14 Superconductivity and BCS theory

14.1 Introduction: early history

Superconductivity, the phenomenon whereby the resistance of a metal spontaneously drops to zero upon cooling below its critical temperature, was discovered over a hundred years ago by Heike Kamerlingh Onnes in 1911. However, it took another 46 years for the development of the conceptual framework required to understand this collective phenomenon as a condensation of electron pairs. During this time, many great physicists, including Bohr, Einstein, Heisenberg, Bardeen, and Feynman, had tried to develop a microscopic theory of the phenomenon. Today, superconductivity has been observed in a wide variety of materials (see Table 14.1), with transition temperatures reaching up as high as high as 134 K.

The development of the theory of superconductivity leading to BCS theory really had two parts – one phenomenological, the second microscopic. Let me mention some highlights:

- The discovery of the Meissner effect in 1933 by Walther Meissner and Robert Ochsenfeld [1]. When a metal is cooled in a small magnetic field, the flux is spontaneously excluded as the metal becomes superconducting (see Figure 14.1). The Meissner effect demonstrates that a superconductor is, in essence, a perfect diamagnet.
- Rigidity of the wavefunction. In 1937 Fritz London, working at Oxford [2, 3], proposed that a persistent supercurrent is a property of the *ground state* associated with its *rigidity* against the application of a field. London's idea applies to the full many-body wavefunction, but he initially developed it using a phenomenological one-particle wavefunction $\psi(x)$ that today we call the *superconducting order parameter*. He noted that the quantum mechanical current contains a *paramagnetic* and a *diamagnetic* component, writing

$$j = \frac{\hbar e}{2im}(\psi^* \vec{\nabla}\psi - \psi\vec{\nabla}\psi^*) - \left(\frac{e^2}{m}\right)\psi^*\psi\vec{A}. \tag{14.1}$$

  In the ground state in the absence of a field ($\vec{A} = 0$), the current vanishes, so the ground-state wavefunction ψ_0 must be uniform. Normally, the wavefunction is highly sensitive to an external magnetic field, but London reasoned that, if the wavefunction is somehow *rigid* and hence unchanged to linear order in the magnetic field, $\psi(x) = \psi_0(x) + O(B^2)$, where ψ_0 is the ground-state wavefunction, then, to leading order in a field, the current carried by the uniform quantum state is

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Table 14.1 Selected superfluids/superconductors.

Symmetry	Superfluid/superconductor	T_c	Mechanism
s	Hg	4.2 K	Phonon-mediated
	Pb	7.2 K	
	$NbGe_3$	23 K	
	MgB_2	39 K	
p	^3He	2.5 mK	Magnetic interactions
	UPt_3	0.51 K	
	Sr_2RuO_4	0.93 K	
d	$CeCu_2Si_2$	0.65 K	
	$PuCoGa_7$	18.5 K	
	$HgBa_2Ca_2Cu_3O_8$	134 K	
$s^{\pm}$	$Sr_{0.5}Sm_{0.5}FeAsF$	56 K	

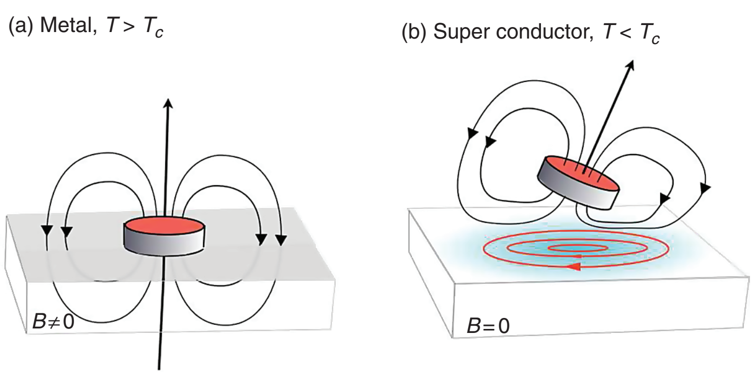

Fig. 14.1 (a) A magnet rests on top of a normal metal, with its field lines penetrating the metal. (b) Once cooled below T_c, the superconductor spontaneously excludes magnetic fields, generating persistent supercurrents at its surface, causing the magnet to levitate.

$$\vec{j} = -\frac{e^2}{m}|\psi_0|^2\vec{A} + \cdots . \tag{14.2}$$

In London's equation we see a remarkable convergence of the classical and the quantum: it is certainly a classical equation of motion in that it involves purely macroscopic variables, yet on the other hand it contains a naked vector potential $\vec{A}$ rather than the magnetic field $\vec{B} = \nabla \times \vec{A}$, a feature which reflects the broken gauge symmetry of the quantum ground state.

London's equation provides a natural explanation of the Meissner effect. To see this, we use Ampère's relation $\vec{j} = \mu_0^{-1}\nabla \times \vec{B}$ to rewrite the current in London's terms of the magnetic field:

$$\nabla \times \vec{B} = -\frac{1}{\lambda_L^2}\vec{A} \qquad \left(\frac{1}{\lambda_L^2} = \mu_0\frac{e^2}{m}|\psi_0|^2\right), \tag{14.3}$$

where the quantity λ_L defined above is the *London penetration depth*. Taking the curl of (14.3), we eliminate the vector potential to obtain

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$$\overbrace{\nabla \times \nabla \times \vec{B}}^{-\nabla^2 \vec{B}} = -\frac{1}{\lambda_L^2} \overbrace{\nabla \times \vec{A}}^{\vec{B}} \tag{14.4}$$

or

$$\nabla^2 B = \frac{1}{\lambda_L^2} \vec{B}, \tag{14.5}$$

where we have substituted $\nabla \times (\nabla \times \vec{B}) = \vec{\nabla}(\nabla \cdot \vec{B}) - \nabla^2 \vec{B} = -\nabla^2 \vec{B}$, using the divergence-free nature of the magnetic field. The solutions of this equation describe magnetic fields $B(x) \sim B_0 e^{\pm x/\lambda_L}$ which decay inside the superconductor over a London penetration depth. This exclusion of magnetic fields inside superconductors is precisely the Meissner effect.

- Ginzburg–Landau theory [4]. In 1950, Lev Landau and Vitaly Ginzburg in Moscow reinterpreted London's phenomenological wavefunction $\psi(x)$ as a *complex-order parameter*. Using arguments of gauge invariance, they reasoned that the free energy must contain a gradient term that instills the rigidity of the order parameter:

$$f = \int d^3x \frac{1}{2m^*} |(-i\hbar\vec{\nabla} - e^*\vec{A})\psi|^2. \tag{14.6}$$

(At this stage, the identification of $e^* = 2e$ as the Cooper pair charge had not been made.) The vitally important aspect of this gauge-invariant functional (see Section 11.5) is that, once $\psi \neq 0$, the electromagnetic field develops a mass, giving rise to a super-current

$$\vec{j}(x) = -\delta f/\delta \vec{A}(x) = -\frac{(e^*)^2}{m^*} |\psi_0|^2 \vec{A}(x) \tag{14.7}$$

for a uniform $\psi = \psi_0$.

Following the Second World War, physicists set to work to try to develop a microscopic theory of superconductivity. The development of quantum field theory and new experimental techniques, such as microwaves – a biproduct of radar – and the availability of isotopes after the Manhattan Project, meant that a new intellectual offensive could begin. The landmark events included:

- Theory of the electron–phonon interaction. In 1949–1950, Herbert Fröhlich at Purdue and Liverpool universities [5] formulated the electron–phonon interaction as a direct analogue of photon exchange in electromagnetism. He showed that it gives rise to a low-energy attractive interaction,

$$V_{eff}(\mathbf{k}, \mathbf{k}') = -g^2_{\mathbf{k}-\mathbf{k}'} \frac{2\omega_{\mathbf{k}-\mathbf{k}'}}{\omega^2_{\mathbf{k}-\mathbf{k}'} - (\epsilon_{\mathbf{k}} - \epsilon_{\mathbf{k}'})^2}, \tag{14.8}$$

where $\epsilon_{\mathbf{k}}$ and $\epsilon_{\mathbf{k}'}$ are the energies of incoming and outgoing electrons, while $\omega_{\mathbf{q}}$ is the phonon frequency. $V_{eff}(\mathbf{k}, \mathbf{k}')$ is attractive for low-energy transfer, $|\epsilon_{\mathbf{k}} - \epsilon_{\mathbf{k}'}| << \omega_{\mathbf{k}-\mathbf{k}'}$.
- Discovery of the isotope effect. In 1950, Emanuel Maxwell at the National Bureau of Standards [7] and the group of Bernard Serin at Rutgers University [8] observed a reduction in the superconducting transition temperature with the isotopic mass in mercury.

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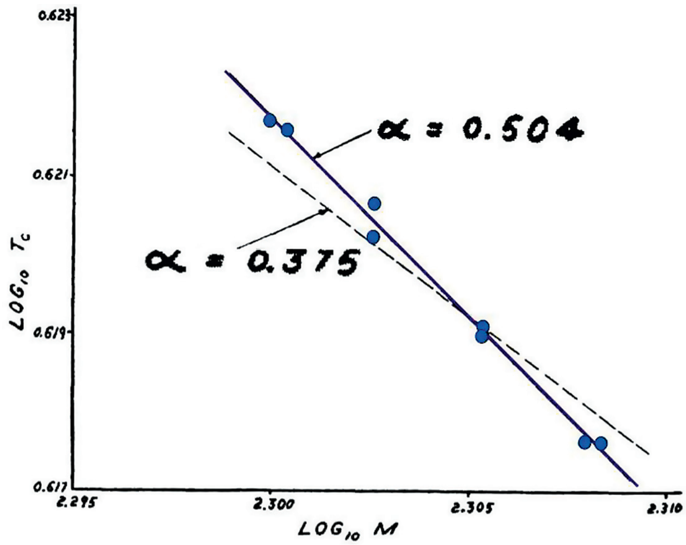

Fig. 14.2 Superconducting transition temperature as a function of isotopic mass for mercury, showing the $-\frac{1}{2}$ exponent, implying phonon-driven superconductivity. Reprinted with permission from B. Serin, *et al.*, *Phys. Rev.*, vol. 80, p. 761, 1950. Copyright 1950 by the American Physical Society.

It now became clear that the electron–phonon interaction provided the key to superconductivity. Indeed, in *any* theory in which the transition temperature is proportional to the Debye temperature, the expected dependence on isotopic mass M is given by [9]

$$T_c \propto \omega_D \sim \frac{1}{\sqrt{M}} \Rightarrow \frac{d \ln T_c}{d \ln M} = -\frac{1}{2}. \tag{14.9}$$

Careful analysis showed agreement with the $-\frac{1}{2}$ exponent [6] (see Figure 14.2), but what was the mechanism?

- Discovery of the coherence length. In 1953 Brian Pippard at the Cavendish Laboratory in Cambridge [10, 11] proposed, based on his thesis work on the anomalous skin depth in dirty superconductors, that the character of superconductivity changes at short distances, below a scale he named the *coherence length* ξ. Pippard showed that, at these short distances, the local London relation between current and vector potential is replaced by a non-local relationship. Pippard's result means that Ginzburg–Landau theory is inadequate at distances shorter than the coherence length ξ, demanding a microscopic theory.
- Gap hypothesis. In 1955 John Bardeen, who had recently resigned from Bell Laboratories to pursue his research into the theory of superconductivity at the University of Illinois Urbana-Champaign, proposed that if a gap Δ developed in the electron spectrum this would account for the wavefunction rigidity proposed by London and would also give rise to Pippard's coherence length $\xi \sim v_F/\Delta$, where v_F is the Fermi velocity [12]. What was now needed was a model and mechanism to create the gap.
- Bardeen–Pines Hamiltonian. In 1955 John Bardeen and David Pines at the University of Illinois Urbana-Champaign [13] rederived the Fröhlich interaction as a second-quantized

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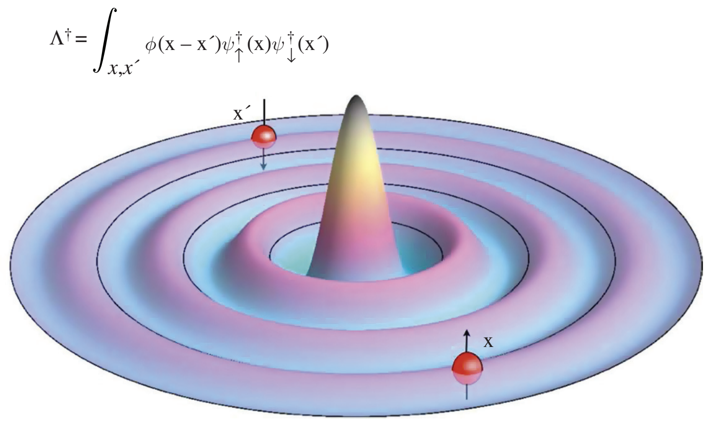

Fig. 14.3 Illustration of a Cooper pair. (Note: the location of the electrons relative to the pair wavefunction involves artistic license since the wavefunction describes the *relative* position of the two electrons.)

model, incorporating the effects of the Coulomb interaction in a "Jellium model" in which the ions form a smeared positive background (see Section 7.7.3). The Bardeen–Pines effective interaction takes the form

$$V_{BP}(\mathbf{q}, \nu) = \frac{e^2}{\epsilon_0(q^2 + \kappa^2)}\left[1 + \frac{\omega_{\mathbf{q}}^2}{\nu^2 - \omega_{\mathbf{q}}^2}\right], \tag{14.10}$$

where κ^{-1} is the Thomas–Fermi screening length and the phonon frequency $\omega_{\mathbf{q}}$ is related to the plasma frequency of the ions $\Omega_p^2 = (Ze)^2 n_{ion}/(\epsilon_0 M)$ via the relation $\omega_{\mathbf{q}} = (q/[q^2 + \kappa^2]^{1/2})\Omega_p$. The Bardeen–Pines interaction is seen to contain two terms: a frequency-independent Coulomb interaction, and a strongly frequency-dependent electron–phonon interaction. In the time domain, the former corresponds to an instantaneous Coulomb repulsion, while the latter is a highly retarded attractive interaction. This interaction became the basis for BCS theory.

The stage was set for Bardeen–Cooper–Schrieffer (BCS) theory.

14.2 The Cooper instability

In the fall of 1956, Bardeen's postdoc Leon Cooper, at the University of Illinois Urbana-Champaign, solved one of the most famous "warm-up" problems of all time. Considering two electrons moving above the Fermi surface of a metal, Cooper found that an arbitrarily weak electron–electron attraction induces a two-particle bound state that will destabilize the Fermi surface [14].

Cooper imagined adding a pair of electrons above the Fermi surface in a state with no net momentum, described by the wavefunction

$$|\Psi\rangle = \Lambda^\dagger|FS\rangle, \tag{14.11}$$

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where

$$\Lambda^{\dagger} = \int d^3x d^3x' \phi(\mathbf{x} - \mathbf{x}') \psi^{\dagger}_{\downarrow}(\mathbf{x}) \psi^{\dagger}_{\uparrow}(\mathbf{x}') \tag{14.12}$$

creates a pair of electrons, while $|FS\rangle = \prod_{k<k_F} c^{\dagger}_{\mathbf{k}\uparrow} c^{\dagger}_{-\mathbf{k}\downarrow}|0\rangle$ defines the filled sea. If we Fourier transform the fields, writing $\psi^{\dagger}_{\sigma}(\mathbf{x}) = \frac{1}{\sqrt{V}} \sum_{\mathbf{k}} c^{\dagger}_{\mathbf{k}\sigma} e^{-i\mathbf{k}\cdot\mathbf{x}}$, then the pair creation operator can be recast as a sum over pairs in momentum space:

$$\Lambda^{\dagger} = \sum_{\mathbf{k}} \phi_{\mathbf{k}} c^{\dagger}_{\mathbf{k}\downarrow} c^{\dagger}_{-\mathbf{k}\uparrow}, \tag{14.13}$$

Cooper pair creation operator

where

$$\phi_{\mathbf{k}} = \int d^3x e^{-i\mathbf{k}\cdot\mathbf{x}} \phi(\mathbf{x}) \tag{14.14}$$

is the Fourier transform of the spatial pair wavefunction. This result tells us that a real-space pair of fermions can be decomposed into a sum of momentum-space pairs, weighted by the amplitude $\phi_{\mathbf{k}}$. The properties of the pair (and the superconductor it will give rise to) are encoded in the pair wavefunction $\phi_{\mathbf{k}}$. In the phonon-mediated superconductors considered by BCS, $\phi_{\mathbf{k}} \sim f(k)$ is an isotropic s-wave function, but in a rapidly growing class of *anisotropically paired superfluids* of great current interest, including superfluid ^{3}He, heavy-fermion, and iron- and copper-based high-temperature superconductors $\phi_{\mathbf{k}}$ is anisotropic changing sign *somewhere* in momentum space to lower the repulsive interaction energy, giving rise to a *nodal pair wavefunction*.

When an electron pair is created, electrons can only be added above the Fermi surface, so that

$$|\Psi\rangle = \Lambda^{\dagger}|FS\rangle = \sum_{|\mathbf{k}|>k_F} \phi_{\mathbf{k}} |\mathbf{k}_P\rangle, \tag{14.15}$$

where $|\mathbf{k}_P\rangle \equiv |\mathbf{k}\uparrow, -\mathbf{k}\downarrow\rangle = c^{\dagger}_{\mathbf{k}\uparrow} c^{\dagger}_{-\mathbf{k}\downarrow}|FS\rangle$. Now suppose that the Hamiltonian has the form

$$H = \sum_{\mathbf{k}} \epsilon_{\mathbf{k}} c^{\dagger}_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} + \hat{V}, \tag{14.16}$$

where $\hat{V}$ contains the details of the electron–electron interaction; if $|\Psi\rangle$ is an eigenstate with energy E, then

$$H|\Psi\rangle = \sum_{|\mathbf{k}|>k_F} 2\epsilon_{\mathbf{k}} \phi_{\mathbf{k}} |\mathbf{k}_P\rangle + \sum_{|\mathbf{k}|,\ |\mathbf{k}'|>k_F} |\mathbf{k}_P\rangle \langle \mathbf{k}_P|\hat{V}|\mathbf{k}'_P\rangle \phi_{\mathbf{k}'}. \tag{14.17}$$

Identifying this with $E|\Psi\rangle = E\sum_{\mathbf{k}} \phi_{\mathbf{k}}|\mathbf{k}_P\rangle$, so comparing the amplitudes to be in the state $|\mathbf{k}_P\rangle$,

$$E\phi_{\mathbf{k}} = 2\epsilon_{\mathbf{k}}\phi_{\mathbf{k}} + \sum_{|\mathbf{k}'|>k_F} \langle \mathbf{k}_P|\hat{V}|\mathbf{k}'_P\rangle \phi_{\mathbf{k}'}. \tag{14.18}$$

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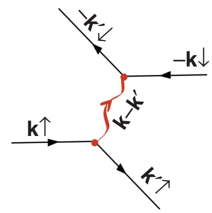

Fig. 14.4 Virtual phonon exchange process responsible for the BCS interaction. The process $|\mathbf{k}\uparrow, -\mathbf{k}\downarrow\rangle \rightarrow |\mathbf{k}'\uparrow, -\mathbf{k}'\downarrow\rangle$ can be thought of as the consequence of Bragg diffraction of a virtual standing wave: one electron in the pair $|\mathbf{k}\uparrow, -\mathbf{k}\downarrow\rangle$ diffracts from $\mathbf{k} \rightarrow \mathbf{k}'$, creating a virtual standing wave (phonon) of momentum $\mathbf{k} - \mathbf{k}'$. Later, the second diffracts from $-\mathbf{k} \rightarrow -\mathbf{k}'$, reabsorbing the virtual phonon.

The beauty of this equation is that the details of the electron interactions are entirely contained in the pair scattering matrix element $V_{\mathbf{k},\mathbf{k}'} = \langle \mathbf{k}_P|\hat{V}|\mathbf{k}'_P\rangle$. Microscopically, this scattering is produced by the exchange of virtual phonons (in conventional superconductors), and the scattering matrix element is determined by the electron–phonon propagator

$$V_{\mathbf{k},\mathbf{k}'} = g^2_{\mathbf{k}-\mathbf{k}'} D(\mathbf{k}' - \mathbf{k}, \epsilon_{\mathbf{k}} - \epsilon_{\mathbf{k}'}), \tag{14.19}$$

as illustrated in Figure 14.4. Cooper noted that this matrix element is not strongly momentum-dependent, only becoming attractive within an energy ω_D of the Fermi surface, and this motivated a simplified model interaction in which

$$V_{\mathbf{k},\mathbf{k}'} = \begin{cases} -g_0/V & (|\epsilon_{\mathbf{k}}|,\ |\epsilon_{\mathbf{k}'}| < \omega_D) \\ 0 & \text{(otherwise).} \end{cases} \tag{14.20}$$

This is a piece of pure physics *haiku*, a brilliant simplification that makes BCS theory analytically tractable. Much more is to come, but for the moment it enables us to simplify (14.18):

$$(E - 2\epsilon_{\mathbf{k}})\phi_{\mathbf{k}} = -\frac{g_0}{V} \sum_{0<\epsilon_{\mathbf{k}'}<\omega_D} \phi_{\mathbf{k}'}, \tag{14.21}$$

so that by solving for $\phi_{\mathbf{k}}$,

$$\phi_{\mathbf{k}} = -\frac{g_0/V}{E - 2\epsilon_{\mathbf{k}}} \sum_{0<\epsilon_{\mathbf{k}'}<\omega_D} \phi_{\mathbf{k}'}, \tag{14.22}$$

then summing both sides over $\mathbf{k}$ and factoring out $\sum_{\mathbf{k}} \phi_{\mathbf{k}}$, we obtain the self-consistent equation

$$1 = -\frac{1}{V} \sum_{0<\epsilon_{\mathbf{k}}<\omega_D} \frac{g_0}{E - 2\epsilon_{\mathbf{k}}}. \tag{14.23}$$

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Replacing the summation by an integral over energy, $\frac{1}{V}\sum_{0<\epsilon_{\mathbf{k}}<\omega_D} \to N(0)\int_0^{\omega_D}$, where $N(0)$ is the density of states per spin per unit volume at the Fermi energy, the resulting equation gives

$$1 = g_0 N(0)\int_0^{\omega_D}\frac{d\epsilon}{2\epsilon - E} = -\frac{1}{2}g_0 N(0)\ln\left[\frac{2\omega_D - E}{-E}\right] \approx -\frac{1}{2}g_0 N(0)\ln\left[\frac{2\omega_D}{-E}\right], \tag{14.24}$$

where, anticipating the smallness of $|E| << \omega_D$, we have approximated $2\omega_D - E \approx 2\omega_D$. In other words, the energy of the Cooper pair is given by

$$E = -2\omega_D e^{-\frac{2}{g_0 N(0)}}. \tag{14.25}$$

Remarks

- The Cooper pair is a bound state beneath the particle–hole continuum (see Figure 14.5).
- In his seminal paper, Cooper notes that the Cooper pair is a boson, an operator governed by a bosonic (commutator) algebra. (We will see shortly that it can be regarded as the transverse component of a very large isospin.) This changes everything, for, as pairs, electrons can *condense macroscopically*.
- A generalization of the above calculation to finite momentum (see Example 14.1) shows that the Cooper pair has a *linear* dispersion $E_{\mathbf{p}} - E = \mathrm{v}_F p$ (see Figure 14.5), reminiscent of a collective mode.

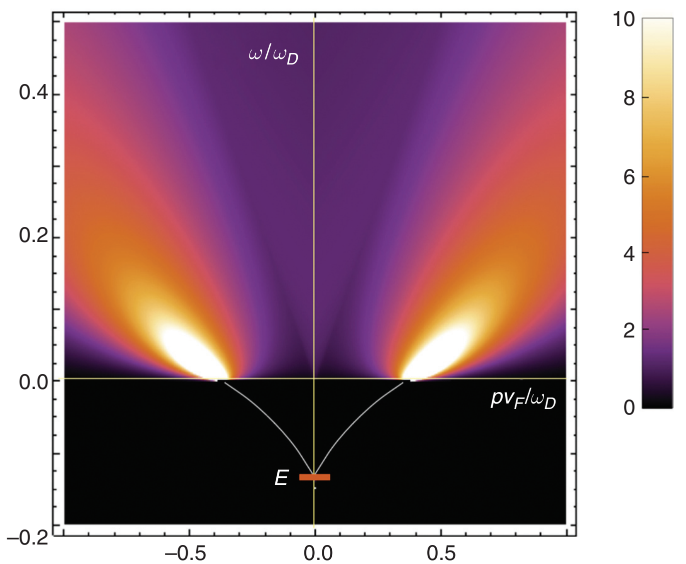

Fig. 14.5 Formation of a Cooper pair beneath the two-particle continuum. This density plot shows the density of states of pair excitations obtained from the imaginary part of the pair susceptibility $\chi''(E, \mathbf{p})$ (see Example 14.1). At a finite momentum, the Cooper pair energy defines a collective bosonic mode beneath the quasiparticle continuum with dispersion $E_{\mathbf{p}} \approx E(0) + \mathrm{v}_F|p|$.

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Example 14.1 Generalize Cooper's calculation to a pair with finite momentum. In particular:

(a) Show that the operator that creates a Cooper pair at a finite momentum $\mathbf{p}$,

$$\Lambda^\dagger(\mathbf{p}) = \int d^3x d^3x' \phi(\mathbf{x}-\mathbf{x}')\psi^\dagger_\uparrow(\mathbf{x})\psi^\dagger_\downarrow(\mathbf{x}')e^{i\mathbf{p}\cdot(\mathbf{x}+\mathbf{x}')/2}, \tag{14.26}$$

can be rewritten in the form

$$\Lambda^\dagger(\mathbf{p}) = \sum_{\mathbf{k}} \phi(\mathbf{k}) c^\dagger_{\mathbf{k}+\mathbf{p}/2\uparrow} c^\dagger_{-\mathbf{k}+\mathbf{p}/2\downarrow}. \tag{14.27}$$

(b) Show that the energy $E_{\mathbf{p}}$ of the pair state $\Lambda^\dagger(\mathbf{p})|FS\rangle$ is given by the roots $z = E_{\mathbf{p}}$ of the equation

$$1 + \frac{g_0}{V} \sum_{0<\epsilon_{\mathbf{k}\pm\mathbf{p}/2}<\omega_D} \frac{1}{z - (\epsilon_{\mathbf{k}+\mathbf{p}/2} + \epsilon_{\mathbf{k}-\mathbf{p}/2})} = 0. \tag{14.28}$$

Demonstrate that this equation predicts a linear dispersion given by

$$E_{\mathbf{p}} = -2\omega_D e^{-\frac{2}{g_0 N(0)}} + \mathrm{v}_F |p|. \tag{14.29}$$

Solution

(a) Introducing center-of-mass variables $\mathbf{X} = (\mathbf{x}+\mathbf{x}')/\mathbf{2}$ and $\mathbf{r} = \mathbf{x}-\mathbf{x}'$, using $d^3x d^3x' = d^3X d^3r$, we rewrite the Cooper pair creation operator in the form

$$\Lambda^\dagger(\mathbf{p}) = \int d^3r d^3X \, e^{i\mathbf{p}\cdot\mathbf{X}} \phi(\mathbf{r}) \, \psi^\dagger_\uparrow(\mathbf{X}+\mathbf{r}/2)\psi^\dagger_\downarrow(\mathbf{X}-\mathbf{r}/\mathbf{2}). \tag{14.30}$$

If we substitute $\psi^\dagger_\sigma(x) = \frac{1}{\sqrt{V}} \sum_{\mathbf{k}} c^\dagger_{\mathbf{k}\sigma} e^{-i\mathbf{k}\cdot\mathbf{x}}$, we then obtain

$$\begin{aligned}\Lambda^\dagger(p) &= \frac{1}{V}\int d^3r d^3X e^{i\mathbf{p}\cdot\mathbf{X}}\phi(\mathbf{r}) \sum_{\mathbf{k}_1,\mathbf{k}_2} c^\dagger_{\mathbf{k}_1\uparrow} c^\dagger_{\mathbf{k}_2\downarrow} e^{-i\mathbf{k}_1\cdot(\mathbf{X}+\mathbf{r}/2)} e^{i\mathbf{k}_2\cdot(\mathbf{X}-\mathbf{r}/2)} \\ &= \sum_{\mathbf{k}_1,\mathbf{k}_2} c^\dagger_{\mathbf{k}_1\uparrow} c^\dagger_{-\mathbf{k}_2\downarrow} \overbrace{\int d^3r \, \phi(\mathbf{r}) e^{i\mathbf{r}\cdot(\mathbf{k}_1+\mathbf{k}_2)/2}}^{\phi((\mathbf{k}_1+\mathbf{k}_2)/2)} \overbrace{\frac{1}{V}\int d^3R \, e^{i[\mathbf{p}-(\mathbf{k}_1-\mathbf{k}_2)]\cdot\mathbf{X}}}^{\delta_{\mathbf{p}-(\mathbf{k}_1-\mathbf{k}_2)}} \\ &= \sum_{\mathbf{k}} \phi(\mathbf{k}) \, c^\dagger_{\mathbf{k}+\mathbf{p}/2\uparrow} c^\dagger_{-\mathbf{k}+\mathbf{p}/2\downarrow},\end{aligned} \tag{14.31}$$

where we have replaced $(\mathbf{k}_1 + \mathbf{k}_2)/2 \to \mathbf{k}$ in the last step.

(b) Denote a Cooper pair with momentum $\mathbf{p}$ by

$$\Lambda^\dagger(\mathbf{p})|FS\rangle \equiv |\psi(\mathbf{p})\rangle = \sum_{\mathbf{k}} \phi_{\mathbf{k}} |\mathbf{k},\mathbf{p}\rangle, \tag{14.32}$$

where $|\mathbf{k},\mathbf{p}\rangle = c^\dagger_{\mathbf{k}+\mathbf{p}/2\uparrow} c^\dagger_{-\mathbf{k}+\mathbf{p}/2\downarrow}|FS\rangle$. Applying $H|\Psi(\mathbf{p})\rangle = E_{\mathbf{p}}|\Psi(\mathbf{p})\rangle$, using (14.16),

$$E_{\mathbf{p}} \sum_{\mathbf{k}} \phi_{\mathbf{k}} |\mathbf{k},\mathbf{p}\rangle = \sum_{|\mathbf{k}\pm\frac{\mathbf{p}}{2}|>k_F} (\epsilon_{\mathbf{k}+\mathbf{p}/2} + \epsilon_{\mathbf{k}-\mathbf{p}/2}) \, \phi_{\mathbf{k}} |\mathbf{k},\mathbf{p}\rangle + \sum_{|\mathbf{k}|,\,|\mathbf{k}'|>k_F} |\mathbf{k},\mathbf{p}\rangle\langle\mathbf{k},\mathbf{p}|\hat{V}|\mathbf{k}',\mathbf{p}\rangle\phi_{\mathbf{k}'}.$$

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Assume that $\langle \mathbf{k}, \mathbf{p}|\hat{V}|\mathbf{k}', \mathbf{p}\rangle \phi_{\mathbf{k}'} = -g_0/V$ is independent of $\mathbf{p}$. Comparing coefficients of $|\mathbf{k}, \mathbf{p}\rangle$,

$$E_{\mathbf{p}}\phi_{\mathbf{k}} = (\epsilon_{\mathbf{k}+\mathbf{p}/2} - \epsilon_{\mathbf{k}-\mathbf{p}/2})\,\phi_{\mathbf{k}} - \frac{g_0}{V} \sum_{0<\epsilon_{\mathbf{k}'\pm\mathbf{p}/2}<\omega_D} \phi_{\mathbf{k}'}. \tag{14.33}$$

Solving for $\phi_{\mathbf{k}}$,

$$\phi_{\mathbf{k}} = \frac{g_0/V}{\epsilon_{\mathbf{k}+\mathbf{p}/2} + \epsilon_{\mathbf{k}-\mathbf{p}/2} - E_{\mathbf{p}}} \sum_{0<\epsilon_{\mathbf{k}'\pm\mathbf{p}/2}<\omega_D} \phi_{\mathbf{k}'}. \tag{14.34}$$

Summing both sides over momentum $\mathbf{k}$ and removing the common factor $\sum_{\mathbf{k}} \phi_{\mathbf{k}}$, we then obtain

$$1 - \frac{g_0}{V} \sum_{0<\epsilon_{\mathbf{k}\pm\mathbf{p}/2}<\omega_D} \frac{1}{\epsilon_{\mathbf{k}+\mathbf{p}/2} + \epsilon_{\mathbf{k}-\mathbf{p}/2} - E_{\mathbf{p}}} = 0. \tag{14.35}$$

It is convenient to cast this as the zero of the function $\mathcal{G}^{-1}[E_{\mathbf{p}}, \mathbf{p}] = 0$, where

$$\mathcal{G}^{-1}[z, \mathbf{p}] = 1 - g_0\chi_0(z, \mathbf{p}), \tag{14.36}$$

and

$$\chi_0(z, \mathbf{p}) = \frac{1}{V} \sum_{0<\epsilon_{\mathbf{k}\pm\mathbf{p}/2}<\omega_D} \frac{1}{\epsilon_{\mathbf{k}+\mathbf{p}/2} + \epsilon_{\mathbf{k}-\mathbf{p}/2} - z} \tag{14.37}$$

can be interpreted as the bare pair susceptibility of the conduction sea. Now, taking $\epsilon_{\mathbf{k}} = k^2/2m - \mu$ in the momentum summation, we must impose the condition

$$\epsilon_{\mathbf{k}\pm\mathbf{p}/2} = \epsilon_{\mathbf{k}} \pm \frac{\mathbf{p} \cdot \mathbf{v_F}}{2} + \frac{p^2}{8m} > 0, \tag{14.38}$$

or $\epsilon_k > \frac{pv_F}{2}|\cos\theta| - \frac{p^2}{8m}$. Replacing the momentum summation by an integral over energy and angles,

$$\begin{aligned}
\chi_0[z, p] &= \frac{N(0)}{2} \int_{-1}^{1} \frac{d\cos\theta}{2} \int_{\frac{pv_F}{2}|\cos\theta| - p^2/8m}^{\omega_D} \frac{d\epsilon}{2\epsilon + p^2/4m - z} \\
&= \frac{N(0)}{2} \int_0^1 d\cos\theta \ln\left[\frac{2\omega_D}{pv_F\cos\theta - z}\right].
\end{aligned} \tag{14.39}$$

Finally, carrying out the integral over θ, one obtains

$$\chi_0(z, p) = \frac{N(0)}{2} \tilde{\chi}_0\left[\frac{z}{2\omega_D}, \frac{pv_F}{2\omega_D}\right], \tag{14.40}$$

where

$$\tilde{\chi}_0[\tilde{z}, \tilde{p}] = \ln\left(\frac{1}{\tilde{p} - \tilde{z}}\right) + \left[1 + \frac{\tilde{z}}{\tilde{p}} \ln\left(1 - \frac{\tilde{p}}{\tilde{z}}\right)\right]. \tag{14.41}$$

Thus for small $v_F p << |E|$, using (14.36),

$$\mathcal{G}^{-1}[E, p] = 1 - \frac{g_0 N(0)}{2} \ln\left[\frac{2\omega_D}{v_F p - E}\right], \tag{14.42}$$

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so the bound-state pole occurs at $\mathcal{G}^{-1}(E_{\mathbf{p}}, \mathbf{p}) = 0$ or

$$E_{\mathbf{p}} = -2\omega_D \exp\left[-\frac{2}{g_0 N(0)}\right] + v_F p. \tag{14.43}$$

The linear spectrum is a signature of a collective bosonic mode. Incidentally, the quantity

$$\chi''(E, \mathbf{p}) = \mathrm{Im}[\chi_0(z, \mathbf{p})/(1 - g_0\chi_0(z, \mathbf{p}))]|_{z=E-i\delta} \tag{14.44}$$

can be interpreted as a spectral function giving the density of Cooper pairs above and below the particle–particle continuum. It is this quantity that is plotted in Figure 14.5.

14.3 The BCS Hamiltonian

After Cooper's discovery, it took a further six months of intense exploration of candidate wavefunctions before Bardeen, Cooper and Schrieffer succeeded in formulating the theory of superconductivity in terms of a *pair condensate* [15]. It was the graduate student in the team, J. Robert Schrieffer, who took the next leap.[1] Schrieffer's insight was to identify the superconducting ground state as a coherent state of the Cooper pair operator:

$$|\psi_{BCS}\rangle = \exp[\Lambda^\dagger]|0\rangle, \tag{14.45}$$

where $|0\rangle$ is the electron vacuum and $\Lambda^\dagger = \sum_{\mathbf{k}} \phi_{\mathbf{k}} c^\dagger_{\mathbf{k}\uparrow} c^\dagger_{-\mathbf{k}\downarrow}$ is the Cooper pair creation operator (14.13). If we expand the exponential as a product in momentum space,

$$|\psi_{BCS}\rangle = \prod_{\mathbf{k}} \exp[\phi_{\mathbf{k}} c^\dagger_{\mathbf{k}\uparrow} c^\dagger_{-\mathbf{k}\downarrow}]|0\rangle = \prod_{\mathbf{k}} (1 + \phi_{\mathbf{k}} c^\dagger_{\mathbf{k}\uparrow} c^\dagger_{-\mathbf{k}\downarrow})|0\rangle. \tag{14.46}$$

BCS wavefunction

In the second step, we have truncated the exponential to linear order because all higher powers of the pair operator vanish: $(c^\dagger_{\mathbf{k}\uparrow} c^\dagger_{-\mathbf{k}\downarrow})^n = 0\ (n > 1)$. This remarkable coherent state mixes states of different particle number, giving rise to a state of off-diagonal long-range order in which

$$\langle\psi_{BCS}|c_{-\mathbf{k}\downarrow} c_{\mathbf{k}\uparrow}|\psi_{BCS}\rangle \propto \phi_{\mathbf{k}}. \tag{14.47}$$

[1] Following a conference at the Stevens Institute of Technology on the many–body problem, inspired by a wavefunction that Tomonaga had derived, Schrieffer wrote down a candidate wavefunction for the ground-state superconductivity. He recalls the event in his own words [16]:

> So I guess it was on the subway, I scribbled down the wave function and I calculated the beginning of that expectation value and I realized that the algebra was very simple. I think it was somehow in the afternoon and that night at this friend's house I worked on it. And the next morning, as I recall, I did the variational calculation to get the gap equation and I solved the gap equation for the cutoff potential.

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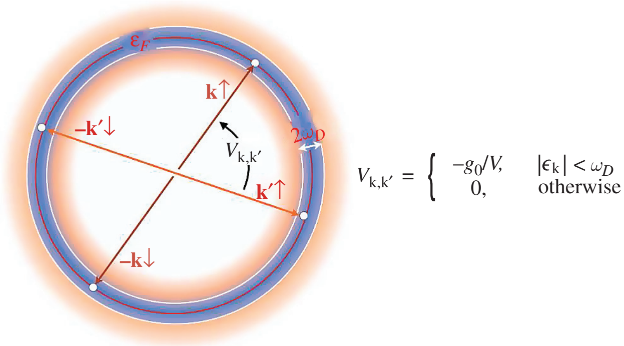

Fig. 14.6

In the BCS Hamiltonian, the matrix $V_{\mathbf{k},\mathbf{k}'}$ acts attractively on pairs of electrons within ω_D of the Fermi surface. Provided the repulsive interaction at higher energies is not too large, a superconducting instability results.

But what Hamiltonian explicitly gives rise to pairing? A clue came from the Cooper instability, which depends on the scattering amplitude $V_{\mathbf{k},\mathbf{k}'} = \langle \mathbf{k}_P|\hat{V}|\mathbf{k}'_P\rangle$ between *zero-momentum pairs*. BCS [15] incorporated this feature into a model Hamiltonian:

$$H = \sum_{\mathbf{k}\sigma} \epsilon_{\mathbf{k}\sigma} c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} + \sum_{\mathbf{k},\mathbf{k}'} V_{\mathbf{k},\mathbf{k}'} c^\dagger_{\mathbf{k}\uparrow} c^\dagger_{-\mathbf{k}\downarrow} c_{-\mathbf{k}'\downarrow} c_{\mathbf{k}'\uparrow}. \tag{14.48}$$

BCS Hamiltonian

In the universe of possible superconductors and superfluids, the interaction $V_{\mathbf{k},\mathbf{k}'}$ can take a wide variety of symmetries, but in its s-wave manifestation it is simply an isotropic attraction that develops within a narrow energy shell of electrons within a Debye energy of the Fermi surface, ω_D (Figure 14.6):

$$V_{\mathbf{k},\mathbf{k}'} = \begin{cases} -g_0/V & (|\epsilon_{\mathbf{k}}| < \omega_D) \\ 0 & (\text{otherwise}). \end{cases} \tag{14.49}$$

The s-wave BCS Hamiltonian then takes the form

$$H = \sum_{|\epsilon_{\mathbf{k}}|<\omega_D,\ \sigma} \epsilon_{\mathbf{k}} c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} - \frac{g_0}{V} A^\dagger A.$$
$$A^\dagger = \sum_{|\epsilon_{\mathbf{k}}|<\omega_D} c^\dagger_{\mathbf{k}\uparrow} c^\dagger_{-\mathbf{k}\downarrow}, \qquad A = \sum_{|\epsilon_{\mathbf{k}'}|<\omega_D} c_{-\mathbf{k}'\downarrow} c_{\mathbf{k}'\uparrow}. \tag{14.50}$$

s-wave BCS Hamiltonian

Remarks

- The BCS Hamiltonian is a *model* Hamiltonian capturing the low-energy pairing physics.

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- The normalizing factor $1/V$ is required in the interaction so that the interaction energy is extensive, growing linearly rather than quadratically with volume V.
- The BCS interaction takes place exclusively at zero momentum, and as such involves an infinite-range interaction between pairs. This long-range aspect of the model permits the exact solution of the BCS Hamiltonian using mean-field theory. In the more microscopic Fröhlich model the effective interaction (Figure (14.6)) is attractive within a narrow momentum shell $|\Delta\mathbf{p}| \sim \omega_D/\mathrm{v}_F$, corresponding to a spatial interaction range of order $1/|\Delta\mathbf{p}| \sim \mathrm{v}_F/\omega_D \sim O(\epsilon_F/\omega_D) \times a$, where a is the lattice spacing. This length scale is typically hundreds of lattice spacings, so the infinite-range mean-field theory is a reasonable rendition of the underlying physics.

14.3.1 Mean-field description of the condensate

The key consequence of the BCS model is the development of a state with off-diagonal long-range order (see Section 11.4.2). The pair operator $\hat{A}$ is extensive, and in a superconducting state its expectation value is proportional to the volume of the system $\langle\hat{A}\rangle \propto V$. The pair density

$$\Delta = |\Delta|e^{i\phi} = -\frac{g_0}{V}\langle\hat{A}\rangle = -g_0\int_{|\epsilon_{\mathbf{k}}|<\omega_D}\frac{d^3k}{(2\pi)^3}\langle c_{-\mathbf{k}\downarrow}c_{\mathbf{k}\uparrow}\rangle \tag{14.51}$$

is an intensive, macroscopic property of superconductors that has both an amplitude $|\Delta|$ *and* a phase ϕ. This is the order parameter. It sets the size of the gap in the excitation spectrum and gives rise to the emergent phase variable whose rigidity supports superconductivity.

Like the pressure in a gas, the order parameter Δ is an emergent many-body property. Just as fluctuations in pressure $\langle\delta P^2\rangle \sim O(1/V)$ become negligible in the thermodynamic limit, fluctuations in Δ can be similarly ignored. Of course, the reasoning needs to be refined to encompass a quantum variable, formally requiring a path-integral approach. The important point is that the change in action $\delta S[\delta\Delta] = S[\Delta + \delta\Delta_0] - S[\Delta]$ associated with a small variation in Δ about a stationary point scales extensively in volume: $\delta S[\delta\Delta] \sim V \times \delta\Delta^2$, so that the corresponding distribution function can be expanded as a Gaussian,

$$\mathcal{P}[\Delta] \propto e^{-S[\delta\Delta]} \sim \exp\left[-\frac{\delta\Delta^2}{O(1/V)}\right], \tag{14.52}$$

which is exquisitely peaked about $\Delta = \Delta_0$, with variance $\langle\delta\Delta^2\rangle \propto 1/V$, justifying a mean-field treatment.

Let us now expand the BCS interaction in powers of the fluctuation operator $\delta\hat{A} = \hat{A} - \langle\hat{A}\rangle$:

$$-\frac{g_0}{V}A^\dagger A = \overbrace{\bar{\Delta}A + A^\dagger\Delta + V\frac{\bar{\Delta}\Delta}{g_0}}^{O(V)} - \overbrace{\frac{g_0}{V}\delta A^\dagger\delta A}^{O(1)}. \tag{14.53}$$

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Now the first three terms are extensive in volume, but since $\langle \delta A^\dagger \delta A\rangle \sim O(V)$ the last term is intensive $O(1)$, and can be neglected in the thermodynamic limit. We shall shortly see how this same decoupling is accomplished in a path integral using a Hubbard–Stratonovich transformation. The resulting mean-field Hamiltonian for BCS theory is then

$$H_{MFT} = \sum_{\mathbf{k}\sigma} \epsilon_{\mathbf{k}} c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} + \sum_{\mathbf{k}} \left[\bar{\Delta} c_{-\mathbf{k}\downarrow} c_{\mathbf{k}\uparrow} + c^\dagger_{\mathbf{k}\uparrow} c^\dagger_{-\mathbf{k}\downarrow} \Delta \right] + \frac{V}{g_0} \bar{\Delta}\Delta, \tag{14.54}$$

BCS theory: mean-field Hamiltonian

in which Δ needs to be determined self-consistently by minimizing the free energy.

14.4 Physical picture of BCS theory: pairs as spins

Let us discuss the physical meaning of the pairing terms in the BCS mean-field Hamiltonian (14.54)

$$H_P(\mathbf{k}) = \left(\bar{\Delta} c_{-\mathbf{k}\downarrow} c_{\mathbf{k}\uparrow} + c^\dagger_{\mathbf{k}\uparrow} c^\dagger_{-\mathbf{k}\downarrow} \Delta \right). \tag{14.55}$$

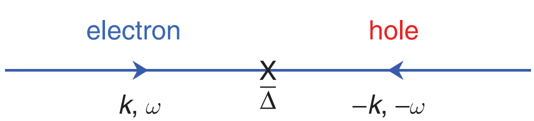
On the one hand, the term $\bar{\Delta} c_{-\mathbf{k}\downarrow} c_{\mathbf{k}\uparrow}$ converts two particles into the condensate:

$$\text{Pair creation}: \qquad e^- + e^- \rightleftharpoons \text{pair}^{2-}. \tag{14.56}$$

Alternatively, by writing $c_{-\mathbf{k}\downarrow} = h^\dagger_{\mathbf{k}\downarrow}$ as a hole creation operator, we see that $H_P(\mathbf{k}) \equiv (h^\dagger_{\mathbf{k}\uparrow}\bar{\Delta})c_{\mathbf{k}\uparrow} + \text{H.c.}$ describes the scattering of a single electron into a condensed pair (represented by $\bar{\Delta}$) and a hole, a process called *Andreev reflection*, named after its discoverer, Alexander Andreev:

$$\text{Andreev reflection}: \qquad e^- \rightleftharpoons \text{pair}^{2-} + h^+. \tag{14.57}$$

While the first process builds the condensate, the second coherently mixes particle and holes. We will denote the Andreev scattering process by a Feynman diagram:



Andreev reflection differs from conventional reflection in that

- it elastically scatters electrons into holes, reversing *all* components of the velocity[2]

[2] Andreev noticed that, although the momentum of the hole is the same as the incoming electron, its group velocity $\nabla_{\mathbf{k}}(-\epsilon_{-\mathbf{k}}) = \nabla_{\mathbf{k}}(-\epsilon_{\mathbf{k}}) = -\nabla_{\mathbf{k}}\epsilon_{\mathbf{k}}$ is reversed. This led him to predict that such scattering at the interface of a superconductor leads to non-specular reflection of electrons, which scatter back as holes moving in the opposite direction to the incoming electrons.

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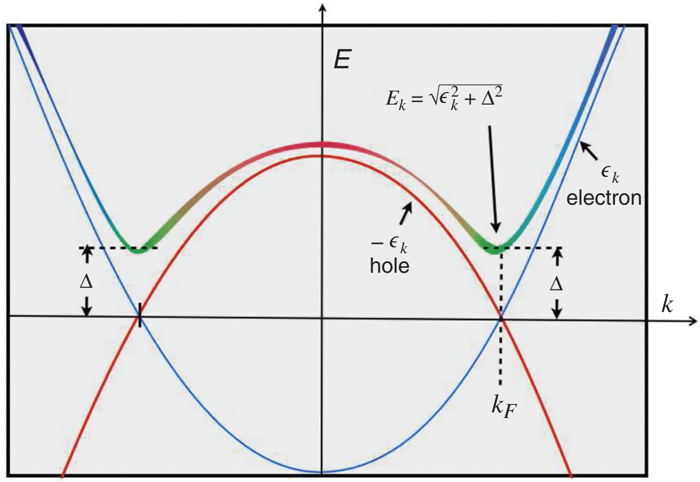

Fig. 14.7 Illustrating the excitation spectrum of a superconductor. Andreev scattering mixes the electron excitation spectrum (blue) with the hole excitation spectrum (red), producing the gap Δ in the quasiparticle excitation spectrum. The quasiparticles at the Fermi momentum are linear combinations of electrons and holes, with an indefinite charge.

- it *conserves* spin, momentum, *and* current, for a hole in the state $(-\mathbf{k}, \downarrow)$ has spin up, momentum $+\mathbf{k}$, and carries a current $I = (-e) \times (-\nabla \epsilon_{\mathbf{k}}) = e\nabla_{\mathbf{k}}\epsilon_{\mathbf{k}}$.

  Now the particle and hole dispersions are given by

$$\begin{array}{rl} \text{particle:} & \epsilon_{\mathbf{k}} \\ \text{hole:} & -\epsilon_{-\mathbf{k}}, \end{array} \tag{14.58}$$

as denoted by the blue and red lines, respectively, in Figure 14.7. These lines intersect at the Fermi surface, so that the Andreev mixing between electrons and holes in a superconductor opens up a gap that eliminates the Fermi surface, giving rise to a dispersion which, we will shortly show, takes the form

$$E_{\mathbf{k}} = \sqrt{\epsilon_{\mathbf{k}}^2 + |\Delta|^2}, \tag{14.59}$$

as illustrated in Figure 14.7. The quasiparticle operators now become linear combinations of electron and hole states with corresponding quasiparticle operators

$$a^\dagger_{\mathbf{k}\sigma} = u_{\mathbf{k}} c^\dagger_{\mathbf{k}\sigma} + \mathrm{sgn}(\sigma) v_{\mathbf{k}} c_{-\mathbf{k}-\sigma}. \tag{14.60}$$

14.4.1 Nambu spinors

We now introduce Nambu's spinor formulation of BCS theory, which we'll employ to expose the beautiful magnetic analogy between pairs and spins, discovered by Yoichiro Nambu [17] working at the University of Chicago and Philip W. Anderson [18] at AT&T Bell Laboratories. The analogue of a superconductor is an antiferromagnet, for both superconductivity and antiferromagnetism involve an order parameter which (unlike ferromagnetism), does *not* commute with the Hamiltonian. Superconductivity involves an

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analogous quantity to spin, which we will call *isospin*, which describes orientations in charge space. The pairing field Δ can be regarded as a transverse field in isospin space.

To bring out this physics, it is convenient to introduce the charge analogue of the electron spinor, the *Nambu spinor*, defined as

$$\psi_{\mathbf{k}} = \begin{pmatrix} c_{\mathbf{k}\uparrow} \\ c^{\dagger}_{-\mathbf{k}.\downarrow} \end{pmatrix} \qquad \begin{matrix} \text{electron} \\ \text{hole} \end{matrix} \tag{14.61}$$

with the corresponding Hermitian conjugate

$$\psi^{\dagger}_{\mathbf{k}} = \left(c^{\dagger}_{\mathbf{k}\uparrow},\ c_{-\mathbf{k}\downarrow}\right). \tag{14.62}$$

Nambu spinors behave like conventional electron fields, with an algebra

$$\{\psi_{\mathbf{k}\alpha},\ \psi^{\dagger}_{\mathbf{k}'\beta}\} = \delta_{\alpha\beta}\delta_{\mathbf{k},\mathbf{k}'}, \tag{14.63}$$

but instead of up and down electrons, they describe electrons and holes. These spinors enable us to unify the kinetic and pairing energy terms into a single *vector* field, analogous to a magnetic field, that acts in isospin space.

The kinetic energy can be written as

$$\sum_{\mathbf{k}} \epsilon_{\mathbf{k}}(c^{\dagger}_{\mathbf{k}\uparrow}c_{\mathbf{k}\uparrow} - c_{-\mathbf{k}\downarrow}c^{\dagger}_{-\mathbf{k}\downarrow} + 1) = \left(c^{\dagger}_{\mathbf{k}\uparrow},\ c_{-\mathbf{k}\downarrow}\right)\begin{bmatrix} \epsilon_{\mathbf{k}} & 0 \\ 0 & -\epsilon_{\mathbf{k}} \end{bmatrix}\begin{pmatrix} c_{\mathbf{k}\uparrow} \\ \bar{c}^{\dagger}_{-\mathbf{k}\downarrow} \end{pmatrix} + \sum_{\mathbf{k}} \epsilon_{\mathbf{k}}, \tag{14.64}$$

where the sign reversal in the lower component derives from anticommuting the down-spin electron operators. The energy $-\epsilon_{\mathbf{k}}$ is the energy to create a hole. We will drop the constant remainder term $\sum_{\mathbf{k}} \epsilon_{\mathbf{k}}$. We can now combine the kinetic and pairing terms into a single matrix:

$$\begin{aligned}
\epsilon_{\mathbf{k}} \sum_{\sigma} c^{\dagger}_{\mathbf{k}\sigma}c_{\mathbf{k}\sigma} + \left[\bar{\Delta}c_{-\mathbf{k}\downarrow}c_{\mathbf{k}\uparrow} + c^{\dagger}_{\mathbf{k}\uparrow}c^{\dagger}_{-\mathbf{k}\downarrow}\Delta\right] &= \left(c^{\dagger}_{\mathbf{k}\uparrow},\ c_{-\mathbf{k}\downarrow}\right)\begin{bmatrix} \epsilon_{\mathbf{k}} & \Delta \\ \bar{\Delta} & -\epsilon_{\mathbf{k}} \end{bmatrix}\begin{pmatrix} c_{\mathbf{k}\uparrow} \\ c^{\dagger}_{-\mathbf{k}\downarrow} \end{pmatrix} \\
&= \psi^{\dagger}_{\mathbf{k}}\begin{bmatrix} \epsilon_{\mathbf{k}} & \Delta_1 - i\Delta_2 \\ \Delta_1 + i\Delta_2 & -\epsilon_{\mathbf{k}} \end{bmatrix}\psi_{\mathbf{k}} \\
&= \psi^{\dagger}_{\mathbf{k}}[\epsilon_{\mathbf{k}}\tau_3 + \Delta_1\tau_1 + \Delta_2\tau_2]\psi_{\mathbf{k}},
\end{aligned} \tag{14.65}$$

where we denote $\Delta = \Delta_1 - i\Delta_2$, $\bar{\Delta} = \Delta_1 + i\Delta_2$ and we have introduced the *isospin matrices*

$$\vec{\tau} = (\tau_1, \tau_2, \tau_3) = \left(\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}, \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}\right). \tag{14.66}$$

By convention the symbol $\vec{\tau}$ is used to distinguish a Pauli matrix in charge space from a spin $\boldsymbol{\sigma}$ acting in spin space. Putting this all together, the mean-field Hamiltonian can now be rewritten

$$H = \sum_{\mathbf{k}} \psi^{\dagger}_{\mathbf{k}}\,(\vec{h}_{\mathbf{k}} \cdot \vec{\tau})\psi_{\mathbf{k}} + V\frac{\bar{\Delta}\Delta}{g_0}, \tag{14.67}$$

where

$$\vec{h}_{\mathbf{k}} = (\Delta_1, \Delta_2, \epsilon_{\mathbf{k}}) \tag{14.68}$$

plays the role of a Zeeman field acting in isospin space.

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14.4.2 Anderson's domain-wall interpretation of BCS theory

Anderson noted that the isospin operators $\psi^\dagger_{\mathbf{k}}\vec{\tau}\psi_{\mathbf{k}}$ have the properties of spin-$\frac{1}{2}$ operators acting in charge space. The z component of the isospin is

$$\tau_{3\mathbf{k}} = \psi^\dagger_{\mathbf{k}}\tau_3\psi_{\mathbf{k}} = (c^\dagger_{\mathbf{k}\uparrow}c_{\mathbf{k}\uparrow} - c_{-\mathbf{k}\downarrow}c^\dagger_{-\mathbf{k}\downarrow}) = (n_{\mathbf{k}\uparrow} + n_{-\mathbf{k}\downarrow} - 1), \tag{14.69}$$

so the up and down states correspond to the doubly occupied and empty pair state, respectively:

$$\begin{array}{lccl} \tau_{3\mathbf{k}} = +1: & |\Uparrow_{\mathbf{k}}\rangle & \equiv & |2\rangle = c^\dagger_{\mathbf{k}\uparrow}c^\dagger_{-\mathbf{k}\downarrow}|0\rangle \\ \tau_{3\mathbf{k}} = -1: & |\Downarrow_{\mathbf{k}}\rangle & \equiv & |0\rangle. \end{array} \tag{14.70}$$

By contrast, the transverse components of the isospin describe pair creation and annihilation:

$$\begin{aligned} \hat{\tau}_{1\mathbf{k}} &= \psi^\dagger_{\mathbf{k}}\tau_1\psi_{\mathbf{k}} = \quad c^\dagger_{\mathbf{k}\uparrow}c^\dagger_{-\mathbf{k}\downarrow} + c_{-\mathbf{k}\downarrow}c_{\mathbf{k}\uparrow} \\ \hat{\tau}_{2\mathbf{k}} &= \psi^\dagger_{\mathbf{k}}\tau_2\psi_{\mathbf{k}} = -i(c^\dagger_{\mathbf{k}\uparrow}c^\dagger_{-\mathbf{k}\downarrow} - c_{-\mathbf{k}\downarrow}c_{\mathbf{k}\uparrow}). \end{aligned} \tag{14.71}$$

In a normal metal, the isospin points "up" in the occupied states below the Fermi surface, and "down" in the empty states above the Fermi surface (Figure 14.8(a)). Now since the Hamiltonian is $H = \sum_{\mathbf{k}} \psi^\dagger_{\mathbf{k}}(\vec{h}_{\mathbf{k}} \cdot \vec{\tau})\psi_{\mathbf{k}}$, the quantity

$$\vec{B}_{\mathbf{k}} = -\vec{h}_{\mathbf{k}} = -(\Delta_1, \Delta_2, \epsilon_{\mathbf{k}}) \tag{14.72}$$

is thus a momentum-dependent Weiss field, setting a natural quantization axis for the electrons at momentum $\mathbf{k}$: in the ground state, the fermion isospins line up with this field. In the normal state, the natural isospin quantization axis is the charge or "z-axis," but in the

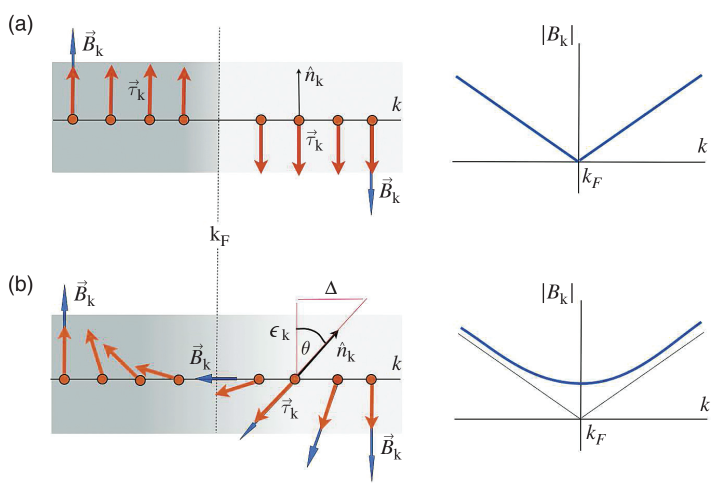

Fig. 14.8 Showing the domain-wall configuration of the isospin $\vec{\tau}_{\mathbf{k}}$ and direction of pairing field $\hat{n}_{\mathbf{k}}$ near the Fermi momentum: (a) a normal metal, in which the Weiss field $B_{\mathbf{k}}$ vanishes linearly at the Fermi energy, and (b) a superconductor in which the Weiss field remains finite at the Fermi energy, giving rise to a gap in the excitation spectrum.

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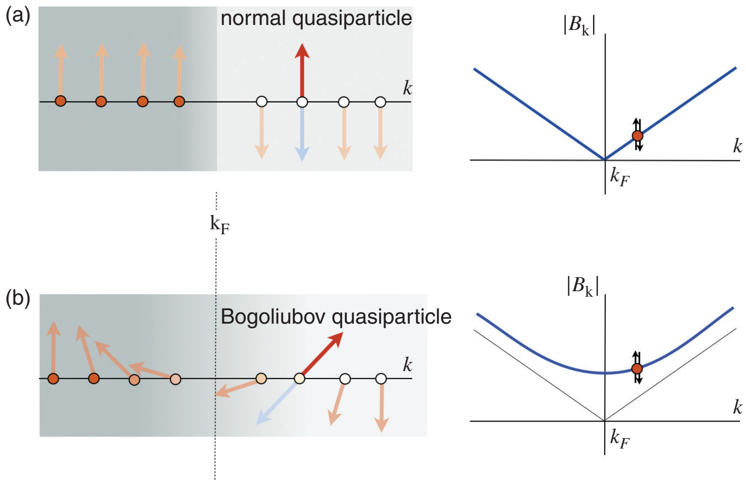

Fig. 14.9 Illustrating how the excitation of quasiparticle pairs corresponds to an "isospin flip," which forms a pair of up and down quasiparticles with energy $2|B_{\mathbf{k}}|$: (a) quasiparticle pair formation in the normal state where the quasiparticle spectrum is gapless; (b) formation of a Bogoliubov quasiparticle pair in the superconducting state where the excitation spectrum is gapped.

superconductor, the presence of a pairing condensate tips the quantization axis, mixing particle and hole states (Figure 14.8(b)).

With this analogy one can identify the reversal of an isospin out of its ground-state configuration as the creation of a pair of quasiparticles "above" the condensate. Since this costs an energy $2|\vec{B}_{\mathbf{k}}|$, the magnitude of the Weiss field

$$E_{\mathbf{k}} \equiv |\vec{B}_{\mathbf{k}}| = \sqrt{\epsilon_{\mathbf{k}}^2 + |\Delta|^2} = \text{quasiparticle energy} \tag{14.73}$$

must correspond to the energy of a single quasiparticle. In a metal ($\Delta = 0$), the Weiss field vanishes at the Fermi surface so it costs no energy to create a quasiparticle there (Figure 14.9(a)), but in a superconductor the Weiss field has magnitude $|\Delta|$ so the quasiparticle spectrum is now gapped (Figure 14.9(b)).

Let us write $\vec{B}_{\mathbf{k}} = -E_{\mathbf{k}}\hat{n}_{\mathbf{k}}$, where the unit vector

$$\hat{n}_{\mathbf{k}} = \left(\frac{\Delta_1}{E_{\mathbf{k}}}, \frac{\Delta_2}{E_{\mathbf{k}}}, \frac{\epsilon_{\mathbf{k}}}{E_{\mathbf{k}}}\right) \tag{14.74}$$

points upwards far above the Fermi surface, and downwards far beneath it. In a normal metal, $\hat{n}_{\mathbf{k}}$ (see Figure 14.8) reverses at the Fermi surface forming a sharp "Ising-like" domain wall, but in a superconductor the $\hat{n}$ vector is aligned at an angle θ to the $\hat{z}$ axis, where

$$\cos\theta_{\mathbf{k}} = \frac{\epsilon_{\mathbf{k}}}{E_{\mathbf{k}}}. \tag{14.75}$$

This angle rotates continuously as one passes through the Fermi energy, so the domain wall is now spread out over an energy range of order Δ, forming a kind of Bloch domain wall in isospin space, as shown in Figure 14.8.

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In the ground state each isospin will align parallel to the field $\vec{B}_{\mathbf{k}} = -E_{\mathbf{k}}\hat{n}_{\mathbf{k}}$, i.e.

$$\langle \psi^{\dagger}_{\mathbf{k}} \vec{\tau} \psi_{\mathbf{k}} \rangle = -\hat{n}_{\mathbf{k}} = -(\sin\theta_{\mathbf{k}}, 0, \cos\theta_{\mathbf{k}}), \tag{14.76}$$

where we have taken the liberty of choosing the phase of Δ so that $\Delta_2 = 0$. In a normal ground state ($\Delta = 0$) the isospin aligns along the z-axis, $\langle \tau_{3\mathbf{k}} \rangle = \langle n_{\mathbf{k}\uparrow} + n_{-\mathbf{k}\downarrow} - 1 \rangle = \mathrm{sgn}(k_F - k)$, but in a superconductor the isospin quantization axis is rotated through an angle $\theta_{\mathbf{k}}$ so that the z component of the isospin is

$$\langle \tau_{3\mathbf{k}} \rangle = \langle n_{\mathbf{k}\uparrow} + n_{-\mathbf{k}\downarrow} - 1 \rangle = -\cos\theta_{\mathbf{k}} = -\frac{\epsilon_{\mathbf{k}}}{\sqrt{\epsilon_{\mathbf{k}}^2 + \Delta^2}}, \tag{14.77}$$

which smears the occupancy around the Fermi surface, while the transverse isospin component, representing the pairing, is now finite:

$$\langle \tau_{1\mathbf{k}} \rangle = \langle (c^{\dagger}_{\mathbf{k}\uparrow} c^{\dagger}_{-\mathbf{k}\downarrow} + c_{-\mathbf{k}\downarrow} c_{\mathbf{k}\uparrow}) \rangle = -\sin\theta_{\mathbf{k}} = -\frac{\Delta}{\sqrt{\epsilon_{\mathbf{k}}^2 + \Delta^2}}. \tag{14.78}$$

Now since we have chosen $\Delta_2 = 0$, $\langle \tau_{2\mathbf{k}} \rangle = -i\langle (c^{\dagger}_{\mathbf{k}\uparrow} c^{\dagger}_{-\mathbf{k}\downarrow} - c_{-\mathbf{k}\downarrow} c_{\mathbf{k}\uparrow}) \rangle = 0$, it follows that $\langle c_{-\mathbf{k}\downarrow} c_{\mathbf{k}\uparrow} \rangle = -\frac{1}{2}\sin\theta_{\mathbf{k}}$. Imposing the self-consistency condition $\Delta = -\frac{g_0}{V}\sum_{\mathbf{k}} \langle c_{-\mathbf{k}\downarrow} c_{\mathbf{k}\uparrow} \rangle$ (14.51), one then obtains the *BCS gap equation*:

$$\Delta = \frac{g_0}{V}\sum_{\mathbf{k}} \frac{1}{2}\sin\theta_{\mathbf{k}} = g_0 \int_{|\epsilon_{\mathbf{k}}|<\omega_D} \frac{d^3k}{(2\pi)^3} \frac{\Delta}{2\sqrt{\epsilon_{\mathbf{k}}^2 + \Delta^2}}. \tag{14.79}$$

BCS gap equation ($T = 0$)

Since the momentum sum is restricted to a narrow region of the Fermi surface, one can replace the momentum sum by an energy integral, to obtain

$$1 = g_0 N(0) \int_{-\omega_D}^{\omega_D} d\epsilon \frac{1}{2\sqrt{\epsilon^2 + \Delta^2}} = g_0 N(0) \sinh^{-1}\left(\frac{\omega_D}{\Delta}\right) \approx g_0 N(0) \ln\left[\frac{2\omega_D}{\Delta}\right], \tag{14.80}$$

so, in the superconducting ground state, the BCS gap is given by

$$\Delta = 2\omega_D e^{-\frac{1}{g_0 N(0)}}. \tag{14.81}$$

Remarks

- Note the disappearance of the factor of 2 in the exponent that appeared in Cooper's original calculation (14.25).
- The magnetic analogy has many intriguing consequences. One can immediately see that, like a magnet, there must be collective pair excitations, in which the isospins fluctuate about their ground-state orientations. Like magnons, these excitations form quantized collective modes. In a neutral superconductor, this leads to a gapless "sound" (Bogoliubov or Goldstone) mode, but in a charged superconductor the condensate phase mixes with the electromagnetic vector potential via the Anderson–Higgs mechanism (see Section 11.6) to produce the massive photon responsible for the Meissner effect.

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14.4.3 The BCS ground state

In the vacuum $|0\rangle$, electron isospin operators all point "down," $\tau_{3\mathbf{k}} = -1$. To construct the ground state in which the isospins are aligned with the Weiss field, we need to construct a state in which each isospin is rotated relative to the vacuum. This is done by rotating the isospin at each momentum $\mathbf{k}$ through an angle $\theta_{\mathbf{k}}$ about the y-axis, as follows:

$$\begin{aligned}|\theta_{\mathbf{k}}\rangle = \exp\left[-i\frac{\theta_{\mathbf{k}}}{2}\psi^\dagger_{\mathbf{k}}\tau_y\psi_{\mathbf{k}}\right]|\Downarrow_{\mathbf{k}}\rangle &= \left(\cos\frac{\theta_{\mathbf{k}}}{2} - i\sin\frac{\theta_{\mathbf{k}}}{2}\psi^\dagger_{\mathbf{k}}\tau_y\psi_{\mathbf{k}}\right)|\Downarrow_{\mathbf{k}}\rangle \\ &= \cos\frac{\theta_{\mathbf{k}}}{2}|\Downarrow_{\mathbf{k}}\rangle - \sin\frac{\theta_{\mathbf{k}}}{2}|\Uparrow_{\mathbf{k}}\rangle. \end{aligned} \tag{14.82}$$

The ground state is a product of these isospin states:

$$|BCS\rangle = \prod_{\mathbf{k}}|\theta_{\mathbf{k}}\rangle = \prod_{\mathbf{k}}\left(\cos\frac{\theta_{\mathbf{k}}}{2} + \sin\frac{\theta_{\mathbf{k}}}{2}c^\dagger_{-\mathbf{k}\downarrow}c^\dagger_{\mathbf{k}\uparrow}\right)|0\rangle, \tag{14.83}$$

where we have absorbed the minus sign by anticommuting the two electron operators. Following BCS, the coefficients $\cos\left(\frac{\theta_{\mathbf{k}}}{2}\right)$ and $\sin\left(\frac{\theta_{\mathbf{k}}}{2}\right)$ are labeled $u_{\mathbf{k}}$ and $\mathrm{v}_{\mathbf{k}}$, respectively, writing

$$|BCS\rangle = \prod_{\mathbf{k}}|\theta_{\mathbf{k}}\rangle = \prod_{\mathbf{k}}\left(u_{\mathbf{k}} + \mathrm{v}_{\mathbf{k}}c^\dagger_{-\mathbf{k}\downarrow}c^\dagger_{\mathbf{k}\uparrow}\right)|0\rangle, \tag{14.84}$$

where

$$\begin{aligned} u_{\mathbf{k}} &\equiv \cos\left(\frac{\theta_{\mathbf{k}}}{2}\right) = \sqrt{\frac{1}{2}\left[1 + \underbrace{\cos\theta_{\mathbf{k}}}_{\epsilon_{\mathbf{k}}/E_{\mathbf{k}}}\right]} = \sqrt{\frac{1}{2}\left[1 + \frac{\epsilon_{\mathbf{k}}}{E_{\mathbf{k}}}\right]} \\ \mathrm{v}_{\mathbf{k}} &\equiv \sin\left(\frac{\theta_{\mathbf{k}}}{2}\right) = \sqrt{\frac{1}{2}\left[1 - \cos\theta_{\mathbf{k}}\right]} = \sqrt{\frac{1}{2}\left[1 - \frac{\epsilon_{\mathbf{k}}}{E_{\mathbf{k}}}\right]}. \end{aligned} \tag{14.85}$$

Remarks

- Dropping the normalization, the BCS wavefunction can be rewritten as a coherent state (14.45),

$$|BCS\rangle = \prod_{\mathbf{k}}\left(1 + \phi_{\mathbf{k}}c^\dagger_{\mathbf{k}\uparrow}c^\dagger_{-\mathbf{k}\downarrow}\right)|0\rangle) = \exp\left[\sum_{\mathbf{k}}\phi_{\mathbf{k}}c^\dagger_{\mathbf{k}\uparrow}c^\dagger_{-\mathbf{k}\downarrow}\right]|0\rangle = \exp\left[\Lambda^\dagger\right]|0\rangle, \tag{14.86}$$

  where $\phi_{\mathbf{k}} = -\frac{\mathrm{v}_{\mathbf{k}}}{u_{\mathbf{k}}}$ determines the Cooper pair wavefunction.
- We can thus expand the exponential in (14.86) as a coherent sum of pair-states:

$$|BCS\rangle = \sum_n \frac{1}{n!}(\Lambda^\dagger)^n|0\rangle = \sum_n \frac{1}{\sqrt{n!}}|n\rangle, \tag{14.87}$$

  where $|n\rangle = \frac{1}{\sqrt{n!}}(\Lambda^\dagger)^n|0\rangle$ is a state containing n pairs.

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The BCS wavefunction breaks gauge invariance, because it is not invariant under gauge transformations $c^\dagger_{\mathbf{k}\sigma} \to e^{i\alpha} c^\dagger_{\mathbf{k}\sigma}$ of the electron operators:

$$|BCS\rangle \to |\alpha\rangle = \prod_{\mathbf{k}} (1 + e^{2i\alpha} \phi_{\mathbf{k}} c^\dagger_{\mathbf{k}\uparrow} c^\dagger_{-\mathbf{k}\downarrow})|0\rangle = \sum \frac{e^{i2n\alpha}}{\sqrt{n!}} |n\rangle. \tag{14.88}$$

Under this transformation, the order parameter $\Delta = -g_0/V \sum_{\mathbf{k}} \langle \alpha | c_{-\mathbf{k}\downarrow} c_{\mathbf{k}\uparrow} |\alpha\rangle$ acquires a phase $\Delta \to e^{2i\alpha}|\Delta|$. On the other hand, the energy of the BCS state is unchanged by a gauge transformation, so the states $|\alpha\rangle$ must form a family of degenerate broken-symmetry states.

The action of the number operator $\hat{N}$ on this state may be represented as a differential with respect to phase:

$$\hat{N}|\alpha\rangle = \sum \frac{1}{\sqrt{n!}} 2n e^{i2n\alpha} |n\rangle = -i \frac{d}{d\alpha} |\alpha\rangle, \tag{14.89}$$

so that

$$\hat{N} \equiv -i \frac{d}{d\alpha}. \tag{14.90}$$

In this way, we see that the particle number is the generator of gauge transformations. Moreover, the phase of the order parameter is conjugate to the number operator, $[\alpha, N] = i$, and like position and momentum, or energy and time, the two variables therefore obey an uncertainty principle,

$$\Delta\alpha \Delta N \gtrsim 1. \tag{14.91}$$

Just as a macroscopic object with a precise position has an ill-defined momentum, a pair condensate with a sharply defined phase (relative to other condensates) is a physical state of matter – a macroscopic Schrödinger cat state – with an *ill-defined particle number*.

For the moment, we're ignoring the charge of the electron, but once we restore it, we will have to keep track of the vector potential, which also changes under gauge transformations.

14.5 Quasiparticle excitations in BCS theory

Let us now construct the quasiparticles of the BCS Hamiltonian. Recall that, for any one-particle Hamiltonian $H = \psi^\dagger_\alpha h_{\alpha\beta} \psi_\beta$, we can transform to an energy basis where the operators $a^\dagger_k = \psi^\dagger_\beta \langle \beta | k \rangle$ diagonalize $H = \sum_k E_k a^\dagger_k a_k$. Now the $\langle \beta | k \rangle$ are the eigenvectors of $h_{\alpha\beta}$, since $\langle \alpha | \hat{H} | k \rangle = E_k \langle \alpha | k \rangle = h_{\alpha\beta} \langle \beta | k \rangle$, so to construct quasiparticle operators we must project the particle operators onto the eigenvectors of $h_{\alpha\beta}$, $a^\dagger_k = \psi^\dagger_\beta \langle \beta | k \rangle$.

We now seek to diagonalize the BCS Hamiltonian, written in Nambu form:

$$H = \sum_{\mathbf{k}} \psi^\dagger_{\mathbf{k}} (\vec{h}_{\mathbf{k}} \cdot \vec{\tau}) \psi_{\mathbf{k}} + \frac{V}{g_0} \bar{\Delta} \Delta.$$

The two-dimensional Nambu matrix

$$\underline{h}_{\mathbf{k}} = \epsilon_{\mathbf{k}} \tau_3 + \Delta_1 \tau_1 + \Delta_2 \tau_2 \equiv E_{\mathbf{k}} \hat{n}_{\mathbf{k}} \cdot \vec{\tau} \tag{14.92}$$

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has two eigenvectors with isospin quantized parallel and antiparallel to $\hat{n}_{\mathbf{k}}$, [3]

$$\hat{n}_{\mathbf{k}} \cdot \vec{\tau} \begin{pmatrix} u_{\mathbf{k}} \\ \mathrm{v}_{\mathbf{k}} \end{pmatrix} = + \begin{pmatrix} u_{\mathbf{k}} \\ \mathrm{v}_{\mathbf{k}} \end{pmatrix}, \qquad \hat{n}_{\mathbf{k}} \cdot \vec{\tau} \begin{pmatrix} -\mathrm{v}^*_{\mathbf{k}} \\ u^*_{\mathbf{k}} \end{pmatrix} = - \begin{pmatrix} -\mathrm{v}^*_{\mathbf{k}} \\ u^*_{\mathbf{k}} \end{pmatrix}, \tag{14.93}$$

and corresponding energies $\pm E_{\mathbf{k}} = \pm\sqrt{\epsilon^2_{\mathbf{k}} + |\Delta_{\mathbf{k}}|^2}$. We can combine (14.93) into a single equation,

$$(\hat{n}_{\mathbf{k}} \cdot \vec{\tau}) U_{\mathbf{k}} = U_{\mathbf{k}} \tau_3, \tag{14.94}$$

where

$$U_{\mathbf{k}} = \begin{pmatrix} u_{\mathbf{k}} & -\mathrm{v}^*_{\mathbf{k}} \\ \mathrm{v}_{\mathbf{k}} & u^*_{\mathbf{k}} \end{pmatrix} \tag{14.95}$$

is the unitary matrix formed from the eigenvectors of $\underline{h}_{\mathbf{k}}$. If we now project $\psi^\dagger_{\mathbf{k}}$ onto the eigenvectors of $h_{\mathbf{k}}$, we obtain the quasiparticle operators for the BCS Hamiltonian:

$$\begin{aligned} a^\dagger_{\mathbf{k}\uparrow} &= \psi^\dagger_{\mathbf{k}} \cdot \begin{pmatrix} u_{\mathbf{k}} \\ \mathrm{v}_{\mathbf{k}} \end{pmatrix} = c^\dagger_{\mathbf{k}\uparrow} u_{\mathbf{k}} + c_{-\mathbf{k}\downarrow} \mathrm{v}_{\mathbf{k}} \\ a_{-\mathbf{k}\downarrow} &= \psi^\dagger_{\mathbf{k}} \cdot \begin{pmatrix} -\mathrm{v}^*_{\mathbf{k}} \\ u^*_{\mathbf{k}} \end{pmatrix} = c_{-\mathbf{k}\downarrow} u^*_{\mathbf{k}} - c^\dagger_{\mathbf{k}\uparrow} \mathrm{v}^*_{\mathbf{k}}. \end{aligned} \tag{14.96}$$

Bogoliubov transformation

This transformation, mixing particles and holes, is named after its inventor, Nikolai Bogoliubov. If one takes the complex conjugate of the quasihole operator and reverses the momentum, one obtains $a^\dagger_{\mathbf{k}\downarrow} = c^\dagger_{\mathbf{k}\downarrow} u_{\mathbf{k}} - c_{-\mathbf{k}\uparrow} \mathrm{v}_{\mathbf{k}}$, which defines the spin-down quasiparticle. The general expression for the spin-up and spin-down quasiparticles can be written

$$a^\dagger_{\mathbf{k}\sigma} = c^\dagger_{\mathbf{k}\sigma} u_{\mathbf{k}} + \mathrm{sgn}(\sigma) c_{-\mathbf{k}-\sigma} \mathrm{v}_{\mathbf{k}}. \tag{14.97}$$

Let us combine the two expressions (14.96) into a single Nambu spinor $a^\dagger_{\mathbf{k}}$:

$$a^\dagger_{\mathbf{k}} = (a^\dagger_{\mathbf{k}\uparrow}, a_{-\mathbf{k}\downarrow}) = \psi^\dagger_{\mathbf{k}} \overbrace{\begin{pmatrix} u_{\mathbf{k}} & -\mathrm{v}^*_{\mathbf{k}} \\ \mathrm{v}_{\mathbf{k}} & u^*_{\mathbf{k}} \end{pmatrix}}^{U_{\mathbf{k}}} = \psi^\dagger_{\mathbf{k}} U_{\mathbf{k}}. \tag{14.98}$$

Taking the Hermitian conjugate $a_{\mathbf{k}} = U^\dagger_{\mathbf{k}} \psi_{\mathbf{k}}$, then $\psi_{\mathbf{k}} = U_{\mathbf{k}} a_{\mathbf{k}}$, since $UU^\dagger = 1$. Using (14.94),

$$\psi^\dagger_{\mathbf{k}} h_{\mathbf{k}} \psi_{\mathbf{k}} = a^\dagger_{\mathbf{k}} U^\dagger_{\mathbf{k}} \overbrace{h_{\mathbf{k}} U_{\mathbf{k}}}^{U_{\mathbf{k}} E_{\mathbf{k}} \tau_3} a_{\mathbf{k}} = a^\dagger_{\mathbf{k}} E_{\mathbf{k}} \tau_3 a_{\mathbf{k}}, \tag{14.99}$$

so that, as expected,

$$H = \sum_{\mathbf{k}} a^\dagger_{\mathbf{k}} E_{\mathbf{k}} \tau_3 a_{\mathbf{k}} + V \frac{\bar{\Delta}\Delta}{g_0} \tag{14.100}$$

[3] Here complex conjugation is required to ensure that the complex eigenvectors are orthogonal when the gap is complex.

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is diagonal in the quasiparticle basis. Written out explicitly,

$$H = \sum_{\mathbf{k}} E_{\mathbf{k}} \left(a^\dagger_{\mathbf{k}\uparrow} a_{\mathbf{k}\uparrow} - a_{-\mathbf{k}\downarrow} a^\dagger_{-\mathbf{k}\downarrow} \right) + V \frac{\bar{\Delta}\Delta}{g_0}. \tag{14.101}$$

If we rewrite the Hamiltonian in the form

$$H = \sum_{\mathbf{k}\sigma} E_{\mathbf{k}} \left(a^\dagger_{\mathbf{k}\sigma} a_{\mathbf{k}\sigma} - \frac{1}{2} \right) + V \frac{\bar{\Delta}\Delta}{g_0}, \tag{14.102}$$

we can interpret the excitation spectrum in terms of quasiparticles of energy $E_{\mathbf{k}} = \sqrt{\epsilon^2_{\mathbf{k}} + |\Delta|^2}$ and a ground-state energy[4]

$$E_g = -\sum_{\mathbf{k}} E_{\mathbf{k}} + V \frac{\bar{\Delta}\Delta}{g_0}. \tag{14.104}$$

Now if the density of Bogoliubov quasiparticles per spin is $N_s(E)$, then, since the number of quasiparticle states is conserved, $N_s(E)dE = N_n(0)d|\epsilon|$ (where $N_n(0) = 2N(0)$ is the quasiparticle density of states in the normal state). It follows that

$$N^*_s(E) = N_n(0)\frac{d|\epsilon_{\mathbf{k}}|}{dE_{\mathbf{k}}} = N_n(0) \left(\frac{E}{\sqrt{E^2 - |\Delta|^2}} \right) \theta(E - |\Delta|), \tag{14.105}$$

where we have written $\epsilon_{\mathbf{k}} = \sqrt{E^2_{\mathbf{k}} - |\Delta|^2}$ to obtain $d\epsilon_{\mathbf{k}}/dE_{\mathbf{k}} = E_{\mathbf{k}}/\sqrt{E^2_{\mathbf{k}} - |\Delta|^2}$. The theta function describes the absence of states in the gap (see Figure 14.10(a)). Notice how the Andreev scattering causes states to pile up in a square-root singularity above the gap; this feature is called a *coherence peak*.

One of the most direct vindications of BCS theory derives from tunneling measurements of the excitation spectrum, in which the differential tunneling conductance is proportional to the quasiparticle density of states:

$$\frac{dI}{dV} \propto N_s(eV) = N_n(0)\frac{eV}{\sqrt{eV^2 - \Delta^2}}\theta(eV - |\Delta|). \tag{14.106}$$

The observation of such tunneling spectra in superconducting aluminum in 1960 by Ivar Giaever [19] provided the first direct confirmation of the energy gap predicted by BCS theory (see Figure 14.10(b)).

4 Note that, if we were to restore the constant term $\sum_{\mathbf{k}} \epsilon_k$ dropped in (14.64), the ground-state energy becomes

$$E_g = \sum_{\mathbf{k}} (\epsilon_{\mathbf{k}} - E_{\mathbf{k}}) + V \frac{\bar{\Delta}\Delta}{g_0}. \tag{14.103}$$

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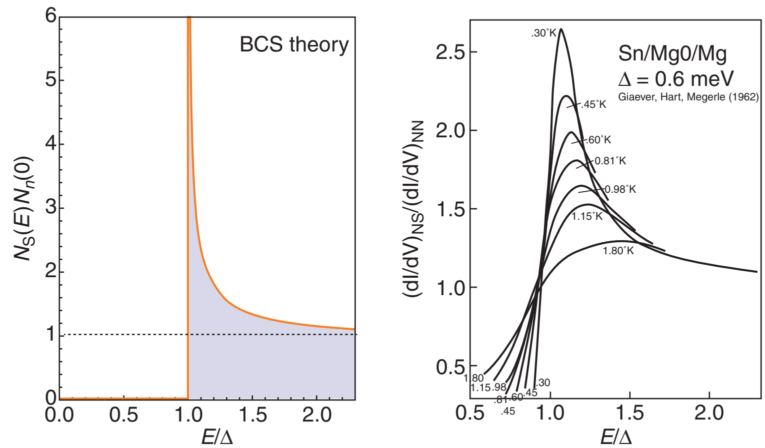

Fig. 14.10

Contrasting (a) quasiparticle density of states with (b) measured tunneling density of states in Sn-Mg0-Mg superconducting-normal tunnel junctions. In practice, finite temperature, disorder, variations in gap size around the Fermi surface, and strong-coupling corrections to BCS theory lead to small deviations from the ideal ground-state BCS density of states. Reprinted with permission from I. Giaever, *et al.*, *Phys. Rev.*, vol. 126, p. 941, 1962. Copyright 1962 by the American Physical Society.

Example 14.2 Show that the BCS ground state is the vacuum for the Bogoliubov quasiparticles, i.e. that the destruction operators $a_{\mathbf{k}\sigma}$ annihilate the BCS ground state.

Solution

One way to confirm this is to directly construct the quasiparticle vacuum $|\psi\rangle$, by repeatedly applying the pair destruction operators to the electron vacuum, so that

$$|\psi\rangle = \prod_{\mathbf{k}} a_{-\mathbf{k}\downarrow} a_{\mathbf{k}\uparrow} |0\rangle$$

$$\Rightarrow a_{\mathbf{k}\sigma} |\psi\rangle = 0 \tag{14.107}$$

for all $\mathbf{k}$, since the square of a destruction operator is zero, so $|\psi\rangle$ is the quasiparticle vacuum. Using the form (14.97),

$$\begin{aligned} a_{\mathbf{k}\uparrow} &= u_{\mathbf{k}} c_{\mathbf{k}\uparrow} + \mathrm{v}_{\mathbf{k}} c^{\dagger}_{-\mathbf{k}\downarrow} \\ a_{-\mathbf{k}\downarrow} &= u_{\mathbf{k}} c_{-\mathbf{k}\downarrow} - \mathrm{v}_{\mathbf{k}} c^{\dagger}_{\mathbf{k}\uparrow}, \end{aligned} \tag{14.108}$$

where for convenience we assume that $u_{\mathbf{k}}$ and $\mathrm{v}_{\mathbf{k}}$ are real, we find

$$\begin{aligned} \prod_{\mathbf{k}} a_{-\mathbf{k}\downarrow} a_{\mathbf{k}\uparrow} |0\rangle &= \prod_{\mathbf{k}} (u_{\mathbf{k}}\, c_{-\mathbf{k}\downarrow} - \mathrm{v}_{\mathbf{k}}\, c^{\dagger}_{\mathbf{k}\uparrow})(\cancel{u_{\mathbf{k}} c_{\mathbf{k}\uparrow}} + \mathrm{v}_{\mathbf{k}}\, c^{\dagger}_{-\mathbf{k}\downarrow})|0\rangle \\ &= \prod_{\mathbf{k}} (u_{\mathbf{k}} \mathrm{v}_{\mathbf{k}} c_{-\mathbf{k}\downarrow} c^{\dagger}_{-\mathbf{k}\downarrow} - (\mathrm{v}_{\mathbf{k}})^2 c^{\dagger}_{\mathbf{k}\uparrow} c^{\dagger}_{-\mathbf{k}\downarrow})|0\rangle \\ &= \prod_{\mathbf{k}} \mathrm{v}_{\mathbf{k}} \times \prod_{\mathbf{k}} (u_{\mathbf{k}} + \mathrm{v}_{\mathbf{k}} c^{\dagger}_{-\mathbf{k}\downarrow} c^{\dagger}_{\mathbf{k}\uparrow})|0\rangle \propto |BCS\rangle, \end{aligned} \tag{14.109}$$

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where terms involving the destruction operator acting on the vacuum vanish and are omitted. Apart from normalization, this is the BCS ground state, confirming that the Bogoliubov quasiparticle operators are the unique operators that annihilate the BCS ground state.

Example 14.3

(a) If the Bogoliubov quasiparticle $\alpha^\dagger_{\mathbf{k}\uparrow} = c^\dagger_{\mathbf{k}\uparrow} u_{\mathbf{k}} + c_{-\mathbf{k}\downarrow} \mathrm{v}_{\mathbf{k}} \alpha_{-\mathbf{k}\downarrow}$, then, starting with the equation of motion of the Bogoliubov quasiparticle,

$$[H, \alpha^\dagger_{\mathbf{k}\uparrow}] = \frac{\partial \alpha^\dagger_{\mathbf{k}\uparrow}}{\partial \tau} = E_{\mathbf{k}} \alpha^\dagger_{\mathbf{k}\uparrow}, \tag{14.110}$$

show that $\begin{pmatrix} u_{\mathbf{k}} \\ \mathrm{v}_{\mathbf{k}} \end{pmatrix}$ must be an eigenvector of $h_{\mathbf{k}}$ that satisfies

$$\underline{h}_{\mathbf{k}} \begin{pmatrix} u_{\mathbf{k}} \\ \mathrm{v}_{\mathbf{k}} \end{pmatrix} = \begin{pmatrix} \epsilon_{\mathbf{k}} & \Delta \\ \Delta & -\epsilon_{\mathbf{k}} \end{pmatrix} \begin{pmatrix} u_{\mathbf{k}} \\ \mathrm{v}_{\mathbf{k}} \end{pmatrix} = E_{\mathbf{k}} \begin{pmatrix} u_{\mathbf{k}} \\ \mathrm{v}_{\mathbf{k}} \end{pmatrix}. \tag{14.111}$$

(b) By solving the eigenvalue problem assuming the gap is real, show that

$$u^2_{\mathbf{k}} = \frac{1}{2}\left[1 + \frac{\epsilon_{\mathbf{k}}}{\sqrt{\epsilon^2_{\mathbf{k}} + \Delta^2}}\right]$$
$$\mathrm{v}^2_{\mathbf{k}} = \frac{1}{2}\left[1 - \frac{\epsilon_{\mathbf{k}}}{\sqrt{\epsilon^2_{\mathbf{k}} + \Delta^2}}\right]. \tag{14.112}$$

Solution

(a) We begin by writing

$$\alpha^\dagger_{\mathbf{k}\uparrow} = \psi^\dagger_{\mathbf{k}} \cdot \begin{pmatrix} u_{\mathbf{k}} \\ \mathrm{v}_{\mathbf{k}} \end{pmatrix} \tag{14.113}$$

where $\psi^\dagger_{\mathbf{k}} = (c^\dagger_{\mathbf{k}\uparrow}, c_{-\mathbf{k}\downarrow})$ is the Nambu spinor. Since $[H, \ \psi^\dagger_{\mathbf{k}}] = \psi^\dagger_{\mathbf{k}} \ \underline{h}_{\mathbf{k}}$, it follows that

$$[H, \alpha^\dagger_{\mathbf{k}\uparrow}] = \psi^\dagger_{\mathbf{k}} \ \underline{h}_{\mathbf{k}} \begin{pmatrix} u_{\mathbf{k}} \\ \mathrm{v}_{\mathbf{k}} \end{pmatrix}. \tag{14.114}$$

Comparing (14.110) and (14.114), we see that the spinor $\begin{pmatrix} u_{\mathbf{k}} \\ \mathrm{v}_{\mathbf{k}} \end{pmatrix}$ is an eigenvector of $h_{\mathbf{k}}$:

$$\underline{h}_{\mathbf{k}} \begin{pmatrix} u_{\mathbf{k}} \\ \mathrm{v}_{\mathbf{k}} \end{pmatrix} = \begin{pmatrix} \epsilon_{\mathbf{k}} & \Delta \\ \Delta & -\epsilon_{\mathbf{k}} \end{pmatrix} \begin{pmatrix} u_{\mathbf{k}} \\ \mathrm{v}_{\mathbf{k}} \end{pmatrix} = E_{\mathbf{k}} \begin{pmatrix} u_{\mathbf{k}} \\ \mathrm{v}_{\mathbf{k}} \end{pmatrix}. \tag{14.115}$$

(b) Taking the determinant of the eigenvalue equation, $\det[\,\underline{h}_{\mathbf{k}} - E_{\mathbf{k}} \underline{1}\,] = E^2_{\mathbf{k}} - \epsilon^2_{\mathbf{k}} - \Delta^2 = 0$, and imposing the condition that $E_{\mathbf{k}} > 0$, we obtain $E_{\mathbf{k}} = \sqrt{\epsilon^2_{\mathbf{k}} + \Delta^2}$.

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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

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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:

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

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

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

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 $\ln\det \to \mathrm{Tr}\ln$. 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:

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

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

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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:

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

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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

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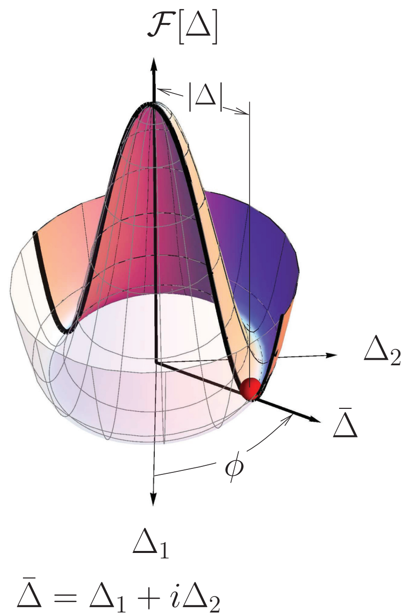

Fig. 14.11 Showing the form of $\mathcal{F}[\Delta]$ for $T < T_c$. The free energy is a minimum at a finite value of $|\Psi|$. The free energy is invariant under changes in phase of the gap, which are generated by the number operator $\hat{N} \propto -i\frac{d}{d\phi}$. See Exercise 14.4.

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

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

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

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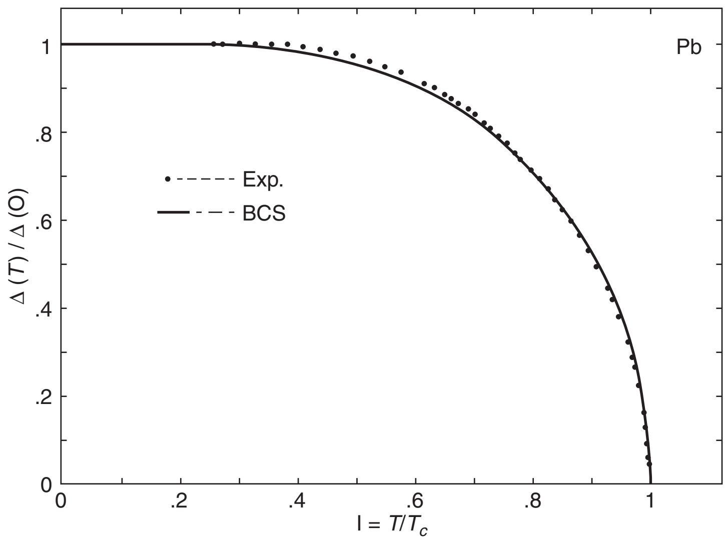

Fig. 14.12 Comparison between the dependence of the gap on the reduced temperature T/T_C and the gap measured by tunneling in superconducting lead. Reprinted with permission from R. F. Gasparovic, *et al.*, *Solid State Commun.*, vol. 4, p. 59, 1966. Copyright 1966 Elsevier.

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

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:

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

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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.

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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

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

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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

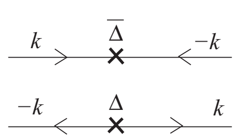
$$\underline{\mathcal{G}}(\mathbf{k}, i\omega_n) = \frac{1}{(i\omega_n)^2 - E^2_{\mathbf{k}}}\begin{bmatrix} i\omega_n + \epsilon_{\mathbf{k}} & \Delta \\ \bar{\Delta} & i\omega_n - \epsilon_{\mathbf{k}}\end{bmatrix}, \tag{14.161}$$

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

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

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



(14.162)

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

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

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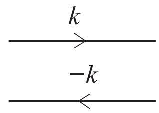
We denote these two components by the diagrams

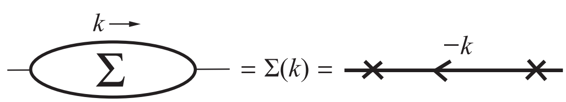


$$\equiv G_0(k) = \frac{1}{i\omega_n - \epsilon_{\mathbf{k}}}$$
$$\equiv -G_0(-k) = \frac{1}{i\omega_n + \epsilon_{\mathbf{k}}}. \tag{14.164}$$

(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

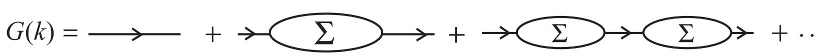
(14.165)

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:



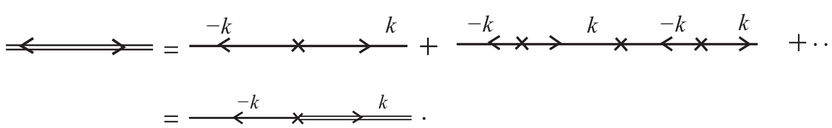
$$= \frac{|\Delta|^2}{i\omega_n + \epsilon_{\mathbf{k}}}. \tag{14.166}$$

We may then redraw the propagator as



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

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

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

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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

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

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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.

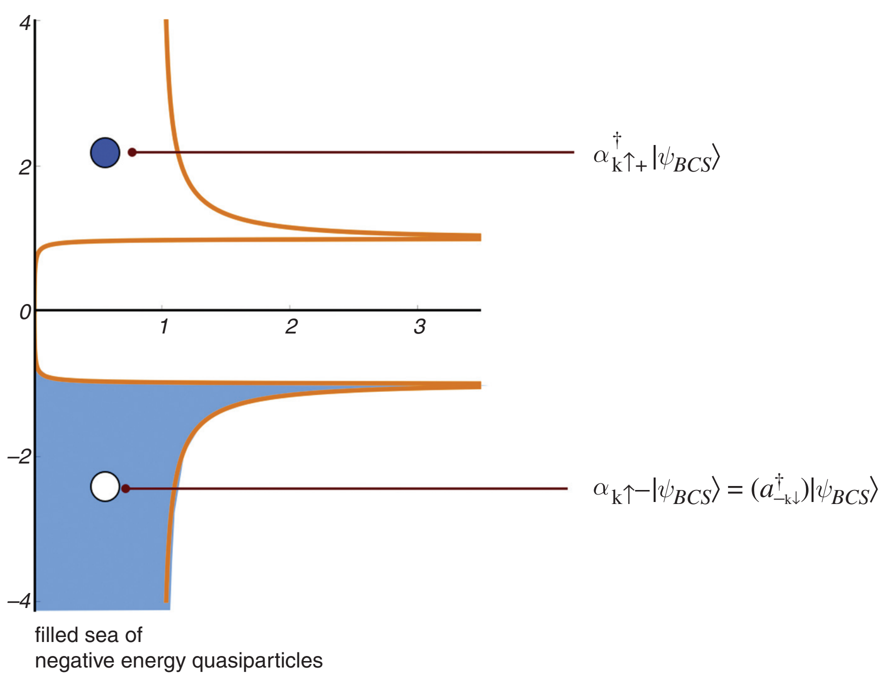

Fig. 14.13 Semiconductor analogy for BCS theory (see Example 14.6). The BCS ground state can be regarded as a filled sea of negative energy quasiparticles. Positive energy excitations are created by adding positive quasiparticles, $\alpha^{\dagger}_{\mathbf{k}\sigma+}|\psi_{BCS}\rangle$, or removing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

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

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

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

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

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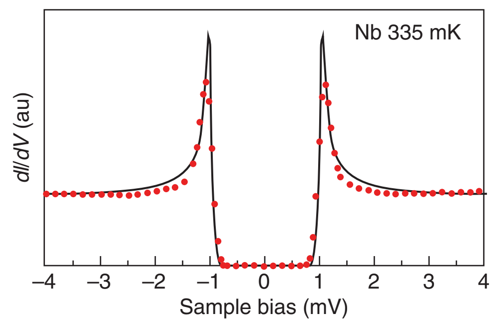

Fig. 14.14 Comparison of the experimental tunneling spectrum and the BCS spectrum in superconducting Nb at $T = 335$ mK [22]. Reprinted with permission from S. H. Pan, *et al.*, *Appl. Phys. Lett.*, vol. 73, p. 2992, 1998. Copyright 1998 by the American Insitute of Physics.

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 $\hat{\rho}_{\mathbf{q}} = e\sum_{\mathbf{k}\sigma} c^\dagger_{\mathbf{k}+\mathbf{q}\sigma}c_{\mathbf{k}\sigma}$, $A_{\alpha\beta}(\mathbf{k},\mathbf{k}') = e\delta_{\alpha\beta}\delta_{\mathbf{k}-(\mathbf{k}'+\mathbf{q})}$

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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, $\theta = -1$.

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- 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,

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

Then

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

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

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

while in this case the matrix elements

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

are unrenormalized, so that the NMR relaxation rate becomes

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

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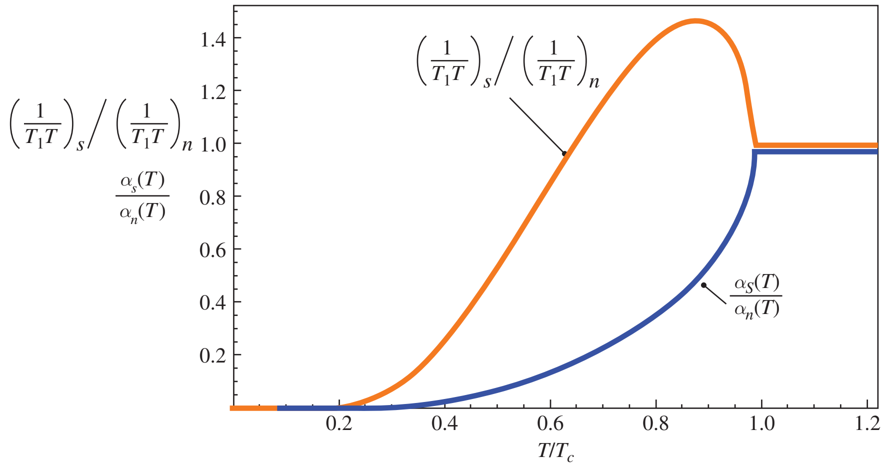

Fig. 14.15 Showing the effect of coherence factors NMR and ultrasonic attenuation in a superconductor, calculated in BCS theory. The orange line displays the NMR relaxation rate, showing the Hebel–Slichter peak. The blue line shows the ultrasound attenuation. The integrals entering the NMR relaxation 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

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

but in the superconductor this becomes

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

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

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

[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.

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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,

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

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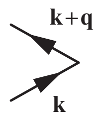
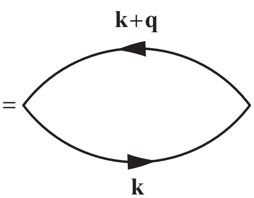
where we have anticommuted the down fermion operators and relabeled $\mathbf{k} \to -\mathbf{k}+\mathbf{q}$. Thus the z component of the magnetization is a unit matrix in Nambu space. The vertex for the magnetization is thus



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

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

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

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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

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

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

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

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

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

thereby proving (14.204).

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

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

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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:

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

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

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

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

$$-g(\psi^\dagger_\uparrow\psi^\dagger_\downarrow\psi_\downarrow\psi_\uparrow)\rightarrow\bar{\Delta}\psi_\downarrow\psi_\uparrow+\psi^\dagger_\uparrow\psi^\dagger_\downarrow\Delta+\frac{\bar{\Delta}\Delta}{g}, \tag{14.224}$$

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

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

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:

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

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

$$\Delta(x)\rightarrow e^{2i\alpha(x)}\Delta(x), \tag{14.227}$$

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:

$$\phi(x)\rightarrow\phi(x)+2\alpha(x). \tag{14.228}$$

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

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

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 $\phi\rightarrow\phi+2\alpha$, $\vec{A}\rightarrow\vec{A}+\frac{\hbar}{e}\vec{\nabla}\alpha(x)$. Indeed, gauge invariance of the free energy under these two transformations requires that the gradient

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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

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

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].

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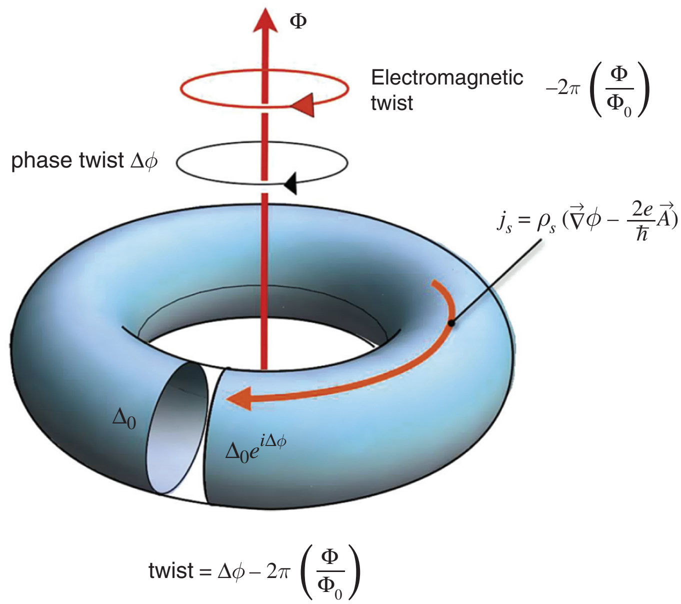

Fig. 14.16 Illustrating the phase-twist in the superconducting order parameter induced by a magnetic flux.

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, $\Phi = n\Phi_0$.

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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

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

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

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

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

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

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

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

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

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

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:

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

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

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

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

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

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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

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

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

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

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(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

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

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

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

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Here, the limit of integration has been moved to infinity. Why can we do this without loss of accuracy?

(c) Use Mathematica or Maple to plot the free energy obtained from the above result, confirming that the minimum is at $\Delta/\Delta_0 = 1$ and the transition occurs at $T_c = 2\Delta_0/3.53$.

References

[1] W. Meissner and R. Ochsenfeld, Ein neuer Effekt bei Eintritt der Supraleitfähigkeit, *Naturwissenschaften*, vol. 21, no. 44, p. 787, 1933.

[2] F. London, New conception of supraconductivity, *Nature*, vol. 140, p. 793, 1937.

[3] F. London, *Superfluids*, vols. 1–2, Dover Publications, 1961–1964.

[4] V. L. Ginzburg and L. D. Landau, On the theory of superconductivity, *Zh. Eksp. Teor. Fiz*, vol. 20, p. 1064, 1950.

[5] H. Fröhlich, Theory of the superconducting state. I The ground state at the absolute zero of temperature, *Phys. Rev.*, vol. 79, p. 845, 1950.

[6] B. Serin, C. A. Reynolds, and L. B. Nesbitt, Mass dependence of the superconducting transition temperature of mercury, *Phys. Rev.*, vol. 80, no. 4, p. 761, 1950.

[7] E. Maxwell, Isotope effect in the superconductivity of mercury, *Phys. Rev.*, vol. 78, no. 4, p. 477, 1950.

[8] C. A. Reynolds, B. Serin, W. H. Wright, and L. B. Nesbitt, Superconductivity of isotopes of mercury, *Phys. Rev.*, vol. 78, no. 4, p. 487, 1950.

[9] H. Fröhlich, Isotope effect in superconductivity, *Proc. Phys. Soc., London*, vol. 63, p. 778, 1950.

[10] *Oral History Transcript: Sir A. Brian Pippard*, Interview with Sir A. Brian Pippard on the history of superconductivity, September 14, 1982, Center for History of Physics, American Institute of Physics.

[11] A. B. Pippard, An experimental and theoretical study of the relation between magnetic field and current in a superconductor, *Proc. R. Soc. A*, vol. A216, p. 547, 1953.

[12] J. Bardeen, Theory of the Meissner effect in superconductors, *Phys. Rev.*, vol. 97, no. 6, p. 1724, 1955.

[13] J. Bardeen and D. Pines, Electron–phonon interaction in metals, *Phys. Rev.*, vol. 99, p. 1140, 1955.

[14] L. N. Cooper, Bound electron pairs in a degenerate Fermi gas, *Phys. Rev.*, vol. 104, no. 4, p. 1189, 1956.

[15] J. Bardeen, L. N. Cooper, and J. R. Schrieffer, Theory of superconductivity, *Phys. Rev.*, vol. 108, no. 5, p. 1175, 1957.

[16] *Schrieffer's Story*: *How We Got an Explanation of Superconductivity*, excerpts from an interview with J. Robert Schrieffer, Moments of Discovery, American Institute of Physics.

https://doi.org/10.1017/CBO9781139020916.016 Published online by Cambridge University Press

[17] Y. Nambu, Quasi-particles and gauge invariance in the theory of superconductivity, *Phys. Rev.*, vol. 117, p. 648, 1960.

[18] P. W. Anderson, Random-phase approximation in the theory of superconductivity, *Phys. Rev.*, vol. 112, no. 6, p. 1900, 1958.

[19] I. Giaever, Energy gap in superconductors measured by electron tunneling, *Phys. Rev. Lett.*, vol. 5, p. 147, 1960.

[20] I. Giaever, H. R. Hart, and K. Megerle, Tunneling into superconductors at temperatures below 1K, *Phys. Rev.*, vol. 126, p. 941, 1962.

[21] R. F. Gasparovic, B. N. Taylor, and R. E. Eck, Temperature dependence of the superconducting energy gap of Pb, *Solid State Commun.*, vol. 4, p. 59, 1966.

[22] S. H. Pan, E. W. Hudson, and J. C. Davis, Vacuum tunneling of superconducting quasiparticles from atomically sharp scanning tunneling microscope tips, *Appl. Phys. Lett.*, vol. 73, p. 2992, 1998.

[23] P. W. Anderson, Plasmons, gauge invariance, and mass, *Phys. Rev.*, vol. 130, no. 1, p. 439, 1963.

[24] P. W. Higgs, Broken symmetries and the masses of gauge bosons, *Phys. Rev. Lett.*, vol. 13, no. 16, p. 508, 1964.

https://doi.org/10.1017/CBO9781139020916.016 Published online by Cambridge University Press