Expanding the eigenvalue equation (14.115),

$$\begin{aligned}(E_{\mathbf{k}} - \epsilon_{\mathbf{k}})u_{\mathbf{k}} &= \Delta \mathrm{v}_{\mathbf{k}} \\ \Delta u_{\mathbf{k}} &= (E_{\mathbf{k}} + \epsilon_{\mathbf{k}})\mathrm{v}_{\mathbf{k}}.\end{aligned} \tag{14.116}$$

Multiplying these two equations, we obtain $(E_{\mathbf{k}}-\epsilon_{\mathbf{k}})u_{\mathbf{k}}^2 = (E_{\mathbf{k}}+\epsilon_{\mathbf{k}})\mathrm{v}_{\mathbf{k}}^2$, or $\epsilon_{\mathbf{k}}(u_{\mathbf{k}}^2+\mathrm{v}_{\mathbf{k}}^2) = \epsilon_{\mathbf{k}} = E_{\mathbf{k}}(u_{\mathbf{k}}^2 - \mathrm{v}_{\mathbf{k}}^2)$, since $u_{\mathbf{k}}^2 + \mathrm{v}_{\mathbf{k}}^2 = 1$. It follows that $u_{\mathbf{k}}^2 - \mathrm{v}_{\mathbf{k}}^2 = \epsilon_{\mathbf{k}}/E_{\mathbf{k}}$. Combining this with $u_{\mathbf{k}}^2 + \mathrm{v}_{\mathbf{k}}^2 = 1$, we obtain the results given in (14.112).

14.6 Path integral formulation

Following our discussion of the physics, let us return to the math to examine how the BCS mean-field theory is succinctly formulated using path integrals. The appearance of single pairing fields A and $A^\dagger$ in the BCS Hamiltonian makes it particularly easy to apply path-integral methods. We begin by writing the problem as a path integral:

$$Z = \int \mathcal{D}[\bar{c}, c]e^{-S}, \tag{14.117}$$

where

$$S = \int_0^\beta \sum_{\mathbf{k}\sigma} \bar{c}_{\mathbf{k}\sigma}(\partial_\tau + \epsilon_{\mathbf{k}})c_{\mathbf{k}\sigma} - \frac{g_0}{V}\bar{A}A. \tag{14.118}$$

Here the condition $|\epsilon_{\mathbf{k}}| < \omega_D$ is implicit in all momentum sums. Next, we carry out the Hubbard–Stratonovich transformation (see Chapter 13):

$$-g\bar{A}A \rightarrow \bar{\Delta}A + A\bar{\Delta} + \frac{V}{g_0}\bar{\Delta}\Delta, \tag{14.119}$$

where $\bar{\Delta}(\tau)$ and $\Delta(\tau)$ are fluctuating complex fields. Inside the path integral this substitution is formally exact, but its real value lies in the static mean-field solution it furnishes for superconductivity. We then obtain

$$\begin{aligned}Z &= \int \mathcal{D}[\bar{\Delta}, \Delta, \bar{c}, c]e^{-S} \\ S &= \int_0^\beta d\tau \left\{ \sum_{\mathbf{k}\sigma} \bar{c}_{\mathbf{k}\sigma}(\partial_\tau + \epsilon_{\mathbf{k}})c_{\mathbf{k}\sigma} + \bar{\Delta}A + A\bar{\Delta} + \frac{V}{g_0}\bar{\Delta}\Delta \right\}.\end{aligned} \tag{14.120}$$

The Hamiltonian part of this expression can be compactly reformulated in terms of Nambu spinors, following precisely the same steps used for the operator Hamiltonian. To transform the Berry phase term (see (12.132)), we note that, since the Nambu spinors satisfy a conventional anticommutation algebra, they must have precisely the same Berry phase term as conventional fermions, i.e. $\int d\tau\, \bar{c}_{\mathbf{k}\sigma}\partial_\tau c_{\mathbf{k}\sigma} = \int d\tau \bar{\psi}_{\mathbf{k}}\partial_\tau \psi_{\mathbf{k}}$.[5]

Putting this all together, the partition function and the action can now be rewritten:

$$Z = \int \mathcal{D}[\bar{\Delta}, \Delta, \bar{\psi}, \psi]e^{-S}$$
$$S = \int_0^\beta d\tau \left\{ \sum_{\mathbf{k}} \bar{\psi}_{\mathbf{k}}(\partial_\tau + \underline{h}_{\mathbf{k}})\psi_{\mathbf{k}} + \frac{V}{g_0}\bar{\Delta}\Delta \right\}, \tag{14.122}$$

where $\underline{h}_{\mathbf{k}} = \epsilon_{\mathbf{k}}\tau_3 + \Delta_1\tau_1 + \Delta_2\tau_2$, with $\Delta = \Delta_1 - i\Delta_2$, $\bar{\Delta} = \Delta_1 + i\Delta_2$. Since the action is explicitly quadratic in the Fermi fields, we can carry out the Gaussian integral of the Fermi fields to obtain

$$Z = \int \mathcal{D}[\bar{\Delta}, \Delta]e^{-S_E[\bar{\Delta},\Delta]}$$
$$e^{-S_E[\bar{\Delta},\Delta]} = \prod_{\mathbf{k}} \det[\partial_\tau + \underline{h}_{\mathbf{k}}(\tau)]e^{-V\int_0^\beta d\tau \frac{\bar{\Delta}\Delta}{g_0}} \tag{14.123}$$

for the effective action, where we have separated the fermionic determinant into a product over each decoupled momentum. Thus

$$S_E[\bar{\Delta}, \Delta] = V\int_0^\beta d\tau \frac{\bar{\Delta}\Delta}{g_0} + \sum_{\mathbf{k}} \mathrm{Tr}\ln(\partial_\tau + \underline{h}_{\mathbf{k}}), \tag{14.124}$$

where we have replaced ln det → Tr ln. This is the action of electrons moving in a *time-dependent* pairing field $\Delta(\tau)$.

14.6.1 Mean-field theory as a saddle point of the path integral

Although we can only explicitly calculate S_E in static configurations of the pair field, in BCS theory it is *precisely* these configurations that saturate the path integral in the thermodynamic limit ($V \to \infty$). To see this, consider the path integral

$$Z = \int \mathcal{D}[\bar{\Delta}, \Delta]e^{-S_E[\bar{\Delta},\Delta]}. \tag{14.125}$$

Every term in the effective action is extensive in the volume V, so if we find a static configuration of $\Delta = \Delta_0$ which minimizes $S_E = VS_0$, so that $\delta S_E/\delta\Delta = 0$, fluctuations $\delta\Delta$

5 We can confirm this result by anticommuting the down-spin Grassmans in the Berry phase, then integrating by parts:

$$S_B = \sum_{\mathbf{k}} \int_0^\beta d\tau \left[\bar{c}_{\mathbf{k}\uparrow}\partial_\tau c_{\mathbf{k}\uparrow} - (\partial_\tau c_{-\mathbf{k}\downarrow})\bar{c}_{-\mathbf{k}\downarrow}\right] = \sum_{\mathbf{k}} \int_0^\beta d\tau \Big[\bar{c}_{\mathbf{k}\uparrow}\partial_\tau c_{\mathbf{k}\uparrow} + c_{-\mathbf{k}\downarrow}\partial_\tau \bar{c}_{-\mathbf{k}\downarrow} - \overbrace{\partial_\tau(c_{-\mathbf{k}\downarrow}\bar{c}_{-\mathbf{k}\downarrow})}^{\to 0}\Big]$$
$$= \sum_{\mathbf{k}} \int_0^\beta d\tau \left[\bar{\psi}_{\mathbf{k}}\partial_\tau \psi_{\mathbf{k}}\right]. \tag{14.121}$$

The antiperiodicity of the Grassman fields in imaginary time causes the total derivative to vanish.

around this configuration will cost a free energy that is of order $O(V)$, i.e. the amplitude for a small fluctuation is given by

$$e^{-S} = e^{-VS_0 + O(V\times|\delta\Delta|^2)}. \tag{14.126}$$

The appearance of V in the coefficient of this Gaussian distribution implies the variance of small fluctuations around the minimum will be of order $\langle \delta\Delta^2\rangle \sim O(1/V)$ so that, to a good approximation,

$$Z \approx Z_{BCS} = e^{-S_E[\bar{\Delta}_0, \Delta_0]}. \tag{14.127}$$

This is why the mean-field approximation to the path integral is essentially exact for the BCS model. Note that we can also expand the effective action as a Gaussian path integral:

$$\begin{aligned} Z_{BCS} &= \int \mathcal{D}[\bar{\psi}, \psi] e^{-S_{MFT}} \\ S_{MFT} &= \int_0^\beta d\tau \left\{ \sum_{\mathbf{k}} \bar{\psi}_{\mathbf{k}} (\partial_\tau + \overbrace{\epsilon_{\mathbf{k}}\tau_3 + \Delta_1\tau_1 + \Delta_2\tau_2}^{h_{\mathbf{k}}}) \psi_{\mathbf{k}} + \frac{V}{g_0}\bar{\Delta}\Delta \right\}, \end{aligned} \tag{14.128}$$

in which the saddle-point solution $\Delta^{(0)}(\tau) \equiv \Delta = \Delta_1 - i\Delta_2$ is assumed to be static. Since this is a Gaussian integral, we can immediately carry out the the integral to obtain

$$Z_{BCS} = \prod_{\mathbf{k}} \det(\partial_\tau + h_{\mathbf{k}}) \exp\left[-\frac{V\beta}{g_0}\bar{\Delta}\Delta\right].$$

It is far easier to work in Fourier space, writing the Nambu fields in terms of their Fourier components:

$$\psi_{\mathbf{k}}(\tau) = \frac{1}{\sqrt{\beta}} \sum_n \psi_{\mathbf{k}n} e^{-i\omega_n\tau}. \tag{14.129}$$

In this basis,

$$\partial_\tau + h \rightarrow [-i\omega_n + \underline{h}_{\mathbf{k}}], \tag{14.130}$$

and the path integral is now diagonal in momentum and frequency:

$$\begin{aligned} Z_{BCS} &= \int \prod_{\mathbf{k}n} d\bar{\psi}_{\mathbf{k}n} d\psi_{\mathbf{k}n} e^{-S_{MFT}[\bar{\psi}_{\mathbf{k}n}, \psi_{\mathbf{k}n}]} \\ S_{MFT}[\bar{\psi}_{\mathbf{k}n}, \psi_{\mathbf{k}n}] &= \sum_{\mathbf{k}\, n} \bar{\psi}_{\mathbf{k}n}(-i\omega_n + h_{\mathbf{k}})\psi_{\mathbf{k}n} + \beta V \frac{\bar{\Delta}\Delta}{g_0}. \end{aligned} \tag{14.131}$$

Remarks

- The distribution function $P[\psi_{\mathbf{k}}]$ for the fermion fields is Gaussian:

$$P[\psi_{\mathbf{k}n}] \sim e^{-S_{MFT}} \propto \exp[-\bar{\psi}_{\mathbf{k}n}(-i\omega_n + h_{\mathbf{k}})\psi_{\mathbf{k}n}], \tag{14.132}$$

so that the amplitude of fluctuations (see 12.144) is given by

$$\langle \psi_{\mathbf{k}n} \bar{\psi}_{\mathbf{k}n} \rangle = -\mathcal{G}(\mathbf{k}, i\omega_n) = [-i\omega_n + h_{\mathbf{k}}]^{-1}, \tag{14.133}$$

which is the electron Green's function in the superconductor. We shall study this in the next section.

- We can now evaluate the determinant

$$\det[\partial_\tau + \underline{h}_{\mathbf{k}}] = \prod_n \det[-i\omega_n + \underline{h}_{\mathbf{k}}] = \prod_n [\omega_n^2 + \epsilon_{\mathbf{k}}^2 + |\Delta|^2]. \tag{14.134}$$

With these results, we can fully evaluate the partition function

$$Z_{BCS} = \prod_n [\omega_n^2 + \epsilon_{\mathbf{k}}^2 + |\Delta|^2] \times e^{-\frac{\beta V |\Delta|^2}{g_0}} = e^{-S_E}, \tag{14.135}$$

and the effective action is then

$$\mathcal{F}[\Delta, T] = \frac{S_E}{\beta} = -T \sum_{\mathbf{kn}} \ln[\omega_n^2 + \epsilon_{\mathbf{k}}^2 + |\Delta|^2] + V \frac{|\Delta|^2}{g_0}. \tag{14.136}$$

free energy: BCS pair condensate

This is the mean-field free-energy for the BCS model.

Remarks

- This quantity provides a microscopic realization of the Landau free energy of a superconductor, discussed in Chapter 11. Notice how $\mathcal{F}$ is invariant under changes in the phase of the gap function so that $\mathcal{F}[\Delta, T] = \mathcal{F}[\Delta e^{i\phi}, T]$, which follows from particle conservation. (The number operator, which commutes with H, is the generator of phase translations.)
- Following our discussion in Chapter 11, we expect that below T_c the free energy $\mathcal{F}[\Delta, T]$ develops a minimum at finite $|\Delta|$, forming a "Mexican hat" potential (Figure 14.11).
- Notice the appearance of the quasiparticle energy $E_{\mathbf{k}} = \sqrt{\epsilon_{\mathbf{k}}^2 + |\Delta|^2}$ inside the logarithm.

To identify the equilibrium gap Δ, we minimize $\mathcal{F}$ with respect to $\bar{\Delta}$, which leads to the BCS gap equation,

$$\frac{\partial \mathcal{F}}{\partial \bar{\Delta}} = -\sum_{\mathbf{k}n} \frac{\Delta}{\omega_n^2 + E_{\mathbf{k}}^2} + V \frac{\Delta}{g_0} = 0 \tag{14.137}$$

or

$$\frac{1}{g_0} = \frac{1}{\beta V} \sum_{\mathbf{k}n} \frac{1}{\omega_n^2 + E_{\mathbf{k}}^2}.$$

BCS gap equation

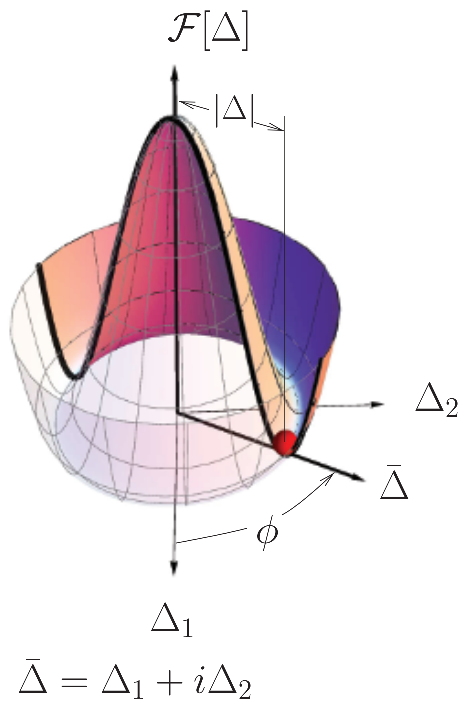


Fig. 14.11 Showing the form of $\mathcal{F}[\Delta]$ for $T < T_c$. The free energy is a minimum at a finite value of $|\Psi|$. The free energy is invariant under changes in phase of the gap, which are generated by the number operator $\hat{N} \propto -i\frac{d}{d\phi}$. See Exercise 14.4.

If we now convert the Matsubara sum to a contour integral, we obtain

$$\frac{1}{\beta}\sum_n \frac{1}{\omega_n^2 + E_{\mathbf{k}}^2} = -\oint \frac{dz}{2\pi i} f(z) \frac{1}{z^2 - E_{\mathbf{k}}^2} = -\oint \frac{dz}{2\pi i} f(z) \frac{1}{2E_{\mathbf{k}}}\left[\frac{1}{z - E_{\mathbf{k}}} - \frac{1}{z + E_{\mathbf{k}}}\right]$$
$$= -\sum_{\mathbf{k}} \overbrace{(f(E_{\mathbf{k}}) - f(-E_{\mathbf{k}}))}^{=2f(E_{\mathbf{k}})-1} \frac{1}{2E_{\mathbf{k}}} = \frac{\tanh(\beta E_{\mathbf{k}}/2)}{2E_{\mathbf{k}}}, \tag{14.138}$$

where the integral runs counterclockwise around the poles at $z = \pm E_{\mathbf{k}}$. Thus the gap equation can be rewritten as

$$\frac{1}{g_0} = \int_{|\epsilon_{\mathbf{k}}|<\omega_D} \frac{d^3k}{(2\pi)^3}\left[\frac{\tanh(\beta E_{\mathbf{k}}/2)}{2E_{\mathbf{k}}}\right], \qquad \text{BCS gap equation II} \tag{14.139}$$

where we have reinstated the implicit energy shell restriction $|\epsilon_{\mathbf{k}}| < \omega_D$. If we approximate the density of states by a constant $N(0)$ per spin over the narrow shell of states around the Fermi surface, we may replace the momentum sum by an energy integral, so that

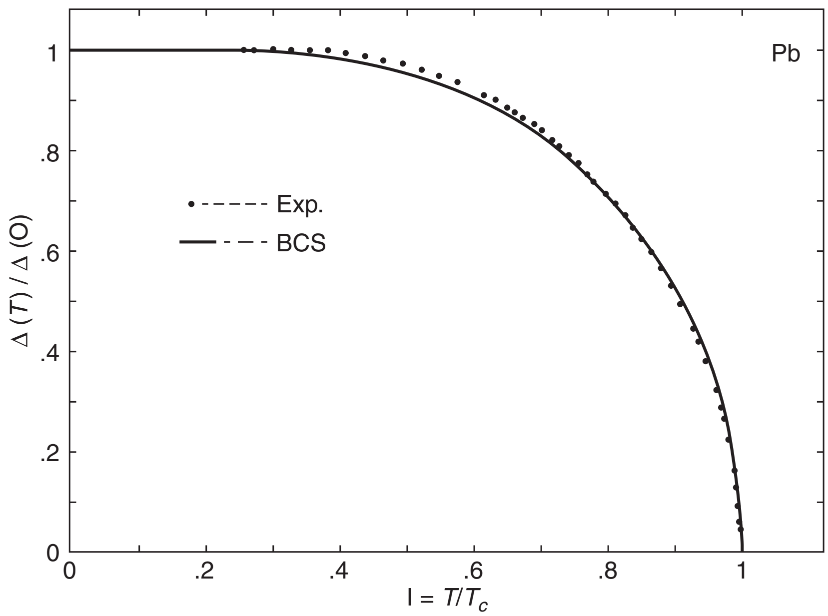


Fig. 14.12 Comparison between the dependence of the gap on the reduced temperature T/T_C and the gap measured by tunneling in superconducting lead. Reprinted with permission from R. F. Gasparovic, *et al.*, *Solid State Commun.*, vol. 4, p. 59, 1966. Copyright 1966 Elsevier.

$$\frac{1}{g_0 N(0)} = \int_0^{\omega_D} d\epsilon \left[\frac{\tanh(\beta\sqrt{\epsilon^2+\Delta^2}/2)}{\sqrt{\epsilon^2+\Delta^2}}\right]. \tag{14.140}$$

At absolute zero, the hyperbolic tangent becomes unity. If we subtract this equation from its zero-temperature value, it becomes

$$\int_0^{\infty} d\epsilon \left[\frac{\tanh(\beta\sqrt{\epsilon^2+\Delta^2}/2)}{\sqrt{\epsilon^2+\Delta^2}} - \frac{1}{\sqrt{\epsilon^2+\Delta_0^2}}\right] = 0, \tag{14.141}$$

where $\Delta_0 = \Delta(T=0)$ is the zero-temperature gap. Since the argument of the integrand now rapidly converges to zero at high energies, we can set the upper limit of integration to zero. This is a useful form for the numerical evaluation of the temperature dependence of the gap. Figure 14.12 contrasts the BCS prediction of the temperature-dependent gap obtained from (14.141), with the gap measured from tunneling in lead.

Example 14.4 Carry out the Matsubara sum in (14.136) to derive a an explicit form for the free energy of the superconducting condensate in terms of the quasiparticle excitation energies:

$$\mathcal{F} = -2TV \int_{|\epsilon_{\mathbf{k}}|<\omega_D} \frac{d^3k}{(2\pi)^3}\Big[\ln[2\cosh(\beta E_{\mathbf{k}}/2)]\Big] + V\frac{|\Delta|^2}{g_0}. \tag{14.142}$$

Solution

Using the contour integration method, we can rewrite (14.136) as

$$\mathcal{F} = -\sum_{\mathbf{k}} \oint \frac{dz}{2\pi i} f(z) \ln[z^2 - E_{\mathbf{k}}^2] + V \frac{|\Delta|^2}{g_0}, \tag{14.143}$$

where the integral runs counterclockwise around the poles of the Fermi function. The logarithm inside the integral can be split up into two terms,

$$\ln[z^2 - E_{\mathbf{k}}^2] \to \ln[E_{\mathbf{k}} - z] + \ln[-E_{\mathbf{k}} - z], \tag{14.144}$$

which we immediately recognize as the contributions from fermions with energies $\pm E_{\mathbf{k}}$, so that the result of carrying out the contour integral is

$$\begin{aligned} \mathcal{F} &= -TV \int \frac{d^3k}{(2\pi)^3} \left[\ln[1 + e^{-\beta E_{\mathbf{k}}}] + \ln[1 + e^{\beta E_{\mathbf{k}}}] \right] + V \frac{|\Delta|^2}{g_0} \\ &= -2TV \int_{|\epsilon_{\mathbf{k}}| < \omega_D} \frac{d^3k}{(2\pi)^3} \left[\ln[2\cosh(\beta E_{\mathbf{k}}/2)] \right] + V \frac{|\Delta|^2}{g_0}. \end{aligned} \tag{14.145}$$

14.6.2 Computing Δ and T_c

To compute T_c we shall take the Matsubara form of the gap equation (14.136), which we rewrite by replacing the sum over momenta by an integral near the Fermi energy, $\frac{1}{V}\sum_{\mathbf{k}} \to N(0)\int d\epsilon$, to get

$$\frac{1}{g_0} = TN(0) \sum_n \int_{-\infty}^{\infty} d\epsilon \frac{1}{\omega_n^2 + \epsilon_{\mathbf{k}}^2 + \Delta^2} = \pi TN(0) \sum_{|\omega_n| < \omega_D} \frac{1}{\sqrt{\omega_n^2 + \Delta^2}}, \tag{14.146}$$

where we have extended the limits of integration over energy to infinity. By carrying out the integral over energy first, we are forced to impose the cut-off on the Matsubara frequencies.

If we now take $T \to 0$ in this expression, we may replace

$$T \sum_n = T \sum \frac{\Delta\omega_n}{2\pi T} \to \int \frac{d\omega}{2\pi}, \tag{14.147}$$

so that at zero temperature (setting $T = 0$) we obtain

$$1 = gN(0) \int_0^{\omega_D} \frac{d\epsilon}{\sqrt{\epsilon^2 + \Delta^2}} = gN(0) \left[\sinh^{-1}\left(\frac{\omega_D}{\Delta} \right) \right] \approx gN(0) \ln\left(\frac{2\omega_D}{\Delta} \right), \tag{14.148}$$

where we have assumed $gN(0)$ is small, so that $\omega_D/\Delta >> 1$. We may now solve for the zero-temperature gap, to obtain

$$\Delta = 2\omega_D e^{-\frac{1}{gN(0)}}. \tag{14.149}$$

This recovers the form of the gap first derived in Section 14.4.2.

To calculate the transition temperature T_c, we note that, just below the transition temperature, the gap becomes infinitesimally small, so that $\Delta(T_c^-) = 0$. Substituting this into (14.147), we obtain

$$\frac{1}{gN(0)} = \pi T_c \sum_{|\omega_n|<\omega_D} \frac{1}{|\omega_n|} = 2\pi T_c \sum_{n=0}^{\infty} \left(\frac{1}{\omega_n} - \frac{1}{\omega_n + \omega_D} \right), \tag{14.150}$$

where we have imposed the limit on ω_n by subtracting an identical term, with $\omega_n \to \omega_n + \omega_D$. Simplifying this expression gives

$$\frac{1}{gN(0)} = \sum_{n=0}^{\infty} \left(\frac{1}{n+\frac{1}{2}} - \frac{1}{\omega_n + \frac{1}{2} + \frac{\omega_D}{2\pi T_c}} \right). \tag{14.151}$$

At this point we can use an extremely useful identity of the digamma function $\psi(z) = \frac{d}{dz} \ln \Gamma(z)$,

$$\psi(z) = -\zeta - \sum_{n=0}^{\infty} \left(\frac{1}{z+n} - \frac{1}{1+n} \right), \tag{14.152}$$

where $\zeta = 0.577216 = -\psi(1)$ is the Euler constant, so that

$$\frac{1}{gN(0)} = \overbrace{\psi(\frac{1}{2} + \frac{\omega_D}{2\pi T_c})}^{\approx \ln(\omega_D/(2\pi T_c))} - \psi(\frac{1}{2}) = \ln\left(\frac{\omega_D e^{-\psi(\frac{1}{2})}}{2\pi T_c} \right). \tag{14.153}$$

We have approximated $\psi(z) \approx \ln z$ for large $|z|$. Thus,

$$T_c = \overbrace{\left(\frac{e^{-\psi(1/2)}}{2\pi} \right)}^{\approx 1.13} \omega_D e^{-\frac{1}{g_0 N(0)}}. \tag{14.154}$$

Notice that the details of the way we introduced the cut-off into the sums affects both the gap Δ in (14.149) and the transition temperature in (14.154). However, the ratio of twice the gap to T_C,

$$\frac{2\Delta}{T_c} = 8\pi e^{\psi(\frac{1}{2})} \approx 3.53 \tag{14.155}$$

is *universal* for BCS superconductors, because the details of the cut-off cancel out of this ratio. Experiments confirm that this ratio of gap to transition is indeed observed in phonon-mediated superconductors.

14.7 The Nambu–Gor'kov Green's function

To describe the propagation of electrons and the Andreev scattering between electron and hole requires a matrix Green's function, formed from two Nambu spinors. This object, written

$$\mathcal{G}_{\alpha\beta}(\mathbf{k}, \tau) = -\langle T\psi_{\mathbf{k}\alpha}(\tau)\psi^\dagger_{\mathbf{k}\beta}(0)\rangle, \tag{14.156}$$

is called the *Nambu–Gor'kov Green's function*. Written out more explicitly, it takes the form

$$\begin{aligned}\mathcal{G}(\mathbf{k},\tau) &= -\left\langle T\begin{pmatrix} c_{\mathbf{k}\uparrow}(\tau) \\ \bar{c}^{\dagger}_{-\mathbf{k}\downarrow}(\tau)\end{pmatrix} \otimes (c^{\dagger}_{\mathbf{k}\uparrow}(0), c_{-\mathbf{k}\downarrow}(0))\right\rangle \\ &= -\begin{bmatrix} \langle Tc_{\mathbf{k}\uparrow}(\tau)c^{\dagger}_{\mathbf{k}\uparrow}(0)\rangle & \langle Tc_{\mathbf{k}\uparrow}(\tau)c_{-\mathbf{k}\downarrow}(0)\rangle \\ \langle Tc^{\dagger}_{-\mathbf{k}\downarrow}(\tau)c^{\dagger}_{\mathbf{k}\uparrow}(0)\rangle & \langle Tc^{\dagger}_{-\mathbf{k}\downarrow}(\tau)c_{-\mathbf{k}\downarrow}(0)\rangle \end{bmatrix}.\end{aligned} \tag{14.157}$$

The unusual off-diagonal components

$$F(\mathbf{k},\tau) = -\langle Tc_{\mathbf{k}\uparrow}(\tau)c_{-\mathbf{k}\downarrow}(0)\rangle, \qquad \bar{F}(\mathbf{k},\tau) = -\langle Tc^{\dagger}_{-\mathbf{k}\downarrow}(\tau)c^{\dagger}_{\mathbf{k}\uparrow}(0)\rangle \tag{14.158}$$

in $\mathcal{G}(\mathbf{k},\tau)$ describe the amplitude for an electron to convert to a hole as it Andreev scatters off the condensate.

Now from (12.142) and (14.131) the Green's function is given by the inverse of the Gaussian action, $\mathcal{G} = -(\partial_\tau - \mathcal{H})^{-1}$, or, in Matsubara space,

$$\mathcal{G}(\mathbf{k}, i\omega_n) = [i\omega_n - h_{\mathbf{k}}]^{-1} \equiv \frac{1}{(i\omega_n - h_{\mathbf{k}})}, \tag{14.159}$$

where we use the notation $\frac{1}{M} \equiv M^{-1}$ to denote the inverse of the matrix M. Now since $\underline{h}_{\mathbf{k}} = \epsilon_{\mathbf{k}}\tau_3 + \Delta_1\tau_1 + \Delta_2\tau_2$ (14.92) is a sum of Pauli matrices, its square is diagonal: $\underline{h}^2_{\mathbf{k}} = \epsilon^2_{\mathbf{k}} + \Delta_1^2 + \Delta_2^2 = E^2_{\mathbf{k}}$ and thus $(i\omega_n - h_{\mathbf{k}})(i\omega_n + h_{\mathbf{k}}) = (i\omega_n)^2 - E^2_{\mathbf{k}}$. Using the matrix identity $\frac{1}{B} = A\frac{1}{BA}$, we may then write

$$\underline{\mathcal{G}}(k) = (i\omega_n + h_{\mathbf{k}})\frac{1}{(i\omega_n - h_{\mathbf{k}})(i\omega_n + h_{\mathbf{k}})} = \frac{(i\omega_n + h_{\mathbf{k}})}{[(i\omega_n)^2 - E^2_{\mathbf{k}}]}. \tag{14.160}$$

Written out explicitly, this is

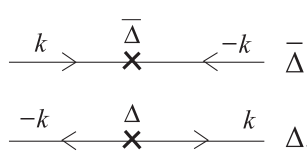
$$\underline{\mathcal{G}}(\mathbf{k}, i\omega_n) = \frac{1}{(i\omega_n)^2 - E^2_{\mathbf{k}}}\begin{bmatrix} i\omega_n + \epsilon_{\mathbf{k}} & \Delta \\ \bar{\Delta} & i\omega_n - \epsilon_{\mathbf{k}} \end{bmatrix}, \tag{14.161}$$

where $E_{\mathbf{k}} = \sqrt{\epsilon^2_{\mathbf{k}} + \Delta^2}$ is the quasiparticle energy.

To gain insight, let us obtain the same results diagrammatically. Andreev scattering converts a particle into a hole, which we denote by the Feynman scattering vertices

$\bar{\Delta} c_{-\mathbf{k}\downarrow} c_{\mathbf{k}\uparrow} \equiv$

$\Delta c^{\dagger}_{\mathbf{k}\uparrow} c^{\dagger}_{-\mathbf{k}\downarrow} \equiv$

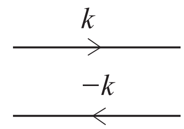


(14.162)

The bare propagators for the electron and hole are the diagonal components of the bare Nambu propagator:

$$\underline{\mathcal{G}}_0(k) = \frac{1}{i\omega_n - \epsilon_{\mathbf{k}}\tau_3} = \begin{bmatrix} \frac{1}{i\omega_n - \epsilon_{\mathbf{k}}} & \\ & \frac{1}{i\omega_n + \epsilon_{\mathbf{k}}} \end{bmatrix}. \tag{14.163}$$

We denote these two components by the diagrams

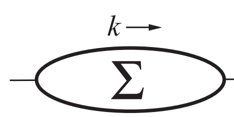


$$
\begin{aligned}
&\equiv G_0(k) = \frac{1}{i\omega_n - \epsilon_{\mathbf{k}}} \\
&\equiv -G_0(-k) = \frac{1}{i\omega_n + \epsilon_{\mathbf{k}}} .
\end{aligned}
\tag{14.164}
$$

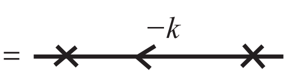
(There is a minus sign in the second term because we have commuted creation and annihilation operators to construct the hole propagator.) The Feynman diagrams for the conventional propagator are given by

(14.165)

involving an even number of Andreev reflections. This enables us to identify a self-energy term that describes the Andreev scattering off a hole state:



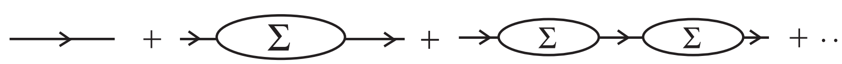
$$= \Sigma(k) =$$



$$= \frac{|\Delta|^2}{i\omega_n + \epsilon_{\mathbf{k}}} . \tag{14.166}$$

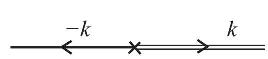
We may then redraw the propagator as

$G(k) =$



$$= \frac{1}{i\omega_n - \epsilon_{\mathbf{k}} - \Sigma(i\omega_n)} = \frac{1}{i\omega_n - \epsilon_{\mathbf{k}} - \frac{|\Delta|^2}{i\omega_n+\epsilon_{\mathbf{k}}}} = \frac{i\omega_n + \epsilon_{\mathbf{k}}}{(i\omega_n)^2 - E_{\mathbf{k}}^2} . \tag{14.167}$$

In a similar way, the anomalous propagator is given by



(14.168)

so that

$$F(k) = \frac{\Delta}{i\omega_n + \epsilon_{\mathbf{k}}} \frac{1}{i\omega_n - \epsilon_{\mathbf{k}} - \frac{|\Delta|^2}{i\omega_n+\epsilon_{\mathbf{k}}}} = \frac{\Delta}{(i\omega_n)^2 - E_{\mathbf{k}}^2} . \tag{14.169}$$

Example 14.5 Decompose the Nambu–Gor'kov Green's function in terms of its quasiparticle poles, and show that the diagonal part can be written

$$G(k) = \frac{u_{\mathbf{k}}^2}{i\omega_n - E_{\mathbf{k}}} + \frac{\mathrm{v}_{\mathbf{k}}^2}{i\omega_n + E_{\mathbf{k}}} . \tag{14.170}$$

Solution

To carry out this decomposition, it is convenient to introduce the projection operators

$$P_+(\mathbf{k}) = \frac{1}{2}(\underline{1} + \hat{n}\cdot\vec{\tau}), \qquad P_-(\mathbf{k}) = \frac{1}{2}(\underline{1} - \hat{n}\cdot\vec{\tau}), \tag{14.171}$$

which satisfy $P_+^2 = P_+$, $P_-^2 = P_-$, and $P_+ + P_- = 1$, and furthermore,

$$P_+(\mathbf{k})(\hat{n}_\mathbf{k}\cdot\vec{\tau}) = P_+(\mathbf{k}), \qquad P_-(\mathbf{k})(\hat{n}_\mathbf{k}\cdot\vec{\tau}) = -P_-(\mathbf{k}), \tag{14.172}$$

so that these operators conveniently project the isospin onto the directions $\pm n_\mathbf{k}$.

We can use the projectors $P_\pm(\mathbf{k})$ to project the Nambu propagator as follows:

$$\begin{aligned}\underline{\mathcal{G}} &= (P_+ + P_-)\frac{1}{i\omega_n - E_\mathbf{k}\hat{n}\cdot\vec{\tau}} \\ &= P_+\frac{1}{i\omega_n - E_\mathbf{k}} + P_-\frac{1}{i\omega_n + E_\mathbf{k}}.\end{aligned} \tag{14.173}$$

We can interpret these two terms as the quasiparticle and quasihole parts of the Nambu propagator. If we explicitly expand this expression, using

$$\hat{n} = \left(\frac{\epsilon}{E_\mathbf{k}}, \frac{\Delta_1}{E_\mathbf{k}}, \frac{\Delta_2}{E_\mathbf{k}}\right), \tag{14.174}$$

then

$$P_\pm = \frac{1}{2}\underline{1} \pm \begin{bmatrix} \frac{\epsilon_\mathbf{k}}{E_\mathbf{k}} & \frac{\Delta}{2E_\mathbf{k}} \\ \frac{\Delta}{2E_\mathbf{k}} & -\frac{\epsilon_\mathbf{k}}{2E_\mathbf{k}} \end{bmatrix}, \tag{14.175}$$

where $\Delta = \Delta_1 - i\Delta_2$, and we find that the diagonal part of the Green's function is given by

$$\begin{aligned}G(k) &= \frac{1}{2}\left(1 + \frac{\epsilon_\mathbf{k}}{E_\mathbf{k}}\right)\frac{1}{i\omega_n - E_\mathbf{k}} + \frac{1}{2}\left(1 - \frac{\epsilon_\mathbf{k}}{E_\mathbf{k}}\right)\frac{1}{i\omega_n + E_\mathbf{k}} \\ &= \frac{u_\mathbf{k}^2}{i\omega_n - E_\mathbf{k}} + \frac{\mathrm{v}_\mathbf{k}^2}{i\omega_n + E_\mathbf{k}},\end{aligned} \tag{14.176}$$

confirming that $u_\mathbf{k}$ and $\mathrm{v}_\mathbf{k}$ determine the overlap between the electron and the quasiparticle and quasihole, respectively.

Example 14.6 The semiconductor analogy

One useful way to regard superconductors is via the *semiconductor analogy*, in which the quasiparticles are treated like the positive and negative energy excitations of a semiconductor.

(a) Divide the Brillouin zone up into two equal halves and redefine a set of positive and negative energy quasiparticle operators according to

$$\left.\begin{aligned}\alpha^\dagger_{\mathbf{k}\sigma+} &= a^\dagger_{\mathbf{k}\sigma} \\ \alpha^\dagger_{\mathbf{k}\sigma-} &= \mathrm{sgn}(\sigma)a_{-\mathbf{k}-\sigma}\end{aligned}\right\} \qquad (\mathbf{k} \in \tfrac{1}{2}\mathrm{BZ}). \tag{14.177}$$

Rewrite the BCS Hamiltonian in terms of these new operators, and show that the excitation spectrum can be interpreted in terms of an empty band of positive energy excitations and a filled band of negative energy excitations.

(b) Show that the BCS ground-state wavefunction can be regarded as a filled sea of negative energy quasiparticle states and an empty sea of positive energy quasiparticle states.

Solution

(a) Dividing the Brillouin zone into two halves, the BCS Hamiltonian can be rewritten

$$\begin{aligned} H &= \sum_{\mathbf{k}\in\frac{1}{2}BZ} E_{\mathbf{k}}(a^\dagger_{\mathbf{k}\uparrow}a_{\mathbf{k}\uparrow} - a_{-\mathbf{k}\downarrow}a^\dagger_{-\mathbf{k}\downarrow}) + \sum_{\mathbf{k}\in\frac{1}{2}BZ} E_{\mathbf{k}}(a^\dagger_{-\mathbf{k}\uparrow}a_{-\mathbf{k}\uparrow} - a_{\mathbf{k}\downarrow}a^\dagger_{\mathbf{k}\downarrow}) \\ &= \sum_{\mathbf{k}\in\frac{1}{2}BZ,\sigma} E_{\mathbf{k}}(a^\dagger_{\mathbf{k}\sigma}a_{\mathbf{k}\sigma} - a_{-\mathbf{k}\sigma}a^\dagger_{-\mathbf{k}\sigma}) \\ &= \sum_{\mathbf{k}\in\frac{1}{2}BZ,\sigma} E_{\mathbf{k}}(\alpha^\dagger_{\mathbf{k}\sigma+}\alpha_{\mathbf{k}\sigma+} - \alpha^\dagger_{\mathbf{k}-}\alpha_{\mathbf{k}\sigma-}), \end{aligned} \tag{14.178}$$

corresponding to two bands of positive and negative energy quasiparticles.

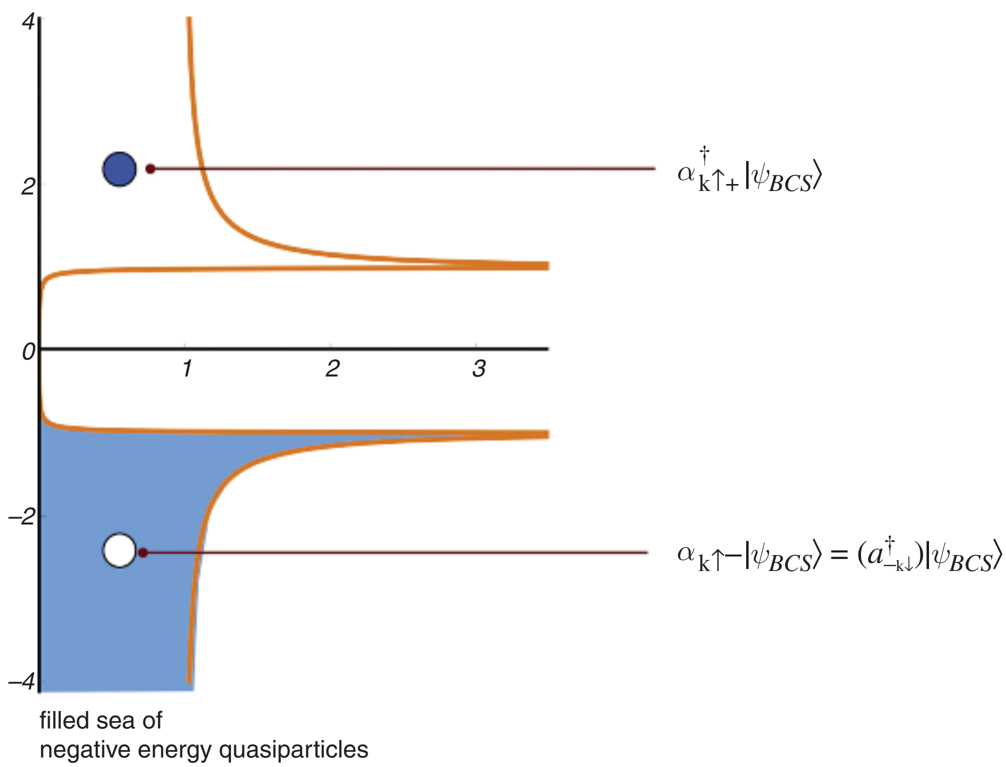


Fig. 14.13 Semiconductor analogy for BCS theory (see Example 14.6). The BCS ground state can be regarded as a filled sea of negative energy quasiparticles. Positive energy excitations are created by adding positive quasiparticles, $\alpha^\dagger_{\mathbf{k}\sigma+}|\psi_{BCS}\rangle$, or removing negative energy quasiparticles, $\alpha_{\mathbf{k}\sigma-}|\psi_{BCS}\rangle$.

(b) Following Example 14.2, the BCS ground state can be written (up to a normalization) as

$$|\psi_{BCS}\rangle = \prod_{\mathbf{k}} a_{-\mathbf{k}\downarrow} a_{\mathbf{k}\uparrow} |0\rangle. \tag{14.179}$$

Factoring the product into the two halves of the Brillouin zone, we may rewrite this as

$$\begin{aligned} |\psi_{BCS}\rangle &= \prod_{\mathbf{k}\in\frac{1}{2}BZ} (a_{\mathbf{k}\downarrow} a_{\mathbf{k}\uparrow})(a_{-\mathbf{k}\downarrow} a_{-\mathbf{k}\uparrow})|0\rangle \\ &= \overbrace{\prod_{\mathbf{k}\in\frac{1}{2}BZ,\sigma} \alpha_{\mathbf{k}\sigma+}}^{\text{empty sea of positive energy quasiparticles}} \underbrace{\prod_{\mathbf{k}\in\frac{1}{2}BZ,\sigma} \alpha^\dagger_{\mathbf{k}\sigma-}}_{\text{filled sea of negative energy quasiparticles}} |0\rangle, \end{aligned} \tag{14.180}$$

corresponding to an empty sea of positive energy quasiparticles and a filled sea of negative energy quasiparticles (see Figure 14.13).

14.7.1 Tunneling density of states and coherence factors

In a superconductor, the particle–hole mixing transforms the character of the quasiparticle, changing the matrix elements for scattering, introducing terms we call *coherence factors* into the physical response functions. These effects produce dramatic features in the various spectroscopies of the superconducting condensate.

Let us begin by calculating the tunneling density of states, which probes the spectrum to add and remove particles from the condensate. In a tunneling experiment the differential conductance is directly proportional to the local spectral function:

$$\frac{dI}{dV} \propto A(\omega)|_{\omega=eV}, \tag{14.181}$$

where

$$A(\omega) = \frac{1}{\pi}\mathrm{Im}\sum_{\mathbf{k}} G(\mathbf{k}, \omega - i\delta). \tag{14.182}$$

The mixed particle–hole character of the quasiparticle $a^\dagger_{\mathbf{k}\uparrow} = u_{\mathbf{k}} c^\dagger_{\mathbf{k}\uparrow} + \mathrm{v}_{\mathbf{k}} c_{-\mathbf{k}\downarrow}$ means that quasiparticles can be created by adding or removing electrons from the condensate. Taking the decomposition of the Green's function in terms of its poles (14.176),

$$\begin{aligned} G(\mathbf{k}, z) &= \frac{\omega + \epsilon_{\mathbf{k}}}{z^2 - E^2_{\mathbf{k}}} = \frac{1}{2}\left(1 + \frac{\epsilon_{\mathbf{k}}}{E_{\mathbf{k}}}\right)\frac{1}{z - E_{\mathbf{k}}} + \frac{1}{2}\left(1 - \frac{\epsilon_{\mathbf{k}}}{E_{\mathbf{k}}}\right)\frac{1}{z + E_{\mathbf{k}}} \\ &= \frac{u^2_{\mathbf{k}}}{z - E_{\mathbf{k}}} + \frac{\mathrm{v}^2_{\mathbf{k}}}{z + E_{\mathbf{k}}}, \end{aligned} \tag{14.183}$$

it follows that

$$A(\mathbf{k}, \omega) = \frac{1}{\pi}\mathrm{Im}\, G(\mathbf{k}, \omega - i\delta) = u^2_{\mathbf{k}}\delta(\omega - E_{\mathbf{k}}) + \mathrm{v}^2_{\mathbf{k}}\delta(\omega + E_{\mathbf{k}}). \tag{14.184}$$

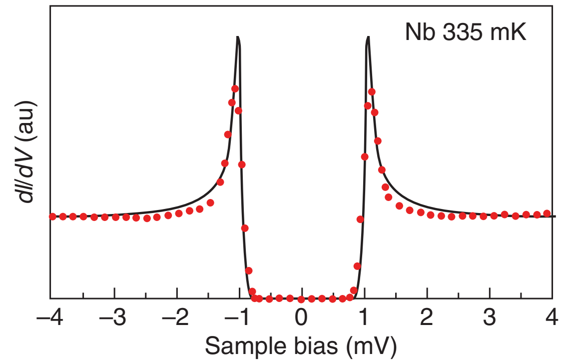


Fig. 14.14 Comparison of the experimental tunneling spectrum and the BCS spectrum in superconducting Nb at $T = 335$ mK [22]. Reprinted with permission from S. H. Pan, *et al.*, *Appl. Phys. Lett.*, vol. 73, p. 2992, 1998. Copyright 1998 by the American Insitute of Physics.

The positive energy part of this expression corresponds to the process of creating a quasiparticle by adding an electron, while the negative energy part corresponds to the creation of a quasiparticle by adding a hole. The amplitudes

$$
\begin{aligned}
|u_{\mathbf{k}}|^2 &= |\langle \mathrm{qp} : \mathbf{k}\sigma | c^{\dagger}_{\mathbf{k}\sigma} | \psi_{BCS} \rangle|^2 \\
|\mathrm{v}_{\mathbf{k}}|^2 &= |\langle \mathrm{qp} : \mathbf{k}\sigma | c_{-\mathbf{k}-\sigma} | \psi_{BCS} \rangle|^2
\end{aligned}
\tag{14.185}
$$

describe the probability to create a quasiparticle through the addition or removal of an electron, respectively. In this way, the tunneling density of states contains both negative and positive energy components.

Now we can sum over the momenta in (14.182), replacing the momentum sum by an integral over energy. In this case,

$$
\begin{aligned}
A(\omega) &= \frac{N(0)}{\pi}\mathrm{Im}\int_{-\infty}^{\infty} d\epsilon \frac{\omega+\epsilon}{(\omega - i\delta)^2 - \epsilon^2 - |\Delta|^2} = -N(0)\mathrm{Im}\frac{\omega}{\sqrt{\Delta^2 - (\omega - i\delta)^2}} \\
&= N(0)\,\mathrm{Re}\left[\frac{|\omega|}{\sqrt{(\omega - i\delta)^2 - \Delta^2}}\right] = N(0)\frac{|\omega|}{\sqrt{\omega^2 - \Delta^2}}\theta(|\omega| - \Delta),
\end{aligned}
\tag{14.186}
$$

where we have used $\mathrm{Im}[\sqrt{\Delta^2 - (\omega - i\delta)^2}] = \sqrt{\omega^2 - \Delta^2}\,\mathrm{sgn}(\omega)\,\theta(|\omega| - \Delta)$. Curiously, this result is identical (up to a factor of ½ derived from the energy average of the coherence factors) to the quasiparticle density of states, except that there is both a positive and a negative energy component to the spectrum. In weakly coupled phonon-paired superconductors such as niobium, experimental tunneling spectra are in good accord with BCS theory (see Figure 14.14). In more strongly coupled electron–phonon superconductors, wiggles develop in the spectrum related to the detailed phonon spectrum.

Other forms of spectroscopy probe the condensate by scattering electrons. In general a one-particle observable $\hat{A}$, such as spin or charge density, can be written as

$$
\hat{A} = \sum_{\mathbf{k}\alpha,\mathbf{k}'\beta} A_{\alpha\beta}(\mathbf{k},\mathbf{k}') c^{\dagger}_{\mathbf{k}\alpha} c_{\mathbf{k}'\beta},
\tag{14.187}
$$

where $A_{\alpha\beta}(\mathbf{k},\mathbf{k}') = \langle \mathbf{k}\alpha|\hat{A}|\mathbf{k}'\beta\rangle$ are the electron matrix elements of the operator $\hat{A}$. For example, for the charge operator $\hat{\rho}_{\mathbf{q}} = e\sum_{\mathbf{k}\sigma} c^{\dagger}_{\mathbf{k}+\mathbf{q}\sigma} c_{\mathbf{k}\sigma}$, $A_{\alpha\beta}(\mathbf{k},\mathbf{k}') = e\delta_{\alpha\beta}\delta_{\mathbf{k}-(\mathbf{k}'+\mathbf{q})}$

Table 14.2 Coherence factors.

Name	$\hat{A}$	$A_{\alpha\beta}(\mathbf{k},\mathbf{k}')$	θ	Coherence factor
Density	$\hat{\rho}_{\mathbf{q}}$	$\delta_{\alpha\beta}\delta_{\mathbf{k}-(\mathbf{k}'+\mathbf{q})}$	$+1$	$uu' - vv'$
Magnetization	$\vec{M}_{\mathbf{q}}$	$\left(\frac{g\mu_B}{2}\right)\vec{\sigma}_{\alpha\beta}\delta_{\mathbf{k}-(\mathbf{k}'+\mathbf{q})}$	-1	$uu' + vv'$
Current	$\vec{J}_{\mathbf{q}}$	$\delta_{\alpha\beta}[(\mathbf{k}'+\mathbf{q}/2) - e\vec{A}]\delta_{\mathbf{k}-(\mathbf{k}'+\mathbf{q})}$	-1	$uu' + vv'$

(see Table 14.2). Let us now rewrite this expression in terms of Bogoliubov quasiparticle operators, substituting $c^{\dagger}_{\mathbf{k}\alpha} = u_{\mathbf{k}}a_{\mathbf{k}\alpha} - \mathrm{sgn}(\alpha)\mathrm{v}_{\mathbf{k}}a^{\dagger}_{-\mathbf{k}-\alpha}$ (where we have taken the gap, $u_{\mathbf{k}}$, and $v_{\mathbf{k}}$ to be real), so that the operator expands into the long expression

$$\hat{A} = \sum_{\mathbf{k}\alpha\mathbf{k}'\beta} A_{\alpha\beta}(\mathbf{k},\mathbf{k}')\Big[(uu'a^{\dagger}_{\mathbf{k}\alpha}a_{\mathbf{k}'\beta} - \mathrm{vv}'\tilde{\alpha}\tilde{\beta}a_{-\mathbf{k}-\alpha}a^{\dagger}_{-\mathbf{k}'-\beta}) - (u\mathrm{v}'\tilde{\beta}a^{\dagger}_{\mathbf{k}\alpha}a^{\dagger}_{-\mathbf{k}'-\beta} + \mathrm{H.c.})\Big]. \tag{14.188}$$

We have used the shorthand $\tilde{\alpha} = \mathrm{sgn}(\alpha)$, $\tilde{\beta} = \mathrm{sgn}(\beta)$, and $u \equiv u_{\mathbf{k}}$, $u' \equiv u_{\mathbf{k}'}$ and so on. This expression can be simplified by taking account of the time-reversal properties of $\hat{A}$. Under time reversal, $A \to -i\sigma_2 A^T i\sigma_2 = \theta A$, where $\theta = \pm 1$ is the parity of the operator under time reversal. In longhand,[6]

$$A_{\alpha\beta}(\mathbf{k},\mathbf{k}') \to \tilde{\alpha}\tilde{\beta}A_{-\beta\ -\alpha}(-\mathbf{k}',-\mathbf{k}) = \theta A_{\alpha\beta}(\mathbf{k},\mathbf{k}'). \tag{14.189}$$

Using this property, we can rewrite $\hat{A}$ as

$$\hat{A} = \sum_{\mathbf{k}\alpha,\mathbf{k}'\beta} A(\mathbf{k},\mathbf{k}')_{\alpha\beta}\Big[(uu' - \theta\mathrm{vv}')a^{\dagger}_{\mathbf{k}\alpha}a_{\mathbf{k}'\beta} + \frac{1}{2}\Big((uv' - \theta vu')a^{\dagger}_{\mathbf{k}\alpha}a^{\dagger}_{-\mathbf{k}-\beta}\,\tilde{\beta} + \mathrm{H.c.}\Big)\Big]. \tag{14.190}$$

We see that, in the pair condensate, the matrix element for quasiparticle scattering is renormalized by the *coherence factor*

$$A_{\alpha\beta}(\mathbf{k},\mathbf{k}') \to A_{\alpha\beta}(\mathbf{k},\mathbf{k}') \times (u_{\mathbf{k}}u_{\mathbf{k}'} - \theta\mathrm{v}_{\mathbf{k}}\mathrm{v}_{\mathbf{k}'}), \tag{14.191}$$

while the matrix element for creating a pair of quasiparticles has been modified by the factor

$$A_{\alpha\beta}(\mathbf{k},\mathbf{k}') \to A_{\alpha\beta}(\mathbf{k},\mathbf{k}') \times (u_{\mathbf{k}}\mathrm{v}_{\mathbf{k}'} - \theta\mathrm{v}_{\mathbf{k}}u_{\mathbf{k}'}). \tag{14.192}$$

Remarks

- At the Fermi energy, $|u_{\mathbf{k}}| = |v_{\mathbf{k}}| = \frac{1}{\sqrt{2}}$, so that for time-reversed even operators ($\theta = 1$) the coherence factors vanish on the Fermi surface.

[6] For example, for the magnetization density at wavevector $\mathbf{q}$, where $\vec{A}(\mathbf{k},\mathbf{k}') = \vec{\sigma}\delta_{\mathbf{k}-(\mathbf{k}'+\mathbf{q})}$, using the result $\vec{\sigma}^T = i\sigma_2\vec{\sigma}i\sigma_2$, we obtain $-i\sigma_2\vec{A}^T(-\mathbf{k}',-\mathbf{k})i\sigma_2 = -i\sigma_2\vec{\sigma}i\sigma_2\delta_{-\mathbf{k}'-(-\mathbf{k}+\mathbf{q})} = -\vec{\sigma}\delta_{\mathbf{k}-(\mathbf{k}'+\mathbf{q})}$, corresponding to an odd time-reversal parity, $\theta = -1$.

- If we square the quasiparticle scattering coherence factor, we obtain

$$
\begin{aligned}
(uu' - \theta \mathrm{v}\mathrm{v}')^2 &= u^2(u')^2 + \mathrm{v}^2(\mathrm{v}')^2 - 2\theta(u\mathrm{v})(u'\mathrm{v}') \\
&= \frac{1}{4}\left(1+\frac{\epsilon}{E}\right)\left(1+\frac{\epsilon'}{E'}\right) + \frac{1}{4}\left(1-\frac{\epsilon}{E}\right)\left(1-\frac{\epsilon'}{E'}\right) - 2\theta\left(\frac{\Delta^2}{4EE'}\right) \\
&= \frac{1}{2}\left(1+\frac{\epsilon\epsilon'}{EE'} - \theta\frac{\Delta^2}{EE'}\right),
\end{aligned} \tag{14.193}
$$

  with the notation $\epsilon = \epsilon_{\mathbf{k}}$, $\epsilon' = \epsilon_{\mathbf{k}'}$, $E = E_{\mathbf{k}}$, and $E' = E_{\mathbf{k}'}$.
- If we employ the semiconductor analogy, using positive ($\lambda = +$) and negative energy ($\lambda = -$) quasiparticles (see Example 14.6), with energies $E_{\mathbf{k}\lambda} = \mathrm{sgn}\,(\lambda)E_{\mathbf{k}}$ ($\lambda = \pm$) and modified Bogoliubov coefficients,

$$
u_{\mathbf{k}\lambda} = \sqrt{\frac{1}{2}\left(1+\frac{\epsilon_{\mathbf{k}}}{E_{\mathbf{k}\lambda}}\right)}, \qquad v_{\mathbf{k}\lambda} = \sqrt{\frac{1}{2}\left(1-\frac{\epsilon_{\mathbf{k}}}{E_{\mathbf{k}\lambda}}\right)}. \tag{14.194}
$$

  Then

$$
(u_{\mathbf{k}}\mathrm{v}_{\mathbf{k}'} - \theta \mathrm{v}_{\mathbf{k}}u_{\mathbf{k}'})a^{\dagger}_{\mathbf{k}\sigma}a^{\dagger}_{-\mathbf{k}'} = (u_{\mathbf{k}+}u_{\mathbf{k}'-} - \theta \mathrm{v}_{\mathbf{k}+}v_{\mathbf{k}'-})\alpha^{\dagger}_{\mathbf{k}\sigma+}a_{\mathbf{k}'\sigma'-}, \tag{14.195}
$$

  so that the creation of a pair of quasiparticles can be regarded as an interband scattering of a valence negative energy quasiparticle into a conduction positive energy quasiparticle state. This has the advantage that all processes can be regarded as quasiparticle scattering, with a single coherent factor for all processes:

$$
\hat{A} = \frac{1}{2}\sum_{\mathbf{k}\sigma\lambda,\,\mathbf{k}'\sigma'\lambda'} A_{\sigma\sigma'}(\mathbf{k},\mathbf{k}')(uu' - \theta\mathrm{v}\mathrm{v}') \times \alpha^{\dagger}_{\mathbf{k}\sigma\lambda}\alpha_{\mathbf{k}\sigma'\lambda'}. \tag{14.196}
$$

Once the condensate forms, the coherence factors renormalize the charge, spin, and current matrix elements of a superconductor. For example, in a metal the NMR relaxation rate is determined by the thermal average of the density of states:

$$
\frac{1}{T_1T} \propto \int\left(-\frac{df}{dE}\right)N(E)^2|\langle E\uparrow|S^+|E\downarrow\rangle|^2 = \int\left(-\frac{df}{dE}\right)N(E)^2 = N(0)^2 \tag{14.197}
$$

at temperatures much smaller than the Fermi energy. However, in a superconductor we need to take account of the strongly energy-dependent quasiparticle density of states

$$
N(E) \to N(0)\frac{|E|}{\sqrt{E^2-\Delta^2}}, \tag{14.198}
$$

while in this case the matrix elements

$$
|\langle E\uparrow|S^+|E\downarrow\rangle|^2 \to |\langle E\uparrow|S^+|E\downarrow\rangle|^2(u(E)^2 + \mathrm{v}(E)^2) = 1
$$

are unrenormalized, so that the NMR relaxation rate becomes

$$
\begin{aligned}
\left(\frac{1}{T_1T}\right)_s \Big/ \left(\frac{1}{T_1T}\right)_n &= \int dE\left(-\frac{df}{dE}\right)\frac{E^2}{E^2-\Delta^2}\theta(|E|-\Delta) \\
&= \frac{1}{2}\int_{\Delta}^{\infty} dE\left(-\frac{df}{dE}\right)\frac{E^2}{E^2-\Delta^2}.
\end{aligned} \tag{14.199}
$$

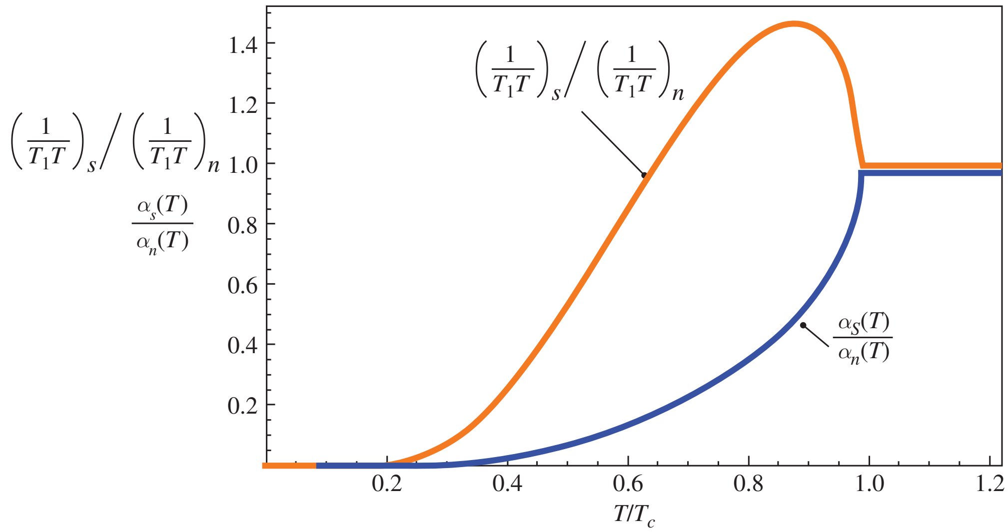


Fig. 14.15 Showing the effect of coherence factors NMR and ultrasonic attenuation in a superconductor, calculated in BCS theory. The orange line displays the NMR relaxation rate, showing the Hebel–Slichter peak. The blue line shows the ultrasound attenuation. The integrals entering the NMR relaxation rate are formally divergent for $T < T_c$ and were regulated by introducing a small imaginary damping rate $i\delta$ to the frequency where $\delta/\Delta = 0.005$.

The NMR relaxation rate is thus sensitive to the coherence peak in the density of states, which leads to a sharp peak in the NMR relaxation rate just below the transition temperature, known as the *Hebel–Slichter peak* (Figure 14.15).[7] By contrast, the absorption coefficient for ultrasound is proportional to the imaginary part of the charge susceptibility at $\mathbf{q} = 0$, which in a normal metal is given by

$$\alpha_n(T) \propto \int dE \left(-\frac{df}{dE}\right) N(E) \overbrace{|\langle E|\rho_{\mathbf{q}=0}|E\rangle|^2}^{=1} \sim N(0), \tag{14.200}$$

but in the superconductor this becomes

$$\alpha_s(T) \propto \int dE \left(-\frac{df}{dE}\right) N_s(E)|\langle E|\rho_{\mathbf{q}=0}|E\rangle|^2 \times (u(E)^2 - \mathrm{v}(E)^2). \tag{14.201}$$

However, in this case the renormalization of the matrix elements identically cancels the renormalization of the density of states:

$$N_s(E)(u^2 - v^2) = N(0)\theta(|E| - \Delta).$$

So there is no net coherence factor effect and

$$\alpha_s(T) \propto N(0) \int_{-\infty}^{\infty} dE \left(-\frac{df}{dE}\right) \theta(|E| - \Delta) = N(0)2f(\Delta), \tag{14.202}$$

[7] Equation (14.199) contains a logarithmic divergence from the coherence peak. In practice, this is cut off by the quasiparticle scattering. To obtain a finite result, one can replace $E \to E - i/(2\tau)$ and use the expression $N(E) = \mathrm{Im}(E/\sqrt{\Delta^2 - (E - i/(2\tau))^2})$ to regulate the logarithmic divergence.

so that

$$\frac{\alpha_s(T)}{\alpha_n(T)} = \frac{2}{e^{\Delta/T}+1}. \tag{14.203}$$

Figure 14.15 contrasts the temperature dependence of NMR with the ultrasound attenuation for a BCS superconductor.

Example 14.7

(a) Calculate the dynamical spin susceptibility of a superconductor using the Nambu Green's function, and show that it takes the form $\chi_{ab}(q) = \delta_{ab}\chi(q)$, where

$$\begin{aligned}\chi(q) &= 2\sum_{\mathbf{k},\eta,\eta'}(uu'+vv')^2\frac{f(E')-f(E)}{\nu-(E'-E)}\\ &= 2\sum_{\mathbf{k},\eta,\eta'}\left(\frac{1}{2}\left(1+\frac{\epsilon\epsilon'+\Delta^2}{EE'}\right)\right)^2\frac{f(E')-f(E)}{\nu-(E'-E)},\end{aligned} \tag{14.204}$$

where $\eta = \pm$, $\eta' = \pm$ and we have employed the (semiconductor analogy) notation $u \equiv u_{\mathbf{k}\eta}$, $u' \equiv u_{\mathbf{k}+\mathbf{q}\eta'}$, $E \equiv E_{\mathbf{k}}\mathrm{sgn}(\eta)$, $E' \equiv E_{\mathbf{k}+\mathbf{q}}\mathrm{sgn}(\eta')$, and so on.

(b) Assuming that the NMR relaxation rate is given by the expression

$$\frac{1}{T_1T} \propto \sum_{\mathbf{q}}\left.\frac{\chi''(\mathbf{q},\nu-i\delta)}{\nu}\right|_{\nu\to 0}, \tag{14.205}$$

show that

$$\frac{1}{T_1T} \propto \int\left(-\frac{df}{dE}\right)N(E)^2. \tag{14.206}$$

Solution

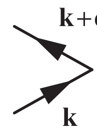
(a) The dynamical susceptibility in imaginary time is given by

$$\chi_{ab}(\mathbf{q},i\nu_n) = \langle M_a(q)M_b(-q)\rangle = \int_0^\beta d\tau\,\langle TM_a(\mathbf{q},\tau)M_b(-\mathbf{q},0)\rangle e^{i\nu_n\tau}. \tag{14.207}$$

Since the system is spin isotropic, we can write $\chi_{ab}(q) = \delta_{ab}\chi(q)$, using the z component of the magnetic susceptibility to calculate $\chi(q) = \langle M_z(q)M_z(-q)\rangle$. In Nambu notation,

$$\begin{aligned}M_z(-\mathbf{q}) &= \sum_{\mathbf{k}}(c^\dagger_{\mathbf{k}+\mathbf{q}\uparrow}c_{\mathbf{k},\uparrow} - c^\dagger_{\mathbf{k}+\mathbf{q}\downarrow}c_{\mathbf{k},\downarrow}) = \sum_{\mathbf{k}}(c^\dagger_{\mathbf{k}+\mathbf{q}\uparrow}c_{\mathbf{k}\uparrow} + c_{\mathbf{k}\downarrow}c^\dagger_{\mathbf{k}+\mathbf{q}\downarrow})\\ &= \sum_{\mathbf{k}}(c^\dagger_{\mathbf{k}+\mathbf{q}\uparrow}c_{\mathbf{k}\uparrow} + c_{-\mathbf{k}-\mathbf{q}\downarrow}c^\dagger_{-\mathbf{k}\downarrow})\\ &= \sum_{\mathbf{k}}\psi^\dagger_{\mathbf{k}+\mathbf{q}}\cdot\psi_{\mathbf{k}},\end{aligned} \tag{14.208}$$

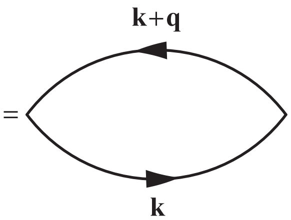
where we have anticommuted the down fermion operators and relabeled $\mathbf{k} \to -\mathbf{k}+\mathbf{q}$. Thus the z component of the magnetization is a unit matrix in Nambu space. The vertex for the magnetization is thus



$$= M_z(-q), \tag{14.209}$$

and we can guess that the Feynman diagram for the susceptibility is

$$\langle M_z(q) M_z(-q)\rangle =$$



$$= -\frac{1}{\beta}\sum_k \mathrm{Tr}\left[\mathcal{G}(k+q)\mathcal{G}(k)\right],$$

where the fermion lines represent the Nambu propagator.

Let us confirm this result. The dynamical susceptibility is written

$$\chi(\mathbf{q},\tau) = \sum_{\mathbf{k},\mathbf{k}'} \langle T\psi^\dagger_{\mathbf{k}'-\mathbf{q}}(\tau)\cdot\psi_{\mathbf{k}'}(\tau)\ \psi^\dagger_{\mathbf{k}+\mathbf{q}}(0)\cdot\psi_{\mathbf{k}}(0)\rangle. \tag{14.210}$$

Since the mean field theory describes a non-interacting system, we can evaluate this expression using Wick's theorem:

$$\begin{aligned}
\chi(\mathbf{q},\tau) &= \sum_{\mathbf{k},\mathbf{k}'} \langle T\psi^\dagger_{\mathbf{k}'-\mathbf{q}\alpha}(\tau)\psi_{\mathbf{k}'\alpha}(\tau)\psi^\dagger_{\mathbf{k}+\mathbf{q}\beta}(0)\psi_{\mathbf{k}\beta}(0)\rangle \\
&= -\sum_{\mathbf{k}} \mathcal{G}_{\alpha\beta}(\mathbf{k}+\mathbf{q},\tau)\mathcal{G}_{\beta\alpha}(\mathbf{k},-\tau) \\
&= -\sum_{\mathbf{k}} \mathrm{Tr}[\mathcal{G}(\mathbf{k}+\mathbf{q},\tau)\mathcal{G}(\mathbf{k},-\tau)].
\end{aligned} \tag{14.211}$$

Notice that the anomalous contractions of the Nambu spinors, such as $\langle T\psi_{\mathbf{k}\alpha}(\tau)\psi_{\mathbf{k}'\beta}(0)\rangle$, equal 0 because these terms describe triplet correlations that vanish in a singlet superconductor. For example, $\langle T\psi_{\mathbf{k}1}(\tau)\psi_{\mathbf{k}'2}(0)\rangle = \langle Tc_{\mathbf{k}\uparrow}(\tau)c^\dagger_{\mathbf{k}'\downarrow}(0)\rangle = 0$.

If we Fourier analyze this, $\chi(q) \equiv \chi(\mathbf{q}, i\nu_r) = \int_0^\beta \chi(\mathbf{q},\tau)e^{i\nu_r\tau}$, we obtain

$$\begin{aligned}
\chi(\mathbf{q},i\nu_r) &= -T^2\sum_{\mathbf{k},n,m}\int_0^\beta d\tau\,\mathrm{Tr}\left[\mathcal{G}(\mathbf{k}+\mathbf{q},i\omega_m)\mathcal{G}(\mathbf{k},i\omega_n)\right]e^{i(\nu_r-\omega_m+\omega_n)\tau} \\
&= -T\sum_{\mathbf{k},i\omega_n}\mathrm{Tr}\left[\mathcal{G}(\mathbf{k}+\mathbf{q},i\omega_n+i\nu_r)\mathcal{G}(\mathbf{k},i\omega_n)\right] \\
&= -T\sum_k \mathrm{Tr}\left[\mathcal{G}(k+q)\mathcal{G}(k)\right].
\end{aligned} \tag{14.212}$$

Now if we choose a real gap,

$$\mathcal{G}(\mathbf{k}, z) = \frac{z + \epsilon_{\mathbf{k}}\tau_3 + \Delta\tau_1}{z^2 - E_{\mathbf{k}}^2}, \tag{14.213}$$

we deduce that

$$\begin{aligned}\mathrm{Tr}\left[\mathcal{G}(k')\mathcal{G}(k)\right] &= \mathrm{Tr}\left[\frac{z'+\epsilon_{\mathbf{k}'}\tau_3+\Delta\tau_1}{z'^2-E_{\mathbf{k}}^2}\frac{z+\epsilon_{\mathbf{k}}\tau_3+\Delta\tau_1}{z^2-E_{\mathbf{k}}^2}\right]\\ &= 2\left[\frac{zz'+\epsilon_{\mathbf{k}}\epsilon_{\mathbf{k}'}+\Delta^2}{(z^2-E_{\mathbf{k}}^2)(z'^2-E_{\mathbf{k}'}^2)}\right].\end{aligned} \tag{14.214}$$

If we first carry out the Matsubara summation in the expression of the susceptibility, then by converting the summation to a contour integral we obtain

$$\chi(q) = -2\sum_{\mathbf{k}}\oint\frac{dz}{2\pi i}f(z)\left[\frac{z(z+i\nu_r)+\epsilon_{\mathbf{k}}\epsilon_{\mathbf{k}+\mathbf{q}}+\Delta^2}{(z^2-E_{\mathbf{k}}^2)((z+i\nu_r)^2-E_{\mathbf{k}+\mathbf{q}}^2)}\right], \tag{14.215}$$

where the contour passes clockwise around the poles in the Green's functions.

To do this integral, it is useful to rewrite the denominators of the Green's functions using the relation

$$\begin{aligned}\frac{1}{z^2-E_{\mathbf{k}}^2} &= \frac{1}{2E_{\mathbf{k}}}\frac{1}{z-E_{\mathbf{k}}} - \frac{1}{2E_{\mathbf{k}}}\frac{1}{z+E_{\mathbf{k}}}\\ &= \sum_{\lambda=\pm 1}\frac{1}{z-E_{\mathbf{k}\lambda}}\frac{1}{2E_{\mathbf{k}\lambda}},\end{aligned} \tag{14.216}$$

where we have introduced (cf. semiconductor analogy, Example 14.6) $E_{\mathbf{k}\lambda} = \mathrm{sgn}(\lambda)E_{\mathbf{k}}$. Similarly,

$$\frac{z}{z^2-E_{\mathbf{k}}^2} = \sum_{\lambda=\pm}\frac{1}{2(z-E_{\mathbf{k}\lambda})}.$$

With this device, the integral becomes

$$\begin{aligned}\chi(q) &= -2\sum_{\mathbf{k},\lambda=\pm,\lambda'=\pm}\oint\frac{dz}{2\pi i}f(z)\left[\frac{1}{4}+\frac{\epsilon_{\mathbf{k}}\epsilon_{\mathbf{k}+\mathbf{q}}+\Delta^2}{(4E_{\mathbf{k}\lambda}E_{\mathbf{k}+\mathbf{q}\lambda'})}\right]\frac{1}{(z-E_{\mathbf{k}\lambda})(z+i\nu_r-E_{\mathbf{k}+\mathbf{q}\lambda'})}\\ &= \sum_{\mathbf{k},\lambda=\pm,\lambda'=\pm}\overbrace{\left[\frac{1}{2}+\frac{\epsilon_{\mathbf{k}}\epsilon_{\mathbf{k}+\mathbf{q}}+\Delta^2}{2E_{\mathbf{k}\lambda}E_{\mathbf{k}+\mathbf{q}\lambda'}}\right]}^{(uu'+vv')^2}\frac{f(E_{\mathbf{k}+\mathbf{q}\lambda'})-f(E_{\mathbf{k}\lambda})}{i\nu_r-(E_{\mathbf{k}+\mathbf{q}\lambda'}-E_{\mathbf{k}\lambda})}\\ &= \sum_{\mathbf{k},\lambda=\pm,\lambda'=\pm}(u_{\mathbf{k}\lambda}u_{\mathbf{k}+\mathbf{q}\lambda'}+v_{\mathbf{k}\lambda}v_{\mathbf{k}+\mathbf{q}\lambda'})^2\frac{f(E_{\mathbf{k}+\mathbf{q}\lambda'})-f(E_{\mathbf{k}\lambda})}{i\nu_r-(E_{\mathbf{k}+\mathbf{q}\lambda'}-E_{\mathbf{k}\lambda})},\end{aligned} \tag{14.217}$$

thereby proving (14.204).

(b) If we analytically continue the susceptibility onto the real axis, then

$$\chi(\mathbf{q},\nu-i\delta) = \sum_{\mathbf{k},\lambda=\pm,\lambda'=\pm}(u_{\mathbf{k}\lambda}u_{\mathbf{k}+\mathbf{q}\lambda'}+v_{\mathbf{k}\lambda}v_{\mathbf{k}+\mathbf{q}\lambda'})^2\frac{f(E_{\mathbf{k}+\mathbf{q}\lambda'})-f(E_{\mathbf{k}\lambda})}{\nu-i\delta-(E_{\mathbf{k}+\mathbf{q}\lambda'}-E_{\mathbf{k}\lambda})}. \tag{14.218}$$

Taking the imaginary part,

$$\frac{\chi''(\mathbf{q}, \nu - i\delta)}{\nu} = \pi \sum_{\mathbf{k},\lambda=\pm,\lambda'=\pm} (uu' + vv')^2 \frac{f(E_{\mathbf{k}\lambda} + \nu) - f(E_{\mathbf{k}\lambda})}{\nu} \delta(E_{\mathbf{k}+\mathbf{q}\lambda'} - E_{\mathbf{k}\lambda}) \tag{14.219}$$

so that

$$\left.\frac{\chi''(\mathbf{q}, \nu - i\delta)}{\nu}\right|_{\nu\to 0} = \pi \sum_{\mathbf{k},\lambda=\pm,\lambda'=\pm} \left(-\frac{df(E_{\mathbf{k}\lambda})}{dE_{\mathbf{k}\lambda}}\right) \delta(E_{\mathbf{k}+\mathbf{q}\lambda'} - E_{\mathbf{k}\lambda}). \tag{14.220}$$

Summing over momentum,

$$\begin{aligned} \frac{1}{T_1 T} &\propto \sum_{\mathbf{q}} \left.\frac{\chi''(\mathbf{q}, \nu - i\delta)}{\nu}\right|_{\nu\to 0} \\ &= \pi \sum_{\mathbf{k},\lambda=\pm} \sum_{\mathbf{k}',\ \lambda=\pm'} \left(-\frac{df(E_{\mathbf{k}\lambda})}{dE_{\mathbf{k}\lambda}}\right) \delta(E_{\mathbf{k}+\mathbf{q}\lambda'} - E_{\mathbf{k}\lambda}) \\ &= \pi N(0)^2 \int dE \left(\frac{|E|}{\sqrt{E^2 - \Delta^2}}\right)^2 \left(-\frac{df(E)}{dE}\right), \end{aligned} \tag{14.221}$$

where we have replaced the summation over momentum and semiconductor index λ by an integral over the quasiparticle and quasihole density of states:

$$\sum_{\mathbf{k},\lambda=\pm} \to \int dE N_s(|E|) = N(0) \int dE \left(\frac{|E|}{\sqrt{E^2 - \Delta^2}}\right). \tag{14.222}$$

14.8 Twisting the phase: the superfluid stiffness

One of the key features in a superconductor is the emergence of a complex order parameter, with a phase. It is the rigidity of this phase that endows the superconductor with its ability to sustain a superflow, a feature held in common between superfluids and superconductors. However, superconductors stand apart from their neutral counterparts because the phase of the condensate is directly coupled to the electromagnetic field. The important point, as we saw in Chapter 11, is that the phase of the order parameter and the vector potential are linked by gauge invariance, so that a twisted phase and a uniform vector are gauge-equivalent. This feature implies that, once a gauge stiffness develops, the electromagnetic field acquires a mass. We shall now derive these features from the microscopic perspective of BCS theory.

To explore a twisted phase, we need to consider an order parameter with position dependence, so that now the interaction that gives rise to superconductivity cannot be infinitely long-range. For this purpose we use Gor'kov's coarse-grained continuum version of BCS theory, where

$$H = \int d^3x \left[\psi_\sigma^\dagger \left(\frac{1}{2m} (-i\hbar\nabla - e\vec{A})^2 - \mu \right) \psi_\sigma - g(\psi_\uparrow^\dagger \psi_\downarrow^\dagger \psi_\downarrow \psi_\uparrow) \right]. \quad (14.223)$$

For compactness, the position arguments of the fields are no longer shown explicitly, $\psi_\sigma(x) \equiv \psi_\sigma$. This is a coarse-grained version of the microscopic Hamiltonian, in which the delta-function interaction represents the effective interaction on scales larger than v_F/ω_D.

Under the Hubbard–Stratonovich transformation, the interaction becomes

$$-g(\psi_\uparrow^\dagger \psi_\downarrow^\dagger \psi_\downarrow \psi_\uparrow) \to \bar{\Delta}\psi_\downarrow \psi_\uparrow + \psi_\uparrow^\dagger \psi_\downarrow^\dagger \Delta + \frac{\bar{\Delta}\Delta}{g}, \quad (14.224)$$

where the gap function $\Delta(x)$ can acquire spatial dependence. The transformed Hamiltonian is then

$$H = \int d^3x \left[\psi_\sigma^\dagger \left(\frac{1}{2m} (-i\hbar\nabla - e\vec{A})^2 - \mu \right) \psi_\sigma + \bar{\Delta}\psi_\downarrow \psi_\uparrow + \psi_\uparrow^\dagger \psi_\downarrow^\dagger \Delta + \frac{\bar{\Delta}\Delta}{g} \right], \quad (14.225)$$

where, at the mean-field saddle point, $\Delta(x) = -g\langle \psi_\downarrow(x)\psi_\uparrow(x)\rangle$. The curious thing is that, once the interaction is factorized in this way, we must take account of the transformation of the charged condensate field under the gauge transformation.

14.8.1 Implications of gauge invariance

The kinetic energy part of the Hamiltonian is invariant under the gauge transformations:

$$\begin{aligned} \psi_\sigma(x) &\to e^{i\alpha(x)}\psi_\sigma(x) \\ \vec{A}(x) &\to \vec{A}(x) + \frac{\hbar}{e}\vec{\nabla}\alpha(x). \end{aligned} \quad (14.226)$$

However, in order that the pairing terms remain invariant under a gauge transformation, we must also transform

$$\Delta(x) \to e^{2i\alpha(x)}\Delta(x), \quad (14.227)$$

reflecting the fact that the pair condensate carries charge $2e$. The free energy of the condensate must therefore be invariant under the combined transformations (14.226) and (14.227). If we write the gap as an amplitude and phase term, $\Delta(x) = |\Delta(x)|e^{i\phi(x)}$, we see that under a gauge transformation the phase of the gap picks up twice the shift of a single electron field:

$$\phi(x) \to \phi(x) + 2\alpha(x). \quad (14.228)$$

Now if the phase becomes *rigid* beneath T_c, so that there is an energetic cost to bending the phase, then the free energy must contain a phase-stiffness term

$$\mathcal{F} \sim \frac{\rho_s}{2} \int_x (\nabla\phi)^2 . \quad (14.229)$$

We've seen such terms in the Ginzburg–Landau theory of a neutral superfluid, but now they must appear when we expand the total energy in powers of the gradient of the order parameter. However, in a charged superfluid such a coupling term is not gauge-invariant under the combined transformation $\phi \to \phi + 2\alpha$, $\vec{A} \to \vec{A} + \frac{\hbar}{e}\vec{\nabla}\alpha(x)$. Indeed, gauge invariance of the free energy under these two transformations requires that the gradient of the phase and the vector potential can only appear as the gauge-invariant combination $\vec{\nabla}\phi - \frac{2e}{\hbar}\vec{A}$, so the phase stiffness term must take the form

$$\mathcal{F} = \frac{\rho_s}{2}\int_x \left(\vec{\nabla}\phi(x) - \frac{2e}{\hbar}\vec{A}(x)\right)^2 = \frac{Q}{2}\int_x \left(\vec{A}(x) - \frac{\hbar}{2e}\vec{\nabla}\phi(x)\right)^2, \tag{14.230}$$

where we have substituted[8]

$$Q = \frac{(2e)^2}{\hbar^2}\rho_s. \tag{14.233}$$

If we now look back at (14.230), we see that the electric current carried by the condensate is

$$\vec{j}(x) = -\frac{\delta\mathcal{F}}{\delta\vec{A}(x)} = -Q\left(\vec{A}(x) - \frac{\hbar}{2e}\vec{\nabla}\phi(x)\right), \tag{14.234}$$

so we can identify Q with the *London kernel* in Chapter 10 in the study of electron transport, except that in a superconductor Q is finite in the DC limit.

Imagine a superconductor of length L in which the phase of the order parameter is twisted, so that $\Delta(L) = e^{i\Delta\phi}\Delta(0)$. Let us consider a uniform twist, so that

$$\Delta(x) = e^{i\vec{a}\cdot\vec{x}}\Delta_0, \tag{14.235}$$

where $\vec{a} = \frac{\Delta\phi}{L}\hat{x}$. Now this twist of the order parameter can be removed by a gauge transformation

$$\begin{aligned} \Delta(x) &\to e^{-i\vec{a}\cdot\vec{x}}\Delta(x) = \Delta_0 \\ \vec{A} &\to \vec{A} - \frac{\hbar}{2e}\vec{a}, \end{aligned} \tag{14.236}$$

so a twist in the order parameter is gauge-equivalent to a uniform vector potential $\vec{A} \equiv -\frac{\hbar}{2e}\vec{a} = -\frac{\hbar}{2e}\vec{\nabla}\phi$. We might have guessed this by noting that the combination $\vec{A} - \frac{\hbar}{2e}\vec{\nabla}\phi$ in the supercurrent formula (14.234) has to be the same in all gauges because it represents a physical quantity: it is gauge-invariant. This means that the effective (gauge-invariant) twist between the two ends of a superconductor is given by

$$\text{effective twist} = \overbrace{\Delta\phi}^{\text{phase twist}} - \overbrace{\frac{2e}{\hbar}\int_0^L \vec{A}\cdot d\vec{l}}^{\text{electromagnetic twist}}. \tag{14.237}$$

[8] Notice the sheer power of this argument: by using gauge invariance, we have been able to deduce that a stiffness of the phase in a charged condensate gives rise to an electromagnetic mass term. As we discussed in Section 11.6.2, since $\mathcal{F}_{EM}$ is invariant under gauge transformations, it becomes possible to redefine the vector potential to absorb the phase of the order parameter, forming a massive field with both longitudinal and transverse components:

$$\vec{A}_H(x) = \vec{A}(x) - \frac{\hbar}{2e}\vec{\nabla}\phi(x). \tag{14.231}$$

Once the phase of the order parameter is absorbed into the electromagnetic field,

$$\mathcal{F} \sim \frac{Q}{2}\int_x \vec{A}_H(x)^2 + \mathcal{F}_{EM}[A] \tag{14.232}$$

and the vector potential has acquired a mass. This is the Anderson–Higgs mechanism, whereby a gauge field “eats” the phase of a condensate, losing manifest gauge invariance by acquiring a mass [18, 23, 24].

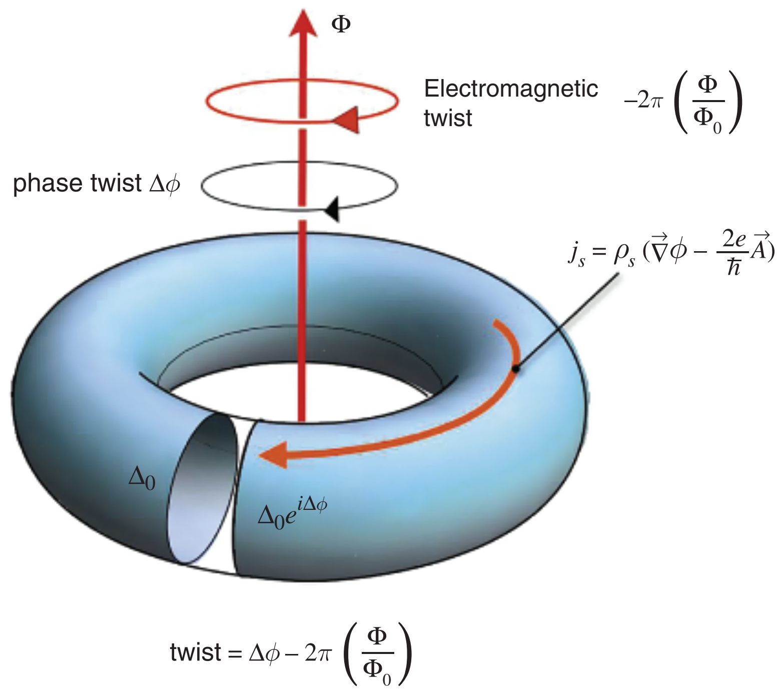


Fig. 14.16 Illustrating the phase-twist in the superconducting order parameter induced by a magnetic flux.

Each of the terms on the right is gauge-dependent, but their sum is a physical quantity. From a computational point of view, it means we can evaluate the phase stiffness without actually changing the phase of the order parameter, by calculating the change in the condensate energy due to an external field of magnitude $\vec{A} = -\frac{\hbar}{2e}\vec{\nabla}\phi$.

This reasoning has interesting consequences when we connect up the two ends of a superconductor to form a torus. Now we can induce an electromagnetic twist by passing a magnetic flux Φ through the torus (see Figure 14.16), inducing a circulating vector potential around the torus such that $\oint \vec{A}\cdot d\vec{l} = \Phi$. The supercurrent and the energy of the condensate will depend on the effective twist,

$$\text{effective twist} = \Delta\phi - \frac{2e}{\hbar}\oint \vec{A}\cdot d\vec{l} = \Delta\phi - \frac{2e}{\hbar}\Phi, \tag{14.238}$$

where Φ is the magnetic flux threading the torus. Whereas the phase change $\Delta\phi$ along a superconducting strip is not gauge-invariant, the phase change around a torus is a topological invariant which must be a multiple of 2π, $\Delta\phi = 2\pi n$, and it is gauge-invariant. The supercurrent around the torus and the total energy of the condensate thus depend on the quantity

$$\Delta\phi - \frac{2e}{\hbar}\Phi = 2\pi\left(n - \frac{\Phi}{\Phi_0}\right), \tag{14.239}$$

where

$$\Phi_0 = \frac{h}{2e} \equiv \frac{2\pi\hbar}{2e} \tag{14.240}$$

is the superconducting flux quantum. In this situation, the supercurrent and the energy are minimized when the flux is quantized as a multiple of Φ_0, $\Phi = n\Phi_0$.

14.8.2 Calculating the phase stiffness

Let us now continue to calculate the phase stiffness or *superfluid density* of a BCS superconductor using the reasoning of the previous section, by applying an equivalent vector potential $\vec{A} = -\frac{\hbar}{2e}\vec{\nabla}\phi$. Such a field changes the dispersion according to $\epsilon_{\vec{k}} \to \epsilon_{\vec{k}-e\vec{A}}$, so, inside $h_{\mathbf{k}}$,

$$\begin{aligned}\epsilon_{\vec{k}}\tau_3 &= \begin{pmatrix}\epsilon_{\vec{k}} & \\ & -\epsilon_{-\vec{k}}\end{pmatrix} \to \begin{pmatrix}\epsilon_{\vec{k}-e\vec{A}} & \\ & -\epsilon_{-\vec{k}-e\vec{A}}\end{pmatrix}\\ &= \begin{pmatrix}\epsilon_{\vec{k}-e\vec{A}} & \\ & -\epsilon_{\vec{k}+e\vec{A}}\end{pmatrix} \equiv \epsilon_{\vec{k}-e\vec{A}\tau_3}\tau_3,\end{aligned} \tag{14.241}$$

i.e.

$$\underline{h}_{\vec{k}} \to \underline{h}_{\vec{k}-e\vec{A}\tau_3} = \epsilon_{\vec{k}-e\vec{A}\tau_3}\tau_3 + \Delta\tau_1. \tag{14.242}$$

The free energy in a field is then

$$F = -T\sum_{\mathbf{k},i\omega_n} \mathrm{Tr}\ln[\epsilon_{\vec{k}-e\vec{A}\tau_3}\tau_3 + \Delta\tau_1 - i\omega_n] + \frac{\Delta^2}{g}. \tag{14.243}$$

We need to calculate

$$Q_{ab} = -\frac{1}{V}\frac{\partial^2 F}{\partial A_a \partial A_b}. \tag{14.244}$$

Taking the first derivative with respect to the vector potential gives us the steady-state diamagnetic current:

$$-\langle J_a\rangle = \frac{1}{V}\frac{\partial F}{\partial A_a} = -\frac{1}{\beta V}\sum_{k\equiv(\mathbf{k},i\omega_n)} \mathrm{Tr}\left[e\nabla_a\epsilon_{\vec{k}-e\vec{A}\tau_3}\, G(k-eA\tau_3)\right], \tag{14.245}$$

where $G(k-eA\tau_3) = [i\omega_n - h_{\vec{k}-e\vec{A}\tau_3}]^{-1} = [i\omega_n - \epsilon_{\vec{k}-e\vec{A}\tau_3}\tau_3 - \Delta\tau_1]^{-1}$.

Taking one more derivative,

$$Q_{ab} = \frac{1}{V}\left.\frac{\partial^2 F}{\partial A_a \partial A_b}\right|_{A=0} = \frac{e^2}{\beta V}\sum_k \left(\overbrace{\left(\nabla^2_{ab}\epsilon_{\vec{k}}\right)\mathrm{Tr}\left[\tau_3 G(k)\right]}^{\text{diamagnetic part}} + \overbrace{\left(\nabla_a\epsilon_{\vec{k}}\nabla_b\epsilon_{\vec{k}}\right)\mathrm{Tr}\left[G(k)G(k)\right]}^{\text{paramagnetic part}}\right). \tag{14.246}$$

Here we have used the fact that $\delta(GG^{-1}) = \delta GG^{-1} + G\delta G^{-1} = 0$ to derive $\delta G = -G\delta G^{-1}G$, which then led to the result $\frac{\partial}{\partial A_b}G(k-eA\tau_3) = -G(k-eA\tau_3)e\nabla_b\epsilon_{\vec{k}-e\vec{A}\tau_3}G(k-eA\tau_3)$, in which we then set $A = 0$. We may identify the above expression as a sum of the diamagnetic and paramagnetic parts of the superfluid stiffness. The first is associated with the instantaneous diamagnetic response of the wavefunction; the second is the retarded paramagnetic correction to the current that occurs as a result of the relaxation of the wavefunction. The diamagnetic part of the response can be integrated by parts, to give

$$\frac{e^2}{\beta V}\sum_{\mathbf{k},n}\left(\nabla^2_{ab}\epsilon_{\vec{k}}\right)\mathrm{Tr}\left[\tau_3 G(k)\right] = -\frac{e^2}{\beta V}\sum_{\mathbf{k},n}\nabla_a\epsilon_{\vec{k}}\mathrm{Tr}\left[\tau_3\nabla_b G(k)\right]$$
$$= -\frac{e^2}{\beta V}\sum_{\mathbf{k},n}\left(\nabla_a\epsilon_{\vec{k}}\nabla_b\epsilon_{\vec{k}}\right)\mathrm{Tr}\left[\tau_3 G(k)\tau_3 G(k)\right], \quad (14.247)$$

where we have used $\nabla_b G = -G\nabla_b G^{-1}G = G\nabla_b\epsilon_k\tau_3 G$ to derive the last line. Notice how this term is identical to the paramagnetic term, apart from the τ_3 insertions. We now add these two terms, to obtain

$$Q_{ab} = -\frac{e^2}{\beta V}\sum_k \nabla_a\epsilon_{\vec{k}}\nabla_b\epsilon_{\vec{k}}\left(\overbrace{\mathrm{Tr}\left[\tau_3 G(k)\tau_3 G(k)\right]}^{\text{diamagnetic part}} - \overbrace{\mathrm{Tr}\left[G(k)G(k)\right]}^{\text{paramagnetic part}}\right). \quad (14.248)$$

Notice that, when pairing is absent, the τ_3 commute with $\mathcal{G}(k)$, and the diamagnetic and paramagnetic contributions exactly cancel. We can make this explicit by writing

$$Q_{ab} = -\frac{e^2}{2\beta V}\sum_k \nabla_a\epsilon_{\vec{k}}\nabla_b\epsilon_{\vec{k}}\mathrm{Tr}\left[\left[\tau_3, G(k)\right]^2\right]. \quad (14.249)$$

Now

$$[\tau_3, G(k)] = 2i\frac{\Delta\tau_2}{(i\omega_n)^2 - E^2_{\mathbf{k}}}, \quad (14.250)$$

so

$$-\mathrm{Tr}\left[[\tau_3, G(k)]^2\right] = 8\frac{\Delta^2}{[\omega_n^2 + \epsilon^2_{\mathbf{k}} + \Delta^2]^2}, \quad (14.251)$$

so that

$$Q_{ab} = \frac{4e^2}{\beta V}\sum_k \nabla_a\epsilon_{\vec{k}}\nabla_b\epsilon_{\vec{k}}\frac{\Delta^2}{[(\omega_n)^2 + \epsilon^2_{\mathbf{k}} + \Delta^2]^2}. \quad (14.252)$$

Remarkably, although the diamagnetic and paramagnetic parts of the superfluid stiffness involve electrons far away from the Fermi surface, the difference between the two is dominated by terms where $\omega_n^2 + \epsilon^2_{\mathbf{k}} \sim \Delta^2$, i.e. by electrons near the Fermi surface. This enables us to replace the summation over $\mathbf{k}$ by an integral over energy:

$$\frac{4}{V}\sum_{\mathbf{k}}\nabla_a\epsilon_{\vec{k}}\nabla_b\epsilon_{\vec{k}}\{\ldots\} = 2N(0)\int_{-\infty}^{\infty}d\epsilon\int\overbrace{\frac{d\Omega_{\hat{\mathbf{k}}}}{4\pi}\mathrm{v}_a\mathrm{v}_b}^{\frac{1}{3}\mathrm{v}_F^2\delta_{ab}}\{\ldots\} = \frac{2\delta_{ab}}{3}N(0)\mathrm{v}_F^2\int_{-\infty}^{\infty}d\epsilon\,\{\ldots\}. \quad (14.253)$$

Note that a factor of 2 is absorbed into the total density of states of up and down electrons. We have taken advantage of the rapid convergence of the integrand to extend the limits of the integral over energy to infinity. Replacing $\frac{1}{3}N(0)\mathrm{v}_F^2 = \frac{n}{m}$, we can now write $Q_{ab} = Q\delta_{ab}$, where

$$Q(T) = \frac{ne^2}{m}T\sum_n\int_{-\infty}^{\infty}d\epsilon\frac{2\Delta^2}{(\epsilon^2 + \omega_n^2 + \Delta^2)^2} = \left(\frac{ne^2}{m}\right)\pi T\sum_n\frac{\Delta^2}{(\omega_n^2 + \Delta^2)^{\frac{3}{2}}}. \quad (14.254)$$

To evaluate this expression, it is useful to note that the argument of the summation is a total derivative, so that

$$Q(T) = \left(\frac{ne^2}{m}\right) \pi T \sum_n \frac{\partial}{\partial \omega_n} \left(\frac{\omega_n}{(\omega_n^2 + \Delta^2)^{1/2}}\right). \tag{14.255}$$

Now at absolute zero we can replace $T\sum_n \to \int \frac{d\omega}{2\pi}$, so that

$$Q(0) \equiv Q_0 = \left(\frac{ne^2}{m}\right) \overbrace{\int_{-\infty}^{\infty} \frac{d\omega}{2} \frac{d}{\partial\omega} \left(\frac{\omega}{(\omega^2 + \Delta^2)^{1/2}}\right)}^{=1} = \left(\frac{ne^2}{m}\right). \tag{14.256}$$

In other words, *all* of the electrons have condensed to form a perfect diamagnet. This is a rather remarkable result, for the pairing only extends within a narrow shell around the Fermi surface and one might have thought that only a tiny fraction T_c/ϵ_F of the Fermi sea would contribute to the stiffness, i.e. that $Q \sim O(T_c/\epsilon_F) \times ne^2/m << ne^2/m$, but this is *not* the case. The fact that all the electrons contribute to the superfluid stiffness means the wavefunction is completely rigid, so that no paramagnetic current develops at absolute zero in response to an applied vector potential.

At a finite temperature this is no longer the case, due to the presence of excited quasiparticles. To evaluate the stiffness at a finite temperature, we rewrite the Matsubara sum as a clockwise contour integral around the poles of the Fermi function:

$$Q(T) = \pi Q_0 \oint_{\text{Im axis}} \frac{dz}{2\pi i} f(z) \frac{d}{dz} \left(\frac{z}{\sqrt{\Delta^2 - z^2}}\right). \tag{14.257}$$

By deforming the integral to run counterclockwise around the branch cuts along the real axis and then integrating by parts, we obtain

$$\begin{aligned}
Q(T) &= Q_0 \pi \oint_{\text{real axis}} \frac{dz}{2\pi i} f(z) \frac{d}{dz} \left(\frac{z}{\sqrt{\Delta^2 - z^2}}\right) \\
&= Q_0 \int_{-\infty}^{\infty} d\omega f(\omega) \frac{d}{d\omega} \,\mathrm{Im} \left(\frac{z}{\sqrt{\Delta^2 - z^2}}\right)_{z=\omega - i\delta} \\
&= Q_0 \left[f(\omega) \mathrm{Im} \left(\frac{z}{\sqrt{\Delta^2 - z^2}}\right)_{z=\omega - i\delta} \right]_{-\infty}^{\infty} \\
&\quad + Q_0 \int_{-\infty}^{\infty} d\omega \left(-\frac{df(\omega)}{d\omega}\right) \mathrm{Im} \left(\frac{z}{\sqrt{\Delta^2 - z^2}}\right)_{z=\omega - i\delta}.
\end{aligned} \tag{14.258}$$

Now a careful calculation of the imaginary part of the integrand gives

$$\begin{aligned}
\mathrm{Im}\left(\frac{\omega}{\sqrt{\Delta^2 - (\omega - i\delta)^2}}\right) &= \mathrm{Im}\left(\frac{\omega}{\sqrt{-(\omega^2 - \Delta^2) + i\delta\, \mathrm{sgn}(\omega)}}\right) \\
&= \left(-\frac{|\omega|}{\sqrt{\omega^2 - \Delta^2}}\right) \theta(\omega^2 - \Delta^2),
\end{aligned} \tag{14.259}$$

so the finite-temperature stiffness can then be written

$$Q(T) = Q_0\left[1 - 2\int_{\Delta(T)}^{\infty} d\omega \left(-\frac{df(\omega)}{d\omega}\right)\left(\frac{\omega}{\sqrt{\omega^2-\Delta^2}}\right)\right], \tag{14.260}$$

where the factor of 2 derives from folding over the contribution from the negative region of the integral. The second term in this expression is nothing more than the thermal average of the quasiparticle density of states $N_{qp}(E) = N(0)\frac{E}{\sqrt{E^2-\Delta^2}}$. This term, with its factor of 2, can thus be interpreted as the reduction in the condensate fraction by a thermal depopulation of the condensate into quasiparticles. We can alternatively rewrite this expression as a formula for the temperature-dependent penetration depth:

$$\frac{1}{\lambda_L^2(T)} = \frac{1}{\lambda_L^2(0)}\left[1 - \overline{\left(\frac{A(E)}{N(0)}\right)}\right], \tag{14.261}$$

where $1/\lambda_L^2(0) = \mu_0 ne^2/m$ and $A(E)$ is the tunneling density of states given in (14.186), thermally averaged over both positive and negative energies.

Exercises

Exercise 14.1 Show, using the Cooper wavefunction, that the mean-squared radius of a Cooper pair is given by

$$\xi^2 = \frac{\int d^3r\, r^2|\phi(\mathbf{r})|^2}{\int d^3r\, |\phi(\mathbf{r})|^2} = \frac{4}{3}\left(\frac{v_F}{E}\right)^3.$$

Exercise 14.2 Generalize the Cooper pair calculation to higher angular momenta. Consider an interaction that has an attractive component in a higher angular momentum channel, such as

$$N(0)V_{\mathbf{k},\mathbf{k}'} = \begin{cases} -g_l(2l+1)P_l(\hat{\mathbf{k}}\cdot\hat{\mathbf{k}}') & (|\epsilon_{\mathbf{k}}|, |\epsilon'_{\mathbf{k}}| < \omega_0) \\ 0 & \text{(otherwise)}, \end{cases} \tag{14.262}$$

where you may assume l is even.

(a) By decomposing the Legendre polynomial in terms of spherical harmonics, $(2l+1)P_l(\hat{\mathbf{k}}, \hat{\mathbf{k}}') = 4\pi\sum_m Y_{lm}(\mathbf{k})Y^*_{lm}(\hat{\mathbf{k}})$, show that this interaction gives rise to bound Cooper pairs with a finite angular momentum given by

$$|\psi_P\rangle = \sum_{\mathbf{k}} \phi_{\mathbf{k}m} Y_{lm}(\hat{\mathbf{k}}) c^\dagger_{\mathbf{k}\uparrow} c^\dagger_{-\mathbf{k}\downarrow}|0\rangle,$$

with a bound-state energy given by

$$E = -2\omega_0 \exp\left[-\frac{2}{g_l N(0)}\right].$$

(b) A general interaction will have several harmonics,

$$V_{\mathbf{k},\mathbf{k}'} = \frac{1}{V}\sum_l g_l(2l+1)P_l(\hat{\mathbf{k}}\cdot\hat{\mathbf{k}}'),$$

not all of them attractive. In which channel(s) will the pairs tend to condense?

(c) Why can't you use this derivation for the case when l is odd?

Exercise 14.3 Generalize the BCS solution to the case where the gap has a finite phase $\Delta = |\Delta|e^{i\phi}$. Show that, in this case, the eigenvectors of the BCS mean-field Hamiltonian are

$$u_{\mathbf{k}} = e^{i\phi/2}\left(\frac{1}{2}+\frac{\epsilon_{\mathbf{k}}}{2E_{\mathbf{k}}}\right)^{\frac{1}{2}}$$

$$\mathrm{v}_{\mathbf{k}} = e^{-i\phi/2}\left(\frac{1}{2}-\frac{\epsilon_{\mathbf{k}}}{2E_{\mathbf{k}}}\right)^{\frac{1}{2}}, \tag{14.263}$$

while the BCS ground state is given by

$$|BCS(\phi)\rangle = \prod_{\mathbf{k}}(u^*_{\mathbf{k}} + \mathrm{v}^*_{\mathbf{k}}c^\dagger_{-\mathbf{k}\downarrow}c^\dagger_{\mathbf{k}\uparrow})|0\rangle. \tag{14.264}$$

Exercise 14.4 Explicit calculation of the free energy.

(a) Assuming that the Debye frequency is a small fraction of the bandwidth, show that the difference between the superconducting and normal-state free energies can be written as the integral

$$\mathcal{F}_S - \mathcal{F}_N = -2TN(0)\int_{-\omega_D}^{\omega_D} d\epsilon \ln\left[\frac{\cosh\left(\frac{\sqrt{\epsilon^2+|\Delta|^2}}{2T}\right)}{\cosh\left(\frac{\epsilon}{2T}\right)}\right] + V\frac{|\Delta|^2}{g_0}.$$

Why is this free energy invariant under changes in the phase of the gap parameter, $\Delta \to \Delta e^{i\phi}$?

(b) By differentiating the above expression with respect to Δ, confirm the zero-temperature gap equation,

$$\frac{V}{gN(0)} = \int_0^{\omega_D}\frac{d\epsilon}{\sqrt{\epsilon^2+\Delta_0^2}},$$

where $\Delta_0 = \Delta(T=0)$ is the zero-temperature gap, and use this result to eliminate g_0, to show that the free energy can be written

$$\mathcal{F}_S - \mathcal{F}_N = N(0)\Delta_0^2\,\Phi\left[\frac{\Delta}{\Delta_0},\frac{T}{\Delta_0}\right],$$

where the dimensionless function

$$\Phi(\delta,t) = \int_0^\infty dx\left\{-4t\ln\left[\frac{\cosh\left(\frac{\sqrt{x^2+\delta^2}}{2t}\right)}{\cosh\left(\frac{x}{2t}\right)}\right] + \frac{\delta^2}{\sqrt{x^2+1}}\right\}.$$