamagnetic component,

$$j_{DIA} = -\frac{ne^2}{m}A = \frac{ne^2}{m}E_0, \qquad (t > 0) \tag{10.19}$$

and a paramagnetic part associated with the relaxation of the electron wavefunction,

$$j_{PARA} = \frac{ne^2}{m}E_0(e^{-t/\tau_{tr}} - 1), \qquad (t > 0) \tag{10.20}$$

which grows to cancel this component. We would now like to see how each of these heuristic features emerges from a microscopic treatment of the conductivity and charge response functions. To do this, we need to relate the conductivity to a response function – and this brings us to the Kubo formula.

10.2 The Kubo formula

Let's now look again at the form of the current density operator. According to (10.5), it can divided into two parts:

$$\vec{j}(x) = \vec{j}_P + \vec{j}_D, \tag{10.21}$$

where

$$\begin{aligned} \vec{j}_P &= -\frac{i\hbar}{m}\psi^\dagger(x)\overset{\leftrightarrow}{\nabla}\psi(x) && \text{paramagnetic current} \\ \vec{j}_D &= -\frac{e^2}{m}\int d^3x\, \rho(x)\vec{A}(x) && \text{diamagnetic current} \end{aligned} \tag{10.22}$$

are the *paramagnetic* and *diamagnetic* parts of the current. The total current operator is invariant under gauge transformations, $\psi(x) \rightarrow e^{i\phi(x)}\psi(x)$, $\vec{A}(x) \rightarrow \vec{A} + \frac{\hbar}{e}\vec{\nabla}\phi(x)$, and, strictly speaking, the two terms in this expression for the current can't be separated in a gauge-invariant fashion. However, we can separate these two terms if we work in a specific gauge. We shall choose to work in the London gauge:

$$\vec{\nabla}\cdot\vec{A} = 0. \qquad \text{London gauge} \tag{10.23}$$

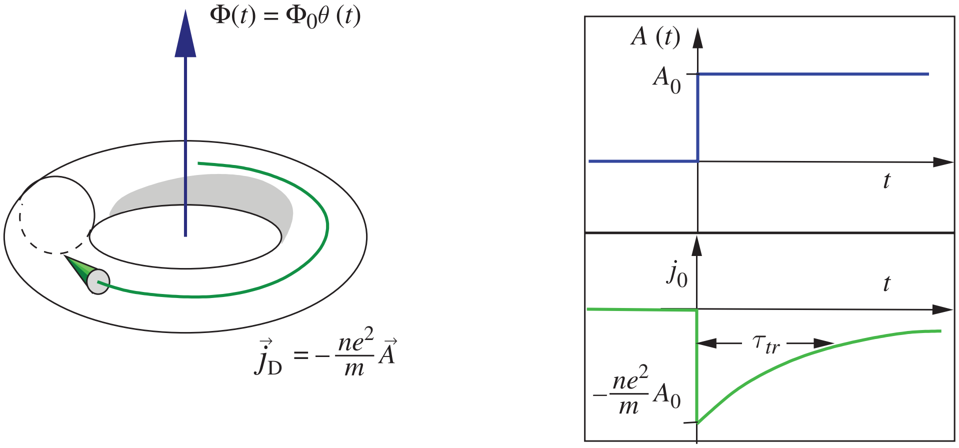


Fig. 10.2 Schematic illustration of a diamagnetic current pulse produced by a sudden change of flux through the conducting loop.

In this gauge, the vector potential is completely transverse, $\vec{q}\cdot\vec{A}(\vec{q}) = 0$. The equations of the electromagnetic field in the London gauge are

$$\left(\frac{1}{c^2}\partial_t^2 - \nabla^2\right)\vec{A}(x) = \mu_0\,\vec{j}(x)$$
$$-\nabla^2\phi(x) = \frac{\rho(x)}{\epsilon_0}, \tag{10.24}$$

so that the potential field $\rho(x)$ is entirely determined by the distribution of charges inside the material, and the only independent external dynamical field coupling to the material is the vector potential. We shall then regard the vector potential as the only external field coupling to the material.

We shall now follow London's argument for the interpretation of these two terms. Let us carry out a thought experiment in which we imagine a toroidal piece of metal, as in Figure 10.2, in which a magnetic flux passing up through the conducting ring is turned on at $t = 0$, creating a vector potential around the ring given by $A = A_0\theta(t) = \frac{\phi_0}{2\pi r}\theta(t)$, where r is the radius of the ring. The electric field is related to the external vector potential via the relation

$$\vec{E} = -\frac{\partial\vec{A}}{\partial t} = -A_0\delta(t), \tag{10.25}$$

so $\vec{E} = -\vec{A}_o\delta(t)$ is a sudden inductively induced electrical pulse.

Suppose the system is described in the Schrödinger representation by the wavefunction $|\psi(t)\rangle$. Then the current flowing after time t is given by

$$\langle\vec{j}(t)\rangle = \langle\psi(t)|\,\vec{j}_P|\psi(t)\rangle - \frac{ne^2}{m}A_o\theta(t), \tag{10.26}$$

where we have assumed that $\langle\rho(x)\rangle = n$ is the equilibrium density of electrons in the material. We see that the second, diamagnetic term switches on immediately after the pulse. This is nothing more than the diamagnetic response – the effect of the field induced by Faraday's effect. What is so interesting is that this component of the current remains *indefinitely* after the initial step in the flux through the toroid. But the current must decay! How?

The answer is that the initial paramagnetic contribution to the current starts to develop after the flux is turned on. Once the vector potential is present, the wavefunction $|\psi(t)\rangle$ starts to evolve, producing a paramagnetic current that rises and, in a regular conductor, ultimately *exactly cancels* the time-independent diamagnetic current. From this point of view, the only difference between an insulator and a metal is the time scale required for the paramagnetic current to cancel the diamagnetic component. In an insulator this time scale is of the order of the inverse (direct) gap Δ_g, $\tau \sim \hbar/\Delta_g$, whereas in a metal it is the transport relaxation time, $\tau \sim \tau_{tr}$.

These arguments were first advanced by London. He noticed that if for some unknown reason the wavefunction of the material could become "rigid," so that it would not respond to the applied vector potential, in this special case the paramagnetic current would never build up, and one would then have a perfect diamagnet – a *superconductor*. Let's now look at this in more detail. We need to compute

$$\vec{j}(\vec{x},t) = \langle \vec{j}_P(x,t)\rangle - \frac{ne^2}{m}\vec{A}(x,t). \tag{10.27}$$

If we are to compute the response of the current to the applied field, we need to compute the build-up of the paramagnetic part of the current. Here we can use linear response theory. The coupling of the vector potential to the paramagnetic current is simply–$\int d^3x\vec{j}(x)\cdot\vec{A}(x)$, so the response of this current is given by

$$\langle j_P^\alpha(t)\rangle = \int_{t'<t} d^3x'dt'\, i\langle[\, j_P^\alpha(x), j_P^\beta(x')]\rangle A^\beta(x'). \tag{10.28}$$

In other words, we may write

$$\begin{aligned} \vec{j}(1) &= -\int d2\underline{Q}(1-2)\vec{A}(2) \\ Q^{\alpha\beta}(1-2) &= \frac{ne^2}{m}\delta^{\alpha\beta}\delta(1-2) - i\langle[\, j_P^\alpha(1), j_P^\beta(2)]\rangle\theta(t_1-t_2). \end{aligned} \tag{10.29}$$

The quantity $\underline{Q}(1-2)$ is the *London response kernel*. In the most general case, this response is non-local in both space and time. In a metal, this response is non-local over a distance given by the electron mean free path $l = v_F\tau_{tr}$. In a superconductor the response to the vector potential is non-local over the *Pippard coherence length* $\xi = v_F/\Delta$, where Δ is the superconducting gap. We can write the above result in Fourier space as

$$\vec{j}(q) = -\underline{Q}(q)\vec{A}(q), \tag{10.30}$$

where

$$Q^{\alpha\beta}(q) = \frac{ne^2}{m}\delta^{\alpha\beta} - i\langle[j^\alpha(q), j^\beta(-q)]\rangle. \tag{10.31}$$

We have used the cavalier notation

$$\langle[j^\alpha(q), j^\beta(-q)]\rangle = \int d^3x \int_0^\infty dt\langle[j^\alpha(x,t), j^\beta(0)]\rangle e^{-i(\vec{q}\cdot\vec{x}-\nu t)}. \tag{10.32}$$

Finally, if we write $\vec{E} = -\frac{\partial A}{\partial t}$, or $A(q) = \frac{1}{i\nu}E(q)$, we deduce that

$$\vec{j}(q) = \underline{\sigma}(q)\vec{E}(q)$$

$$\sigma^{\alpha\beta}(q) = -\frac{1}{i\nu}Q^{\alpha\beta}(q) = \frac{1}{-i\nu}\left\{\frac{ne^2}{m}\delta^{\alpha\beta} - i\langle[j^\alpha(q), j^\beta(-q)]\rangle\right\}. \tag{10.33}$$

Kubo formula

This is the famous *Kubo formula* [4] that allows us to relate current fluctuations to the conductivity. In practice, the high velocity of light means that $q = \nu/c << k_F$ is much shorter than an electronic wavevector, so that in electronic condensed matter physics we may consider the limit $\vec{q} = 0$, writing $\sigma(\nu) = \sigma(\vec{q} = 0, \nu)$. This is the quantity that is measured in optical conductivity measurements. The DC conductivity is given by the zero-frequency limit of the uniform conductivity, i.e. $\sigma_{DC} = \lim_{\nu\to 0}\sigma(\nu)$.

In a metal, σ_{DC} is finite, which implies that $Q(\nu = 0) = 0$, so that

$$i\langle[j^\alpha(q), j^\beta(-q)]\rangle|_{q=0} = \frac{ne^2}{m}\delta^{\alpha\beta}. \tag{10.34}$$

We shall see that this identity breaks down in a system with broken gauge invariance – and this is the origin of superconductivity. In a normal fluid, however, we can use this identity to rewrite the expression for the conductivity as

$$\sigma^{\alpha\beta}(\nu) = \frac{1}{-i\nu}\left[- i\langle[j^\alpha(\nu'), j^\beta(-\nu')]\rangle\right]_{\nu'=0}^{\nu'=\nu}. \tag{10.35}$$

A practical calculation of conductivity depends on our ability to extract this quantity from the imaginary-time response function. We can quickly generalize expression (10.29) to imaginary time by replacing $i\langle[A(1), B(2)]\rangle \to \langle TA(1)B(2)\rangle$, so that, in imaginary time,

$$\begin{aligned}\vec{j}(1) &= -\int d2\,\underline{Q}(1-2)\vec{A}(2) \qquad (1 \equiv (\vec{x}_1, \tau_1))\\ Q^{\alpha\beta}(1-2) &= \frac{ne^2}{m}\delta^{\alpha\beta}\delta(1-2) - \langle Tj_P^\alpha(1)\, j_P^\beta(2)\rangle,\end{aligned} \tag{10.36}$$

so that in Fourier space our expression for the optical conductivity is given by

$$\sigma^{\alpha\beta}(i\nu_n) = -\frac{1}{\nu_n}\left[\ \langle j^\alpha(\nu')j^\beta(-\nu')\rangle\right]_{\nu'=0}^{\nu'=i\nu_n}, \tag{10.37}$$

where we have used the shorthand notation

$$\langle j^\alpha(i\nu_n)j^\beta(-i\nu_n)\rangle = \int_0^\beta d\tau\, e^{i\nu_n\tau}\langle Tj^\alpha(\tau)j^\beta(0)\rangle. \tag{10.38}$$

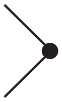
10.3 Drude conductivity: diagrammatic derivation

In the previous section we showed how the fluctuations of the electric current can be related to the optical conductivity. Let us now see how these fluctuations can be computed using

Feynman diagrams, in a disordered electron gas with dispersion $\epsilon_{\mathbf{k}} = \frac{k^2}{2m}$. First, let us review the Feynman rules. We shall assume that we have taken the leading-order effects of disorder into account in the electron propagator, denoted by

$$\longrightarrow = G(k) = \frac{1}{i\omega_n - \epsilon_{\mathbf{k}} + i\ \mathrm{sgn}\ \omega_n \frac{1}{2\tau}} \cdot \tag{10.39}$$

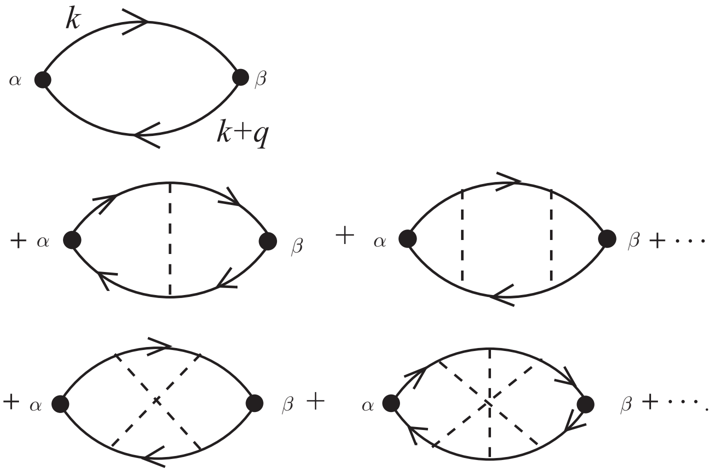
The current operator is $j^{\alpha}(q) = \sum e\frac{k^{\alpha}}{m}\psi^{\dagger}_{k-q/2\sigma}\psi_{k+q/2\sigma}$, which we denote by the vertex



$$\alpha \equiv e\frac{k^{\alpha}}{m} \cdot \tag{10.40}$$

The set of diagrams that represents the current fluctuations can then be written

$$\langle \mathbf{j}^{\alpha}(q)\mathbf{j}^{\beta}(-q)\rangle =$$



(10.41)

In the above expansion, we have identified three classes of diagrams. The first diagram denotes the simplest contribution to the current fluctuation: we shall see shortly that this is already sufficient to capture the Drude conductivity. The second set of diagrams represents the leading impurity corrections to the current vertex: these terms take account of the fact that low-angle scattering does not affect the electric current, and it is these terms that are responsible for the replacement of the electron scattering rate τ by the transport relaxation rate τ_{tr}. We shall see that these terms vanish for isotropically scattering impurities, justifying our neglect of these contributions in our warm-up calculation of the conductivity.

The last set of diagrams involves crossed impurity scattering lines. We have already encountered these types of diagrams in passing, and the momentum restrictions associated with crossed diagrams lead to a reduction factor of order $O(\frac{1}{k_F l}) \sim \frac{\lambda}{l}$, or the ratio of the electron wavelength to the mean free path. These are the *quantum corrections* to the conductivity. These maximally crossed diagrams were first investigated by Langer and Neal in 1966 [5], during the early years of research into electron transport, but it was not until the late 1970s that they became associated with the physics of electron localization. More on this later.