15 Retardation and anisotropic pairing

This chapter continues our discussion of superconductivity, considering the effects of repulsive interactions and the physics of anisotropic Cooper pairing. According to an apocryphal story, Landau is reputed to have said that "nobody has yet repealed Coulomb's law" [1]. In the BCS theory of superconductors, there is no explicit appearance of the the repulsive Coulomb interaction between paired electrons. How then do real-world superconductors produce electron pairs, despite the presence of the strong interaction between them?

This chapter we will examine two routes by which Nature is able to satisfy the Coulomb interaction. In conventional superconductors, the attraction between electrons develops because the positive screening charge created by the ionic lattice around an electron remains in place long after the electron has moved away. This process that gives rise to a short-time repulsion between electrons is followed by a *retarded attraction* which drives s-wave pairing. However, since the 1980s physicists have been increasingly fascinated by *anisotropic superconductors*. In these systems, it is the repulsive interaction between the fermions that drives the pairing. The mechanism by which this takes place is through the development of nodes in the pair wavefunction – often by forming a higher angular momentum Cooper pair. The two classic examples of this physics are the p-wave pairs of superfluid ^{3}He and the d-wave pairs of cuprate high-temperature superconductors.

In truth, the physics community is still trying to understand the full interplay of superconductivity and the Coulomb force. The discovery of room-temperature superconductivity will surely involve finding a quantum material where strong correlations within the electron fluid lead to a large reduction in the sum total of kinetic and Coulomb energy.[1]

15.1 BCS theory with momentum-dependent coupling

We now illustrate these two different ways in which superconductors "overcome" the Coulomb interaction, by returning to the more generalized version of BCS theory with a momentum-dependent interaction:

[1] In weakly interacting systems we are trying to reduce the Coulomb energy in the face of a large kinetic energy, but in strongly interacting systems we are more often trying to reduce the kinetic energy in the face of large Coulomb interactions.

$$H = \sum_{\mathbf{k}\sigma} \epsilon_{\mathbf{k}} c^{\dagger}_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} + \overbrace{\sum_{\mathbf{k},\mathbf{k}'} V_{\mathbf{k},\mathbf{k}'} (c^{\dagger}_{\mathbf{k}\uparrow} c^{\dagger}_{-\mathbf{k}\downarrow})(c_{-\mathbf{k}'\downarrow} c_{\mathbf{k}'\uparrow})}^{H_I}. \tag{15.1}$$

Notice how we have deliberately included a + sign in front of the interaction H_I, to emphasize its predominantly repulsive character. As before, we carry out a Hubbard–Stratonovich decoupling of the interaction:

$$H_I \to \sum_{\mathbf{k}} \left[\bar{\Delta}_{\mathbf{k}} c_{-\mathbf{k}\downarrow} c_{\mathbf{k}\uparrow} + \text{H.c.}\right] - \sum_{\mathbf{k},\mathbf{k}'} \bar{\Delta}_{\mathbf{k}} V^{-1}_{\mathbf{k},\mathbf{k}'} \Delta_{\mathbf{k}'}, \tag{15.2}$$

where $V^{-1}_{\mathbf{k},\mathbf{k}'}$ is the inverse of the matrix $V_{\mathbf{k},\mathbf{k}'}$. While this is formally exact inside a path integral, following s-wave BCS theory we seek a mean-field theory in which the $\Delta_{\mathbf{k}}$ are static. The only place where $V_{\mathbf{k},\mathbf{k}'}$ appears is in the last term, so we can immediately diagonalize the resulting BCS theory to obtain a quasiparticle dispersion $E_{\mathbf{k}} = \sqrt{\epsilon_{\mathbf{k}}^2 + |\Delta_{\mathbf{k}}|^2}$ in which the function $\Delta_{\mathbf{k}}$ is obtained self-consistenly by minimizing the free energy.

We can immediately generalize the mean-field free energy obtained for the momentum-independent interaction (14.145),

$$\mathcal{F} = -2T \sum_{\mathbf{k}} \Big[\ln[2\cosh(\beta E_{\mathbf{k}}/2)] \Big] - \sum_{\mathbf{k},\mathbf{k}'} \bar{\Delta}_{\mathbf{k}} V^{-1}_{\mathbf{k},\mathbf{k}'} \Delta_{\mathbf{k}'}, \tag{15.3}$$

and if we differentiate with respect to $\bar{\Delta}_{\mathbf{k}}$, we obtain

$$\frac{\delta F}{\delta \bar{\Delta}_{\mathbf{k}}} = -\tanh(\beta E_{\mathbf{k}}/2) \frac{\Delta_{\mathbf{k}}}{2E_{\mathbf{k}}} - \sum_{\mathbf{k}'} V^{-1}_{\mathbf{k},\mathbf{k}'} \Delta_{\mathbf{k}'} = 0. \tag{15.4}$$

Inverting this equation by multiplying by $V_{\mathbf{k},\mathbf{k}'}$, we obtain the BCS gap equation:

$$\Delta_{\mathbf{k}} = -\sum_{\mathbf{k}'} V_{\mathbf{k},\mathbf{k}'} \left(\frac{\Delta_{\mathbf{k}'}}{2E_{\mathbf{k}'}} \tanh\left(\frac{\beta E_{\mathbf{k}'}}{2}\right)\right). \tag{15.5}$$

BCS gap equation: momentum-dependent coupling

The zero-temperature limit of this equation takes the simpler form

$$\Delta_{\mathbf{k}} = -\sum_{\mathbf{k}'} V_{\mathbf{k},\mathbf{k}'} \left(\frac{\Delta_{\mathbf{k}'}}{2E_{\mathbf{k}'}} \right). \tag{15.6}$$

Note the minus sign in front of this equation! If the interaction is uniformly attractive, so that $V_{\mathbf{k},\mathbf{k}'} < 0$ is negative, then this equation is satisfied by a uniformly positive gap function. However, in general the interaction $V_{\mathbf{k},\mathbf{k}'}$ will contain repulsive (i.e. positive) terms, so a uniformly positive gap function cannot satisfy the gap equation, giving rise to gap *nodes* where the gap changes sign. The most satisfying kind of solution occurs if the sign of the gap function can satisfy

$$\text{sgn}(\Delta_{\mathbf{k}}) = -\text{sgn}(V_{\mathbf{k},\mathbf{k}'})\,\text{sgn}(\Delta_{\mathbf{k}'}), \tag{15.7}$$

so that *regions of phase space that are linked by a repulsive interaction will have opposite gap signs*, whereas regions linked by an attractive interaction will have the same sign. This is the situation that leads to the largest gap and the largest mean-field transition temperature. We shall see that this can occur in two ways:

- In electron–phonon superconductors, where the interaction is repulsive at high energies, the gap function $\Delta(\epsilon)$ is largely isotropic in momentum space, but is energy-dependent and changes sign at an energy comparable with the Debye frequency.
- In anisotropic superconductors, the gap function $\Delta_{\mathbf{k}}$ becomes strongly momentum-dependent and acquires nodes in momentum space.

This last mechanism appears to be at work in all electronically mediated superconductors: organic, heavy-fermion, high-temperature cuprate and iron-based superconductors. We shall now illustrate this physics by using the BCS gap equation.

Example 15.1 The simplest anisotropic pair potential takes a factorizable form $V_{\mathbf{k},\mathbf{k}'} = -\frac{g_0}{V}\gamma_{\mathbf{k}}\gamma_{\mathbf{k}'}$, where $\gamma_{\mathbf{k}}$ is real and normalized, $\sum_{\mathbf{k}}(\gamma_{\mathbf{k}})^2 = 1$. In this case,

$$H_I = -\frac{g_0}{V}A^{\dagger}A, \tag{15.8}$$

but now the pairs acquire a spatial form factor

$$A = \sum_{\mathbf{k}}\left(\gamma_{\mathbf{k}}c_{-\mathbf{k}\downarrow}c_{\mathbf{k}\uparrow}\right), \qquad A^{\dagger} = \sum_{\mathbf{k}}\left(\gamma_{\mathbf{k}}c^{\dagger}_{\mathbf{k}\uparrow}c^{\dagger}_{-\mathbf{k}\downarrow}\right). \tag{15.9}$$

For example, in a simple model of d-wave pairing in a square two-dimensional lattice of side length a, $\gamma_{\mathbf{k}} = \cos(k_x a) - \cos(k_y)$.

(a) Show that the action for this case is identical to that of s-wave pairing, except that the gap $\Delta \to \Delta_{\mathbf{k}} = \Delta\gamma_{\mathbf{k}}$ now acquires a form-factor $\gamma_{\mathbf{k}}$. Write the action for the path integral.

(b) Derive the gap equation for the factorizable interaction above.

Solution

(a) We carry out a Hubbard–Stratonovich decoupling of the interaction that is formally the same as for s-wave pairing:

$$H_I = -\frac{g_0}{V}\bar{A}A \to \bar{\Delta}A + \bar{A}\Delta + \frac{V}{g_0}\bar{\Delta}\Delta. \tag{15.10}$$

Now we substitute $\bar{A} = \sum_{\mathbf{k}}\gamma_{\mathbf{k}}\bar{c}_{\mathbf{k}\uparrow}\bar{c}_{-\mathbf{k}\downarrow}$ and $A = \sum_{\mathbf{k}}\gamma_{\mathbf{k}}c_{-\mathbf{k}\downarrow}c_{\mathbf{k}\uparrow}$ to obtain

$$H_I = \sum_{\mathbf{k}}\gamma_{\mathbf{k}}\left(\bar{\Delta}c_{-\mathbf{k}\downarrow}c_{\mathbf{k}\uparrow} + \text{H.c.}\right) + \frac{V}{g_0}\bar{\Delta}\Delta.$$

Following the approach of Section 13.6, written in a Nambu notation the action for the path integral is then

$$
\begin{aligned}
S &= \int_0^\beta d\tau \sum_{\mathbf{k}} \bar{\psi}_{\mathbf{k}}(\partial_\tau + \epsilon_{\mathbf{k}}\tau_3)\psi_{\mathbf{k}} + H_I \\
&= \int_0^\beta d\tau \left\{ \sum_{\mathbf{k}} \bar{\psi}_{\mathbf{k}}(\partial_\tau + \underline{h}_{\mathbf{k}})\psi_{\mathbf{k}} + \frac{V}{g_0}\bar{\Delta}\Delta \right\},
\end{aligned}
\tag{15.11}
$$

where $h_{\mathbf{k}} = \epsilon_{\mathbf{k}}\tau_3 + \gamma_{\mathbf{k}}(\bar{\Delta}\tau_- + \Delta\tau_+)$ and $\tau_\pm = \frac{1}{2}(\tau_1 \pm i\tau_2)$.

(b) Approximating the path integral by a mean-field saddle-point approximation, where $\bar{\Delta}(\tau) = \bar{\Delta}$ is a real constant, the mean-field free energy is then given by

$$
\begin{aligned}
F &= -T \sum_{\mathbf{k}, i\omega_n} \mathrm{Tr} \ln(-i\omega_n + h_{\mathbf{k}}) + \frac{V}{g_0}|\Delta|^2 \\
&= -T \sum_{\mathbf{k}} \ln\left[2\cosh\left(\frac{\beta E_{\mathbf{k}}}{2}\right)\right] + \frac{V}{g_0}|\Delta|^2,
\end{aligned}
\tag{15.12}
$$

where $E_{\mathbf{k}} = \sqrt{\epsilon_{\mathbf{k}}^2 + \gamma_{\mathbf{k}}^2|\Delta|^2}$. Finally, differentiating with respect to $\bar{\Delta}$, we obtain

$$
\frac{\partial F}{\partial \bar{\Delta}} = 0 = -\sum_{\mathbf{k}} \frac{\gamma_{\mathbf{k}}^2 \Delta}{2E_{\mathbf{k}}} \tanh\left(\frac{\beta E_{\mathbf{k}}}{2}\right) + \frac{V}{g_0}\Delta,
\tag{15.13}
$$

from which we have the gap equation

$$
\frac{V}{g_0} = \sum_{\mathbf{k}} \frac{\gamma_{\mathbf{k}}^2}{2E_{\mathbf{k}}} \tanh\left(\frac{\beta E_{\mathbf{k}}}{2}\right).
\tag{15.14}
$$

In the continuum limit, this becomes

$$
\frac{1}{g_0} = \int_{\mathbf{k}} \frac{\gamma_{\mathbf{k}}^2}{2E_{\mathbf{k}}} \tanh\left(\frac{\beta E_{\mathbf{k}}}{2}\right).
\tag{15.15}
$$

15.2 Retardation and the Coulomb pseudopotential

In Chapter 7, we encountered the Bardeen–Pines model interaction,

$$
V_{eff}(\mathbf{q}, \omega) = \left[\frac{e^2}{\epsilon_0(q^2 + \kappa^2)}\right]\left(1 + \frac{\omega_q^2}{\omega^2 - \omega_q^2}\right),
\tag{15.16}
$$

where the first term describes the instantaneous Coulomb interaction and the second static
describes the retarded attractive component due to phonons. Notice that the Bardeen–Pines interaction, taken in its entirety, is *always* repulsive, but is less so at low energies.

A simple BCS model that captures the character of this interaction has the form $V_{\mathbf{k},\mathbf{k}'} = V_{eff}(\omega)|_{\omega=\epsilon_{\mathbf{k}}-\epsilon_{\mathbf{k}'}}$, where

$$V_{eff}(\omega) = N(0)^{-1} \times \begin{cases} \mu - g & (|\omega| < \omega_D) \\ \mu & \text{(otherwise)}, \end{cases} \tag{15.17}$$

corresponding to an attractive electron–phonon interaction of strength $-g/N(0)$ operating at energy scales lower than the Debye frequency ω_D, superimposed on an instantaneous Coulomb repulsive interaction of strength $+\mu/N(0)$ (Figure 15.1), where μ is a dimensionless coupling constant representing the Fermi surface average of the Coulomb interaction.[2]

If we Fourier transform this interaction to the time domain, we obtain

$$\begin{aligned} N(0)V_{eff}(t) &= N(0)\int \frac{d\omega}{2\pi} V_{eff}(\omega)e^{-i\omega t} = \mu \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} e^{-i\omega t} - g \int_{-\omega_D}^{\omega_D} \frac{d\omega}{2\pi} e^{-i\omega t} \\ &= \overbrace{\mu\delta(t)}^{\text{Instantaneous repulsion}} \underbrace{- \frac{g\omega_D}{\pi}\left(\frac{\sin \omega_D t}{\omega_D t}\right)}_{\text{retarded attraction}}, \end{aligned} \tag{15.18}$$

where t is the time between "emission" and "absorption" of the exchange boson. We see that the interaction contains an instantaneous delta-function repulsion and a retarded attraction with an oscillatory tail. It is the second term that drives the pairing.

We now show that the retardation has the effect of renormalizing the effective Coulomb interaction down to a much weaker value,

$$\mu^* = \frac{\mu}{1 + \mu \ln(D/\omega_D)}, \tag{15.19}$$

where D is the half-bandwidth and ω_D is the Debye energy. Typically, the ratio $D/\omega_D \sim 10^5\,\text{K}/500\,\text{K} \sim 10^2$, so that $\ln(D/\omega_D) \sim 5$ and, even if the bare Coulomb coupling constant is of order unity, the renormalized Coulomb coupling constant $\mu^* \sim 1/6$. Provided $g - \mu^* > 0$, the renormalized s-wave pairing interacton is attractive and superconductivity develops.

We shall slightly modify interaction (15.17), and write the BCS interaction in the form

$$V_{eff}(\mathbf{k}, \mathbf{k}') = N(0)^{-1} \times \begin{cases} \mu - g & (|\epsilon_{\mathbf{k}}|,\ |\epsilon_{\mathbf{k}'}| < \omega_D) \\ \mu & \text{(otherwise)}. \end{cases} \tag{15.20}$$

Let us assume a constant density of states $N(\epsilon) = N(0)$, replacing the momentum sum by an energy integral, $\sum_{\mathbf{k}'} \rightarrow N(0)\int d\epsilon$, and denoting $\Delta(\epsilon_{\mathbf{k}}) = \Delta_{\mathbf{k}}$. Then the gap equation (15.6) becomes

$$\Delta(\epsilon) = -N(0)\int_{-D}^{D} d\epsilon' V(\epsilon, \epsilon') \frac{\Delta(\epsilon')}{2E(\epsilon')}, \tag{15.21}$$

[2] Caution: by convention we adopt the "μ" notation for the repulsive interaction, in the full knowledge that it clashes with our notation for the chemical potential.

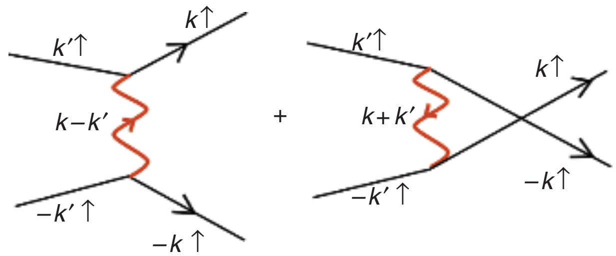


Fig. 15.3 Direct and exchange scattering of a triplet pair.

where we have restricted the sum over momentum space to one-half of momentum space, reflecting the fact that singlet and triplet pairs are only independently defined in half of momentum space ($\mathbf{k} \in \frac{1}{2}BZ$). Now the equal spin pairing terms also involve triplet pairs, which also interact via the triplet interaction $V^T_{\mathbf{k},\mathbf{k}'}$. We find

$$V^{\uparrow\uparrow}_{BCS} + V^{\downarrow\downarrow}_{BCS} = \sum_{\mathbf{k},\mathbf{k}' \in \frac{1}{2}BZ} (V_{\mathbf{k}-\mathbf{k}'} - V_{\mathbf{k}+\mathbf{k}'}) \left[(c^\dagger_{\mathbf{k}\uparrow} c^\dagger_{-\mathbf{k}\uparrow})(c_{-\mathbf{k}'\uparrow} c_{\mathbf{k}'\uparrow}) + (c^\dagger_{\mathbf{k}\downarrow} c^\dagger_{-\mathbf{k}\downarrow})(c_{-\mathbf{k}'\downarrow} c_{\mathbf{k}'\downarrow}) \right]. \tag{15.39}$$

The appearance of scattering of amplitude $V_{\mathbf{k}-\mathbf{k}'}$ and amplitude $V_{\mathbf{k}+\mathbf{k}'}$ can be understood as a result of the exchange scattering term shown in Figure 15.3. A compact way to represent both parallel and unequal spin pair operators is to use the vector of $S = 1$ triplet pair operators:

$$\vec{\Psi}^{T\dagger}_{\mathbf{k}} = c^\dagger_{\mathbf{k}\alpha} \left(\vec{\sigma} i\sigma_2 \right)_{\alpha\beta} c^\dagger_{-\mathbf{k}\beta} = \begin{cases} c^\dagger_{\mathbf{k}\downarrow} c^\dagger_{-\mathbf{k}\downarrow} - c^\dagger_{\mathbf{k}\uparrow} c^\dagger_{-\mathbf{k}\uparrow}, & \text{x} \\ i(c^\dagger_{\mathbf{k}\downarrow} c^\dagger_{-\mathbf{k}\downarrow} + c^\dagger_{\mathbf{k}\uparrow} c^\dagger_{-\mathbf{k}\uparrow}), & \text{y} \\ c^\dagger_{\mathbf{k}\uparrow} c^\dagger_{-\mathbf{k}\downarrow} + c^\dagger_{\mathbf{k}\uparrow} c^\dagger_{-\mathbf{k}\downarrow}, & \text{z} \end{cases} \tag{15.40}$$

refering to the x, y, and z components of the pair operator. The z component describes unequal spin pairing, while the x and y components describe linear combinations of equal spin pairing. Under a rotation, the triplet creation operator $\vec{\Psi}^{T\dagger}_{\mathbf{k}}$ transforms as a vector. In this notation, the BCS interaction is written

$$\hat{V}_{BCS} = \sum_{\mathbf{k},\mathbf{k}' \in \frac{1}{2}BZ} \left(V^S_{\mathbf{k},\mathbf{k}'} \Psi^{S\dagger}_{\mathbf{k}} \Psi^S_{\mathbf{k}'} + V^T_{\mathbf{k},\mathbf{k}'} \vec{\Psi}^{T\dagger}_{\mathbf{k}} \cdot \vec{\Psi}^T_{\mathbf{k}'} \right). \tag{15.41}$$

Note the following:

– If one is only interested in singlet pairing, one can drop the triplet pairing terms and consider the interaction

$$V_{BCS} = \sum V^S_{\mathbf{k},\mathbf{k}'} (c^\dagger_{\mathbf{k}\uparrow} c^\dagger_{-\mathbf{k}\downarrow})(c_{-\mathbf{k}'\downarrow} c_{\mathbf{k}'\uparrow}). \tag{15.42}$$

– One can decompose pairs into their orbital angular momentum components. Since the parity of a pair is related to its orbital angular momentum quantum number L by $P = (-1)^L$, even-parity superconductors involve even L (s, d, ... wave), while odd-parity triplet pairs involve L odd (p, f, ... wave).

Let us now return to consider the pair potential induced by the magnetic interaction

$$\begin{aligned} V_{mag} &= \frac{1}{2}\sum_{\mathbf{q}} J_{\mathbf{q}}\left[\vec{S}_{-\mathbf{q}}\cdot\vec{S}_{\mathbf{q}}\right] \\ &= \frac{1}{2}\sum_{\mathbf{k}_1,\mathbf{k}_2,\mathbf{q}} J_{\mathbf{q}} c^{\dagger}_{\mathbf{k}_1+\mathbf{q}\alpha} c^{\dagger}_{\mathbf{k}_2-\mathbf{q}\gamma}\left(\frac{\vec{\sigma}}{2}\right)_{\alpha\beta}\cdot\left(\frac{\vec{\sigma}}{2}\right)_{\gamma\delta} c_{\mathbf{k}_2\delta}c_{\mathbf{k}_1\beta}, \end{aligned} \tag{15.43}$$

where the $J_{\mathbf{q}}$ is an effective renormalized interaction between the quasiparticles. For example, in the cuprate superconductors, nearest-neighbor antiferromagnetic interactions derive from the vicinity to a Mott transition; these give rise to an antiferromagnetic interaction of the form $J_{\mathbf{q}} = 2J(\cos q_x a + \cos q_y a)$, where a is the separation of Cu atoms in a two-dimensional square lattice.

Now we need to consider the spin dependence of the interaction, determined by the matrices $\left(\frac{\vec{\sigma}}{2}\right)_{\alpha\beta}\cdot\left(\frac{\vec{\sigma}}{2}\right)_{\gamma\delta} \equiv \vec{S}_1\cdot\vec{S}_2$. We note that the eigenvalue of $\vec{S}_1\cdot\vec{S}_2$ is different for singlet and triplet states:

$$\vec{S}_1\cdot\vec{S}_2 = \begin{cases} +\frac{1}{4} & \text{(triplet)} \\ -\frac{3}{4} & \text{(singlet).} \end{cases} \tag{15.44}$$

Since the symmetric and antisymmetric parts of the interaction filter out the singlet and triplet pairs, respectively, these eigenvalues must now enter as prefactors into the pairing potentials, giving

$$\begin{aligned} V^{S}_{\mathbf{k},\mathbf{k}'} &= -\frac{3}{4}\left(\frac{J_{\mathbf{k}-\mathbf{k}'}+J_{\mathbf{k}+\mathbf{k}'}}{2}\right) \\ V^{T}_{\mathbf{k},\mathbf{k}'} &= \frac{1}{4}\left(\frac{J_{\mathbf{k}-\mathbf{k}'}-J_{\mathbf{k}+\mathbf{k}'}}{2}\right). \end{aligned} \tag{15.45}$$

Remarks

- Antiferromagnetic interactions ($J_{\mathbf{k}-\mathbf{k}'} > 0 \Rightarrow V^{S}_{\mathbf{k},\mathbf{k}'} < 0$) attract in the anisotropic singlet channel, whereas ferromagnetic interactions ($J_{\mathbf{k}-\mathbf{k}'} < 0 \Rightarrow V^{T}_{\mathbf{k},\mathbf{k}'} < 0$) attract in the triplet channel:

antiferromagnetic interaction ↔ singlet (mainly d-wave) anisotropic pairing
ferromagnetic interaction ↔ triplet (mainly p-wave) anisotropic pairing.

- The idea that ferromagnetic interactions could drive triplet pairing in nearly ferromagnetic metals, such as palladium, was first proposed by Layzer and Fay in the early 1970s [2]. In 1986 the discovery of antiferromagnetic spin fluctuations in the heavy-fermion superconductor UPt_3 led three separate groups (Zazie Béal Monod, Claude Bourbonnais, and Victor Emery at Orsay, Sherbrooke, and Brookhaven National Laboratory [3]; Kazu Miyake, Stefan Schmitt-Rink, and Chandra Varma at Bell Laboratories [4]; and Douglas Scalapino, Eugene Loh, and Jorge Hirsh at the University of California, Santa Barbara [5]), to propose that antiferromagnetic fluctuations drive d-wave superconductivity.

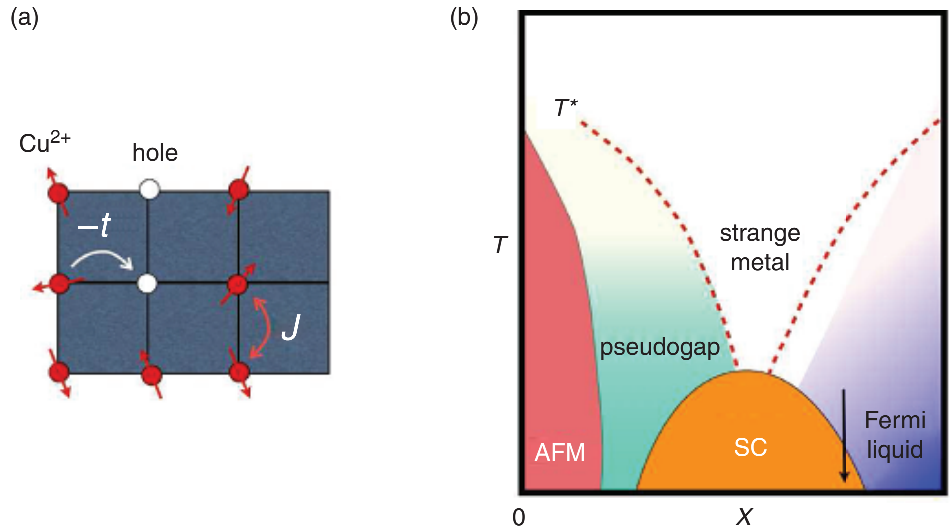


Fig. 15.4

(a) Superconductivity in cuprate superconductors involves the two-dimensional motion of electrons on a square lattice. The undoped material contains a square lattice of Cu^{2+} ions, each carrying a localized $S = \frac{1}{2}$ moment. When holes (or electrons) are introduced into the lattice via doping, the spins become mobile and the residual antiferromagnetic interactions drive d-wave pairing. A simplified model treats this as a single band of electrons of concentration $1 - x$, moving on a square lattice with hopping strength $-t$ and nearest-neighbor antiferromagnetic interaction J. (b) Schematic phase diagram of cuprate superconductors where x is the degree of hole doping. A commensurate antiferromagnetic insulator (pink) forms at small x, while at higher doping a superconducting dome develops. The normal state contains a pseudogap at low doping, forming a strange metal at optimal doping, with a linear resistivity. Fermi-liquid-like properties only develop at high doping, and it is only in this regime that the superconducting instability can be treated as a bona-fide Cooper pair instability of a Fermi liquid.

The basic connection between anisotropic singlet superconductivity and antiferromagnetic interactions is relevant to a wide variety of superconductors.

- If one is only interested in anisotropic singlet pairing, it is sufficient to work with an interaction of the form

$$V_{BCS} = -\frac{3}{4}\sum_{\mathbf{k},\mathbf{k}'}\left(\frac{J_{\mathbf{k}-\mathbf{k}'} + J_{\mathbf{k}+\mathbf{k}'}}{2}\right)(c^{\dagger}_{\mathbf{k}\uparrow}c^{\dagger}_{-\mathbf{k}\downarrow})(c_{-\mathbf{k}'\downarrow}c_{\mathbf{k}'\uparrow}).$$

15.4 d-wave pairing in two-dimensions

One of the most dramatic examples of anisotropic pairing is provided by the d-wave pairing in the copper oxide layers of the cuprate superconductors. These materials form antiferromagnetic Mott insulators, but when electrons or holes are introduced into the layers by doping, the magnetism is destroyed and the doped Mott insulator develops d-wave superconductivity. The normal state of these materials is not well understood, and for most of the phase diagram it cannot be treated as a Fermi liquid. For instance, at optimal doping these materials exhibit a linear resistivity $\rho(T) = AT + \rho_0$ due to electron–electron scattering that cannot be understood within the Fermi liquid framework. However, in the over-doped materials Fermi liquid behavior appears to recover and a BCS treatment is thought to be applicable.

Here we consider a drastically simplified model of a d-wave superconductor in which the fermions move on a two-dimensional tight-binding lattice with a dispersion $\epsilon_{\mathbf{k}} = -2t(\cos k_x a + \cos k_y a) - \mu$, where t is the nearest-neighbor hopping amplitude, interacting via an onsite Coulomb repulsion and a nearest-neighbor antiferromagnetic interaction, so that the Hamiltonian becomes

$$H = \sum_{\mathbf{k}} \epsilon_{\mathbf{k}} c^{\dagger}_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} + \sum_{j} U n_{j\uparrow} n_{j\downarrow} + J \sum_{(i,j)} \vec{S}_i \cdot \vec{S}_j, \tag{15.46}$$

while, in momentum space,

$$\begin{aligned} H &= \sum_{\mathbf{k}} \epsilon_{\mathbf{k}} c^{\dagger}_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} + \frac{1}{2} \sum_{\mathbf{q}} \left[U \rho_{-\mathbf{q}} \cdot \rho_{\mathbf{q}} + J_{\mathbf{q}} \vec{S}_{-\mathbf{q}} \cdot \vec{S}_{\mathbf{q}} \right] \\ J_{\mathbf{q}} &= 2J(\cos q_x a + \cos q_y a). \end{aligned} \tag{15.47}$$

Provided U and J are small compared with the bandwidth of the electron band, we can treat this as a Fermi liquid with a BCS interaction in the singlet channel given by

$$V^{singlet}_{\mathbf{q}} = U - \frac{3J}{2}(\cos q_x a + \cos q_y a).$$

Here, following the previous section, we have multiplied the spin-dependent interaction by $-3/4$ to take care of the expectation value of $\vec{S}_1 \cdot \vec{S}_2 = -3/4$ in the singlet channel. When we replace $\mathbf{q} \rightarrow \mathbf{k} - \mathbf{k}'$ and symmetrize on momenta to obtain the singlet interaction, we obtain

$$V_{\mathbf{k},\mathbf{k}'} = \frac{1}{2}\left[V^{singlet}(\mathbf{k} - \mathbf{k}') + V^{singlet}(\mathbf{k} + \mathbf{k}') \right] = U - \frac{3J}{2}(c_x c_{x'} + c_y c_{y'}), \tag{15.48}$$

where we have used the notation $c_x \equiv \cos k_x$, $c_y \equiv \cos k_y$, and so on. The mean-field BCS Hamiltonian is then

$$H_{BCS} = \sum_{\mathbf{k}\sigma} \epsilon_{\mathbf{k}} c^{\dagger}_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} + \sum_{\mathbf{k},\mathbf{k}'} \left(U - \frac{3J}{2}(c_x c_{x'} + c_y c_{y'}) \right) c^{\dagger}_{\mathbf{k}\uparrow} c^{\dagger}_{-\mathbf{k}\downarrow} c_{-\mathbf{k}'\downarrow} c_{\mathbf{k}'\uparrow}.$$

Let us immediately jump forward to look at the gap equation,

$$\Delta_{\mathbf{k}} = -\int \frac{d^2k'}{(2\pi)^2} V_{\mathbf{k},\mathbf{k}'} \frac{\Delta_{\mathbf{k}'}}{2E_{\mathbf{k}'}} \tanh\left(\frac{\beta E_{\mathbf{k}'}}{2} \right). \tag{15.49}$$

In the gap equation, the interaction will preserve the symmetries of the pair. If we divide the interaction into an s-wave and a d-wave term, $V_{\mathbf{k},\mathbf{k}'} = V^S_{\mathbf{k},\mathbf{k}'} + V^D_{\mathbf{k},\mathbf{k}'}$, as follows,

$$\begin{aligned} V^S_{\mathbf{k},\mathbf{k}'} &= \overbrace{U}^{\text{s-wave}} \overbrace{- \frac{3}{4} J(c_x + c_y)(c_{x'} + c_{y'})}^{\text{extended s-wave}} && \text{(s-wave)} \\ V^D_{\mathbf{k},\mathbf{k}'} &= -\frac{3}{4} J(c_x - c_y)(c_{x'} - c_{y'}) && \text{(d-wave)}, \end{aligned} \tag{15.50}$$

then we see that the s-wave term is invariant under 90° rotations of $\mathbf{k}$ or $\mathbf{k}'$, whereas the d-wave term changes sign:

$$V^S_{\mathbf{k},\mathbf{k}'} = +V^S_{\mathbf{k},R\mathbf{k}'}, \qquad V^D_{\mathbf{k},\mathbf{k}'} = -V^D_{\mathbf{k},R\mathbf{k}'},$$

where $R\mathbf{k} = (-k_y, k_x)$. Notice how the onsite Coulomb interaction is absent from the d-channel. A condensate with d-symmetry,

$$\Delta^D_{\mathbf{k}} = \Delta_D(c_x - c_y),$$

such that $\Delta^D_{R\mathbf{k}} = -\Delta^D_{\mathbf{k}}$, will couple to Cooper pairs via the d-wave interaction, because its integral with s-wave functions must change sign under $\pi/2$ rotations and is hence zero, $\sum_{\mathbf{k}'} V^S_{\mathbf{k},\mathbf{k}'} \Delta^D_{\mathbf{k}'}(\ldots) = 0$. By contrast, a condensate with *extended s-wave symmetry*, with the form

$$\Delta^S_{\mathbf{k}} = \Delta_1 + \Delta_2(c_x + c_y),$$

for which $\Delta^S_{R\mathbf{k}} = +\Delta^S_{\mathbf{k}}$, will vanish when integrated with the d-wave part of the interaction, $\sum_{\mathbf{k}'} V^D_{\mathbf{k},\mathbf{k}'} \Delta^S_{\mathbf{k}'}(\ldots) = 0$. In this case the two types of pairing are symmetry decoupled; moreoever, *the symmetry of the d-wave pair condensate orthogonalizes against the local Coulomb pseudopotential*.

Let us now look more carefully at the d-wave condensate, where the gap function $\Delta^D_{\mathbf{k}} = \Delta_D(c_x - c_y)$ vanishes along *nodes* along the diagonals $k_x = \pm k_y$. The corresponding quasiparticle energy

$$E_{\mathbf{k}} = \sqrt{\epsilon^2_{\mathbf{k}} + \Delta^2_D(c_x - c_y)^2} \tag{15.51}$$

must therefore vanish at the intersection of the nodes (where $\Delta_{\mathbf{k}} = 0$) and the Fermi surface (where $\epsilon_{\mathbf{k}} = 0$), as illustrated in Figure 15.5. At the nodal points the dispersion can be linearized in momentum, so that

$$E \sim \sqrt{(\mathrm{v}_F \delta k^2_{\perp}) + (\mathrm{v}_{\Delta} \delta k_{\parallel})^2}$$

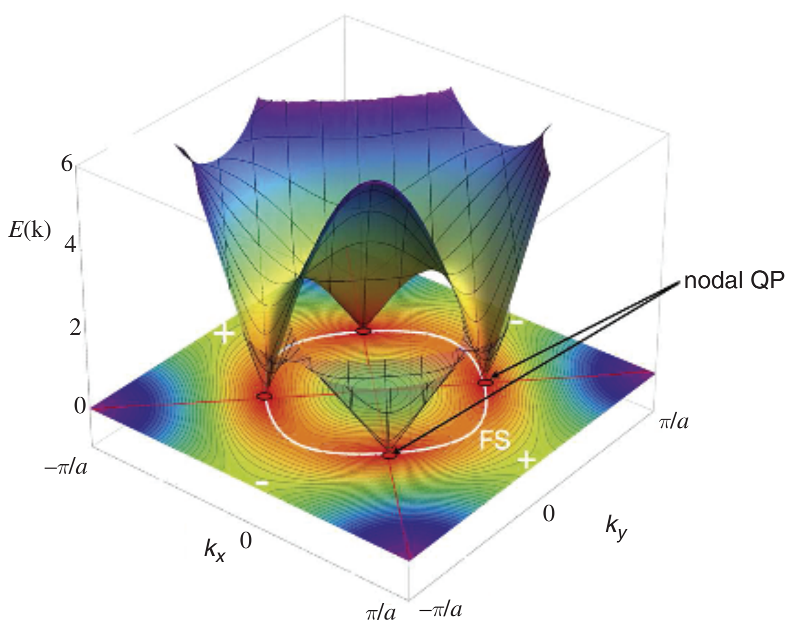


Fig. 15.5 Energy dispersion for a two-dimensional d-wave superconductor with a $d_{x^2-y^2}$ gap function. The upper part of the plot shows a cut-away three-dimensional plot of the dispersion, showing the banana-shaped quasiparticle cones of quasiparticle excitations around the nodes. In the lower contour plot, the position of the nodal excitations is seen to occur at the intersections of the Fermi surface (white line) and the nodal lines of the gap function (red line).

where $v_F = \partial E/\partial k_\perp$ is the Fermi velocity at the node and $v_\Delta = \partial E/\partial k_\parallel = \sqrt{2}\Delta_D a \sin\left(\frac{k_F a}{\sqrt{2}}\right)$ is the group velocity parallel to the Fermi surface created by the pairing. These excitations form a "Dirac cone" of excitations.

Let us now write out the gap equation for the d-wave solution in full:

$$\Delta_D(c_x - c_y) = -\int \frac{d^2k'}{(2\pi)^2} \overbrace{\left(-\frac{3}{4}J(c_x - c_y)(c_{x'} - c_{y'})\right)}^{V^D_{\mathbf{k},\mathbf{k}'}} \frac{\Delta_D(c_{x'} - c_{y'})}{2E_{\mathbf{k}'}} \tanh\left(\frac{\beta E_{\mathbf{k}'}}{2}\right). \tag{15.52}$$

Fortunately, the d-wave form factor $c_x - c_y$ drops out of both sides, to give

$$1 = \frac{3}{4}J \int \frac{d^2k}{(2\pi)^2} \frac{(c_x - c_y)^2}{2E_{\mathbf{k}}} \tanh\left(\frac{\beta E_{\mathbf{k}}}{2}\right). \tag{15.53}$$

Though it is straightforward to evaluate this kind of integral numerically, to get a feel of the physics let us suppose that the interaction only extends by an energy ω_{SF} around the Fermi energy, and that, furthermore, the band-filling around the Γ ($\mathbf{k} = 0$) point is small enough to use a quadratic approximation, $\epsilon_{\mathbf{k}} = -4t - \mu + tk^2$. In this case, the 2D density of states per spin $N(0) = \frac{1}{4\pi t}$ is a constant, while the gap function is

$$\Delta_D(c_y - c_x) = \Delta_D(k_x^2 - k_y^2) = \Delta_0 \cos 2\theta, \tag{15.54}$$

where $\Delta_0 = \Delta_D(k_F a)^2/2$ and a is the lattice spacing. Notice the characteristic $\Delta(\theta) \propto \cos 2\theta$ form, characteristic of an $l = 2$, d-wave Cooper pair. Now the gap equation becomes

$$1 = \frac{3}{4}JN(0) \int_{-\omega_{SF}}^{\omega_{SF}} d\epsilon \int_0^{2\pi} \frac{d\theta}{2\pi} \frac{\cos^2 2\theta}{2E} \tanh\left(\frac{\beta E}{2}\right)$$
$$E = \sqrt{\epsilon^2 + (\Delta_0 \cos 2\theta)^2}. \tag{15.55}$$

BCS gap equation: d-wave pairing

At T_c the average over angle gives $\frac{1}{2}$, so the equation for T_c is

$$1 = \frac{3}{8}JN(0) \int_0^{\omega_{SF}} d\epsilon \frac{1}{\epsilon} \tanh\left(\frac{\epsilon}{2T_c}\right). \tag{15.56}$$

This is identical to the BCS gap equation, but with $g = \frac{3}{8}JN(0)$, with the same formal form for $T_c = 1.13\omega_{SF}e^{-1/g}$.

It is particularly interesting to compute the d-wave density of states. Let us continue to use our approximation $\Delta(\theta) = \Delta_0 \cos 2\theta$. To compute the density of states, we must average the density of states we obtained for an s-wave superconductor (14.186) over angle:

$$N_D^*(E) = N(0)\,\mathrm{Re}\left\langle \frac{|E|}{\sqrt{(E - i\delta)^2 - \Delta^2\cos^2 2\theta}} \right\rangle_\theta, \tag{15.57}$$

where $\langle \ldots \rangle_\theta \equiv \int \frac{d\theta}{2\pi}(\ldots)$ and the real part cleverly builds in the fact that the density of states vanishes when $|E| < |\Delta(\theta)|$. We can recast this expression as a standard elliptic integral by making the change of variable $2\theta \to \phi - \pi/2$. The resulting integral over ϕ is then

$$\frac{N_D^*(E)}{N(0)} = \mathrm{Re}\left[\int_0^{\pi}\frac{d\phi}{\pi}\frac{|E|}{\sqrt{(E-i\delta)^2-\Delta^2\sin^2\phi}}\right] = \Phi\left[\frac{E-i\delta}{\Delta}\right], \tag{15.58}$$

where

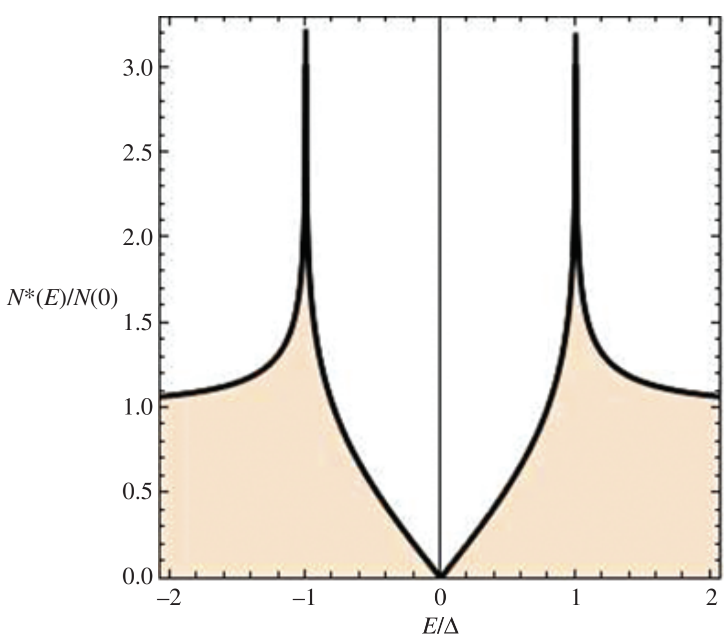
$$\Phi[x] = \frac{2}{\pi}\mathrm{Re}\left[K\left(\frac{1}{x^2}\right)\right] \tag{15.59}$$

is expressed in terms of the elliptic function

$$K(x) = \int_0^{\pi/2}\frac{d\phi}{\sqrt{1-x\sin^2\phi}}, \tag{15.60}$$

known from the study of the pendulum.[3] This function is plotted in Figure 15.6. The clean gap of the s-wave superconductor is now replaced by a V-shaped structure, with a low-lying linear density of states derived from the Dirac cones in the excitation spectrum, and a sharp coherence peak in the density of states around $E \sim \pm\Delta$. We can understand the linear density of states at low energies by remembering that, for a relativistic spectrum $E = ck$, the density of states is $\frac{1}{2\pi}k\frac{dk}{dE} = \frac{|E|}{(2\pi c^2)}$. For these anisotropic Dirac cones, we must replace $c^2 \to \mathrm{v}_F\mathrm{v}_\Delta$; taking into account the four nodal cones and remembering the tricky factor of $\frac{1}{2}$ that enters because of the energy average of the coherence factors in the tunneling density of states (14.184), we obtain

$$N^*(E) = \frac{1}{2}\times 4\times\frac{1}{2\pi}\frac{|E|}{\mathrm{v}_F\mathrm{v}_\Delta} = \overbrace{\frac{k_F}{2\pi\mathrm{v}_F}}^{N(0)}\frac{|E|}{\Delta} = N(0)\frac{|E|}{\Delta}, \tag{15.61}$$



Density of states $N^*(E)/N(0))$ for a d-wave superconductor.

Fig. 15.6

[3] Note: here we use the notation used by Mathematica, with x multiplying $\sin^2\phi$.

where we have put $v_\Delta = \partial E/\partial k_\parallel = (k_F)^{-1}\partial\Delta(\theta)/\partial\theta = 2\Delta/k_F$, identifying $N(0) = \frac{m}{2\pi} = \frac{k_F}{2\pi v_F}$.

Lastly, let us take a brief look at the alternative s-wave solution, where $\Delta_{\mathbf{k}} = \Delta_1 + \Delta_2(c_x + c_y)$. The first, momentum-independent term is entirely local, whereas the second term describes s-waves pairing with nearest neighbors. The gap equation

$$\Delta^S_{\mathbf{k}} = -\int \frac{d^2k'}{(2\pi)^2} \overbrace{\left(U - \frac{3}{4}J(c_x + c_y)(c_{x'} + c_{y'})\right)}^{V^S_{\mathbf{k},\mathbf{k}'}} \frac{\overbrace{\Delta^S_{\mathbf{k}}}^{\Delta_1+\Delta_2(c_{x'}+c_{y'})}}{2E_{\mathbf{k}'}} \tanh\left(\frac{\beta E_{\mathbf{k}'}}{2}\right) \tag{15.62}$$

is more complicated because there is cross-talk between the local and extended s-wave terms. To simplify our discussion, suppose we confine the interaction to within an energy ω_{SF} of the Fermi surface and assume that the filling of the Fermi surface is small enough that we can take $\mathbf{k} = \mathbf{k}' \sim 0$ in the pair potential. Then the effective s-wave coupling constant will be

$$V_{\mathbf{k},\mathbf{k}'} = U - \frac{3}{4}J\overbrace{(c_x + c_y)}^{\sim 2}\overbrace{(c_{x'} + c_{y'})}^{\sim 2} \to U - 3J, \tag{15.63}$$

which is only attractive providing $J > U/3$. We see that, for a single Fermi surface, the attraction in the extended-s-wave channel is suppressed by the Coulomb interaction, entirely vanishing if $J < J_c = U/3$. In fact, extended s-wave solutions are possible, and are believed to occur in the iron-based superconductors, but they require compensating Fermi surfaces in regions where $c_x + c_y$ have opposite signs, so that the Fermi surface average of the gap function vanishes, permitting a decoupling of the pairing from the repulsive Coulomb interaction.

Example 15.2 For a single Dirac cone of excitations with dispersion

$$E_{\mathbf{k}} = \sqrt{(v_x k_x)^2 + (v_y k_y)^2}, \tag{15.64}$$

show that the density of states is given by

$$N(E) = \frac{E}{2\pi v_x v_y}.$$

Solution

We write the density of states as

$$N(E) = \sum_{\mathbf{k}} \delta(E - E_{\mathbf{k}}) = \int \frac{dk_x dk_y}{(2\pi)^2}\delta\left(E - \sqrt{(v_x k_x)^2 + (v_y k_y)^2}\right). \tag{15.65}$$

Changing variables, $x = v_x k_x$, $y = v_y k_y$, then

$$N(E) = \int \frac{dxdy}{(2\pi)^2}\delta\left(E - \sqrt{(x^2 + y^2)}\right). \tag{15.66}$$

Changing $x = r\cos\theta$, $y = r\sin\theta$, then the measure becomes $dxdy \to rdrd\theta$ and the integral is

$$N(E) = \frac{1}{v_x v_y}\int \frac{d\theta\, rdr}{(2\pi)^2}\delta(E - r) = \frac{E}{2\pi v_x v_y}.$$

Example 15.3

(a) Carry out a Hubbard–Stratonovich decoupling of the BCS Hamiltonian on a two-dimensional lattice, where the pair potential is

$$V_{\mathbf{k},\mathbf{k}'} = \mathcal{N}_s^{-1}\left(U - \frac{3}{2}J(c_x c_{x'} + c_y c_{y'})\right), \tag{15.67}$$

($c_x \equiv \cos k_x a$, $c_y \equiv \cos k_y a$), and show that the mean-field action takes the form

$$S_{MFT} = \int_0^\beta \left\{ \sum_{\mathbf{k}} \bar{\psi}_{\mathbf{k}}(\partial_\tau + \overbrace{\epsilon_{\mathbf{k}}\tau_3 + \bar{\Delta}_{\mathbf{k}}\tau_- + \Delta_{\mathbf{k}}\tau_+}^{h_{\mathbf{k}}})\psi_{\mathbf{k}} + \mathcal{N}_s\left[\frac{4}{3J}(\bar{\Delta}_{2S}\Delta_{2S} + \bar{\Delta}_D\Delta_D) - \frac{\Delta_{1S}\Delta_{1S}}{U}\right]\right\}, \tag{15.68}$$

where

$$\Delta_{\mathbf{k}} = \Delta_{1S} + \Delta_{2S}(c_x + c_y) + \Delta_D(c_x - c_y) \tag{15.69}$$

is the momentum-dependent gap function.

(b) Write down the mean-field free energy.

(c) Assuming a d-wave solution (i.e. $\Delta_D \neq 0, \Delta_1 = \Delta_2 = 0$), rederive the gap equation for this problem.

(d) For a single Fermi surface, why will a d-wave condensate have a higher T_c than an extended s-wave condensate?

Solution

(a) Let us factorize the interaction into s- and d-wave component, as follows:

$$V_{\mathbf{k},\mathbf{k}'} = \frac{U}{\mathcal{N}_s}\gamma_{1S}(\mathbf{k})\gamma_{1S}(\mathbf{k}') - \frac{3J}{4\mathcal{N}_s}\left[\gamma_{2S}(\mathbf{k})\gamma_{2S}(\mathbf{k}') + \gamma_D(\mathbf{k})\gamma_D(\mathbf{k}')\right], \tag{15.70}$$

where $\gamma_{1S}(\mathbf{k}) = 1$, $\gamma_{2S}(\mathbf{k}) = c_x + c_y$, $\gamma_D(\mathbf{k}) = c_x - c_y$ are a set of normalized s-, extended s-, and d-wave form factors, respectively. We can then write the interaction Hamiltonian as

$$H_I = \frac{U}{\mathcal{N}_s}A^\dagger_{1S}A_{1S} - \frac{3J}{4\mathcal{N}_s}\left[A^\dagger_{2S}A_{2S} + A^\dagger_D A_D\right], \tag{15.71}$$

where

$$A_\Gamma = \sum_{\mathbf{k}} \phi_\Gamma(\mathbf{k}) c_{-\mathbf{k}\downarrow}c_{\mathbf{k}\uparrow} \qquad (\Gamma \in \{1S, 2S, D\}) \tag{15.72}$$

create s-, extended s-, and d-wave pairs, respectively. If we carry out a Hubbard–Stratonovich decoupling of each of the product terms in this interaction, we then obtain

$$\begin{aligned} H_I \to & \sum_{\Gamma\in\{1S,2S,D\}} \left(\bar{\Delta}_\Gamma A_\Gamma + \text{H.c.}\right) + \frac{4\mathcal{N}_s}{3J}\left(\bar{\Delta}_{2S}\Delta_{2S} + \bar{\Delta}_D\Delta_D\right) - \frac{\mathcal{N}_s}{U}\bar{\Delta}_{1S}\Delta_{1S} \\ &= \sum_{\mathbf{k}}\left(\bar{\Delta}_{\mathbf{k}}c_{-\mathbf{k}\downarrow}c_{\mathbf{k}\uparrow} + \bar{c}_{\mathbf{k}\uparrow}\bar{c}_{-\mathbf{k}\downarrow}\Delta_{\mathbf{k}}\right) + \frac{4\mathcal{N}_s}{3J}\left(\bar{\Delta}_{2S}\Delta_{2S} + \bar{\Delta}_D\Delta_D\right) \\ &\quad - \frac{\mathcal{N}_s}{U}\bar{\Delta}_{1S}\Delta_{1S}, \end{aligned} \tag{15.73}$$

where $\Delta_{\mathbf{k}} = \sum_\Gamma \gamma_\Gamma(\mathbf{k})\Delta_\Gamma = \Delta_{2S}(c_x + c_y) + \Delta_D(c_x - c_y)$. Then the complete transformed Hamiltonian takes the form

$$
\begin{aligned}
H &= \sum_{\mathbf{k}} \epsilon_{\mathbf{k}} c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} + \sum_{\mathbf{k}} (\Delta_{\mathbf{k}} c^\dagger_{\mathbf{k}\uparrow} c^\dagger_{-\mathbf{k}\downarrow} + \text{H.c.}) \\
&\quad + \mathcal{N}_s \left(\frac{4}{3J}(\bar{\Delta}_D \bar{\Delta}_D + \bar{\Delta}_{2S}\Delta_{2S}) - \frac{1}{U}\bar{\Delta}_{1S}\Delta_{1S} \right) \\
&= \sum_{\mathbf{k}} \psi^\dagger_{\mathbf{k}} \left(\epsilon_{\mathbf{k}} \tau_3 + \Delta_{\mathbf{k}} \tau^+ + \bar{\Delta}_{\mathbf{k}} \tau_- \right) \psi_{\mathbf{k}} \\
&\quad + \mathcal{N}_s \left(\frac{4}{3J}(\bar{\Delta}_D \Delta_D + \bar{\Delta}_{2S}\Delta_{2S}) - \frac{1}{U}\bar{\Delta}_{1S}\Delta_{1S} \right),
\end{aligned}
\tag{15.74}
$$

where we've dropped the constant remainder $\sum_{\mathbf{k}} \epsilon_{\mathbf{k}}$. The corresponding action is given by

$$
\begin{aligned}
S = \int_0^\beta \Bigg\{ &\sum_{\mathbf{k}} \bar{\psi}_{\mathbf{k}} (\partial_\tau + \overbrace{\epsilon_{\mathbf{k}}\tau_3 + \bar{\Delta}_{\mathbf{k}}\tau_- + \Delta_{\mathbf{k}}\tau_+}^{h_{\mathbf{k}}}) \psi_{\mathbf{k}} \\
&+ \mathcal{N}_s \left[\frac{4}{3J}(\bar{\Delta}_{2S}\Delta_{2S} + \bar{\Delta}_D \Delta_D) - \frac{\Delta_{1S}\Delta_{1S}}{U} \right] \Bigg\}.
\end{aligned}
$$

(b) Carrying out the Gaussian path integral over the Fermi fields for constant gap functions, we obtain

$$
Z_{MF} = e^{-\beta F_{MF}} = \int \mathcal{D}[\bar{\psi}, \psi] e^{-S},
$$

where

$$
\begin{aligned}
F_{MF} = -T \ln Z_{MF} &= -T \sum_{\mathbf{k}, i\omega_n} \ln \det[-i\omega_n + h_{\mathbf{k}}] \\
&\quad + \mathcal{N}_s \left[\frac{4}{3J}(\bar{\Delta}_{2S}\Delta_{2S} + \bar{\Delta}_D \Delta_D) - \frac{\Delta_{1S}\Delta_{1S}}{U} \right] \\
&= -T \sum_{\mathbf{k}, i\omega_n} 2 \ln[(i\omega_n)^2 - \epsilon^2_{\mathbf{k}} - \bar{\Delta}_{\mathbf{k}}\Delta_{\mathbf{k}}] \\
&\quad + \mathcal{N}_s \left[\frac{4}{3J}(\bar{\Delta}_{2S}\Delta_{2S} + \bar{\Delta}_D \Delta_D) - \frac{\Delta_{1S}\Delta_{1S}}{U} \right] \\
&= -T \sum_{\mathbf{k}} \ln \left[2\cos\left(\frac{\beta E_{\mathbf{k}}}{2} \right) \right] \\
&\quad + \mathcal{N}_s \left[\frac{4}{3J}(\bar{\Delta}_{2S}\Delta_{2S} + \bar{\Delta}_D \Delta_D) - \frac{\Delta_{1S}\Delta_{1S}}{U} \right],
\end{aligned}
\tag{15.75}
$$

where the last line follows from carrying out the Matsubara sum and $E_{\mathbf{k}} = \sqrt{\epsilon_{\mathbf{k}}^2 + |\Delta_{\mathbf{k}}|^2}$.

(c) Suppose Δ_D is the only non-zero component of the gap function. Then

$$F_{MF} = -T \sum_{\mathbf{k}} \ln \left[2 \cos \left(\frac{\beta E_{\mathbf{k}}}{2} \right) \right] + \mathcal{N}_s \frac{4}{3J} (\bar{\Delta}_{2S} \Delta_{2S}), \tag{15.76}$$

where $E_{\mathbf{k}} = \sqrt{\epsilon_{\mathbf{k}}^2 + \gamma_D(\mathbf{k})^2 \bar{\Delta}_D \Delta_D}$.

Taking the derivative of F_{MF} with respect to $\bar{\Delta}_D$, we obtain

$$\frac{\delta F_{MF}}{\delta \bar{\Delta}_D} = 0 = -\sum_{\mathbf{k}} \tanh \left(\frac{\beta E_{\mathbf{k}}}{2} \right) \frac{\gamma_D(\mathbf{k})^2 \Delta_D}{2E_{\mathbf{k}}} + \mathcal{N}_s \frac{4\Delta_D}{3J}, \tag{15.77}$$

giving us the gap equation,

$$\frac{4}{3J} = \int_{\mathbf{k}} \tanh \left(\frac{\beta E_{\mathbf{k}}}{2} \right) \frac{\gamma_D(\mathbf{k})^2}{2E_{\mathbf{k}}}. \tag{15.78}$$

(d) Whereas the d-wave condensate is completely decoupled from the repulsive U, so that $\partial^2 F_{MF}/\partial \Delta_{1S} \Delta_D = 0$, the extended s-wave component always mixes with the local s-wave component, which leads to a reduction of the effective coupling constant, so the d-wave Cooper instability will typically occur at a higher temperature. If we set the differentials of the free energy with respect to Δ_{1S} and Δ_{2S} to zero, we obtain two coupled gap equations, which, written in shorthand, are

$$\begin{aligned} \frac{4\Delta_{2S}}{3J} &= \Delta_{2S} \langle \gamma_{1S}^2 \rangle + \Delta_{1S} \langle \gamma_{1S} \gamma_{2S} \rangle \\ -\frac{\Delta_{1S}}{U} &= \langle \gamma_{1S}^2 \rangle \Delta_{1S} + \langle \gamma_{1S} \gamma_{2S} \rangle \Delta_{2S}, \end{aligned} \tag{15.79}$$

where we have used the shorthand $\langle \ldots \rangle = \sum_{\mathbf{k}} \frac{1}{2E_{\mathbf{k}}} \tanh \left(\frac{\beta E_{\mathbf{k}}}{2} \right) (\ldots)_{\mathbf{k}}$ (although $\gamma_{1S} = 1$, we have kept it in its symbolic form to show the symmetry of the equations). The two equations are coupled, because in general $\langle \gamma_{1S} \gamma_{2S} \rangle \neq 0$ for two s-wave form factors. We can eliminate Δ_{1S} from the second equation, to obtain

$$\Delta_{1S} = -\frac{\langle \gamma_{1S} \gamma_{2S} \rangle}{\langle \gamma_{1S}^2 \rangle + \frac{1}{U}} \Delta_{2S}. \tag{15.80}$$

In other words, providing $\langle \gamma_{1S} \gamma_{2S} \rangle \neq 0$, the extended s-wave solution will always induce a finite onsite s-wave pairing, which costs a lot of Coulomb repulsion energy. Substituting this into the first of the mean-field equations (15.79), we obtain

$$\frac{4}{3J_{eff}} = \left(\frac{4}{3J} + \frac{\langle \gamma_{1S} \gamma_{2S} \rangle^2}{\frac{1}{U} + \langle \gamma_{1S}^2 \rangle} \right) = \langle \gamma_{2S}(\mathbf{k})^2 \rangle = \int_{\mathbf{k}} \tanh \left(\frac{E_{\mathbf{k}}}{2T_c} \right) \gamma_{2S}(\mathbf{k})^2. \tag{15.81}$$

Since $1/J_{eff}$ is increased, we see that the effective coupling constant J_{eff} is reduced by the cross-talk between the extended s-wave channel and the onsite Coulomb interaction, suppressing the extended s-wave T_c. When the higher T_c d-wave condensate develops, this opens up a gap in the spectrum, pre-empting any lower-temperature s-wave instability. This is presumably why d-wave pairing predominates in the cuprate superconductors.

An important exception to this case occurs when there are multiple Fermi surface sheets which live in sectors of the extended s-wave form factor which have opposite sign. In this case, the average $\langle \gamma_{1S}\gamma_{2S}\rangle \sim 0$ and the larger average gap of the s-wave solution then favors extended s-wave over d-wave.

Example 15.4

(a) Show that the Nambu Green's function for a singlet superconductor with a momentum-dependent gap is

$$\mathcal{G}(\mathbf{k}, i\omega_n) = [i\omega_n - \epsilon_{\mathbf{k}}\tau_3 - \Delta_{\mathbf{k}}\tau_1]^{-1}, \tag{15.82}$$

where the gap function $\Delta_{\mathbf{k}} = \Delta_{-\mathbf{k}}$ assumed to be real.

(b) Using the Nambu Green's function, compute the tunneling density of states for a *three-dimensional* d-wave superconductor with gap $\Delta_{\mathbf{k}} = \Delta \cos 2\phi$.

Solution

(a) The Nambu Hamiltonian for a singlet superconductor with a momentum-dependent gap $\Delta_{\mathbf{k}} = \Delta(\phi) = \Delta \cos 2\phi$ is given by

$$\begin{aligned} H &= \sum_{\mathbf{k}} \psi^{\dagger}_{\mathbf{k}} \underline{h}_{\mathbf{k}} \psi_{\mathbf{k}} \\ \underline{h}_{\mathbf{k}} &= \epsilon_{\mathbf{k}}\tau_3 + \Delta \cos 2\theta\, \tau_1, \end{aligned} \tag{15.83}$$

where we taken the gap to be real. The Nambu Green's function is then

$$\mathcal{G}(\mathbf{k}, \omega) = \frac{1}{\omega - h_{\mathbf{k}}} = \frac{\omega + h_{\mathbf{k}}}{\omega^2 - (\epsilon^2_{\mathbf{k}} + \Delta^2 \cos^2 2\phi)}.$$

(b) The diagonal part of the Nambu Green's function is given by

$$[\mathcal{G}(k)]_{11} = \frac{\omega + \epsilon_{\mathbf{k}}}{\omega^2 - (\epsilon^2_{\mathbf{k}} + \Delta^2 \cos^2 2\phi)}$$

and the tunneling density of states is given by

$$\begin{aligned} N(\omega) &= \frac{1}{\pi} \sum_{\mathbf{k}} \mathrm{Im} \left(\frac{\omega + \epsilon_{\mathbf{k}}}{(\omega - i\delta)^2 - E^2_{\mathbf{k}}} \right) \\ &= \frac{1}{\pi} N(0) \int \frac{d\phi}{2\pi} \int d\epsilon\, \mathrm{Im} \left(\frac{\omega + \epsilon}{(\omega - i\delta)^2 - \epsilon^2 + \Delta(\phi)^2} \right) \\ &= -N(0) \int \frac{d\phi}{2\pi} \mathrm{Im} \left(\frac{\omega}{\sqrt{\Delta^2 \cos^2 2\phi - (\omega - i\delta)^2}} \right) \\ &= N(0) \int_0^{\pi/2} \frac{d\phi}{\pi/2} \mathrm{Re} \left(\frac{|\omega|}{\sqrt{(\omega - i\delta)^2 - \Delta^2 \sin^2 \phi}} \right) \\ &= \frac{2N(0)}{\pi} \mathrm{Re}\, K \left(\frac{\Delta}{\omega - i\delta} \right), \end{aligned} \tag{15.84}$$

where

$$K(x) = \int_0^{\pi/2} \frac{dx}{\sqrt{1 - x^2 \sin^2 \phi}}.$$

The last few stages of this calculation are the same as those in the derivation of the s-wave density of states in (14.185). We see that the form of the mean-field density of states of a three-dimensional d-wave system is the same as the density of states of a two-dimensional one.

Example 15.5

(a) By generalizing the approach taken in Section 13.8 for an s-wave superconductor, compute the London stiffness of a d-wave superconductor with gap $\Delta(\phi) = \Delta \cos\phi$, showing that it takes the form

$$Q_D(T) = Q_0 \left[1 - \int_{-\infty}^{\infty} d\omega \int \frac{d\phi}{2\pi} \left(-\frac{df(\omega)}{d\omega} \right) \mathrm{Re} \left(\frac{\omega}{\sqrt{\omega^2 - \Delta(\phi)^2}} \right) \right]$$
$$\Delta(\theta) = \Delta \cos(2\phi). \tag{15.85}$$

(b) Contrast the temperature dependence of the penetration depth in an s-wave and a clean d-wave superconductor.

Solution

This question is a little subtle at the beginning, because the d-wave gap has momentum dependence $\Delta_{\mathbf{k}}$, and it is not immediately clear whether, when a vector potential is included, we should make the Peierls replacement $\Delta_{\mathbf{k}} \to \Delta_{\mathbf{k}-e\mathbf{A}}$ or not.

One way to rationalize this is to notice that, in Nambu notation, the correct gauge-invariant Peierls replacement is $\mathbf{k} \to \mathbf{k} - e\mathbf{A}\tau_3$, so that in pairing terms of the form $\Delta_{\mathbf{k}}\tau_1$ we must replace

$$\Delta_{\mathbf{k}}\tau_1 \to \frac{1}{2}\{\Delta_{\mathbf{k}-e\mathbf{A}\tau_3}, \tau_1\} = \Delta_{\mathbf{k}} - \frac{e}{2}\nabla_{\mathbf{k}}\Delta_{\mathbf{k}} \overbrace{\{\tau_3, \tau_1\}}^{=0} = \Delta_{\mathbf{k}} + O(A^2), \tag{15.86}$$

so there is no correction to the current operator derived from the pairing, and the only important dependence of the BCS Hamiltonian on the vector potential comes from the kinetic energy $\epsilon_{\mathbf{k}-e\mathbf{A}\tau_3}\tau_3$ (14.241).

An alternative and more convincing way to argue the above is to explicitly introduce the vector potential into the pairing interaction using a Peierls substitution in real space. Consider the local pairing interaction, $-g\int_{\mathbf{x}} \Psi_D^\dagger(x)\Psi_D(x)$, where

$$\Psi_D^\dagger = \int_{\mathbf{R}} \gamma_D(\mathbf{R})\psi_\uparrow^\dagger(\mathbf{x} + \mathbf{R}/2)\psi_\downarrow^\dagger(\mathbf{x} - \mathbf{R}/2) \tag{15.87}$$

creates a d-wave pair with spatial form factor $\gamma_D(\mathbf{R})$ centered at $\mathbf{x}$. If we write the interaction out in full, it takes the form

$$
\begin{aligned}
H_I &= -g \int_{\mathbf{x},\mathbf{R},\mathbf{R}'} \gamma_D(\mathbf{R})\gamma_D(\mathbf{R}') \left(\psi^\dagger_\uparrow(\mathbf{x}+\mathbf{R}/2)\psi^\dagger_\downarrow(\mathbf{x}-\mathbf{R}/2)\right)\left(\psi_\downarrow(\mathbf{x}-\mathbf{R}'/2)\psi_\uparrow(\mathbf{x}+\mathbf{R}'/2)\right)\\
&= -g \int_{\mathbf{x},\mathbf{R},\mathbf{R}'} \gamma_D(\mathbf{R})\gamma_D(\mathbf{R}') : \left(\psi^\dagger_\uparrow(\mathbf{x}+\mathbf{R}/2)\psi_\uparrow(\mathbf{x}+\mathbf{R}'/2)\right)\\
&\qquad\qquad \times \left(\psi^\dagger_\downarrow(\mathbf{x}-\mathbf{R}/2)\psi_\downarrow(\mathbf{x}-\mathbf{R}'/2)\right) : \ ,
\end{aligned}
\tag{15.88}
$$

which involves the normal-ordered product of two hopping terms. To make this gauge-invariant, we need to make a Peierls substitution on each hopping term, replacing

$$
\begin{aligned}
\psi^\dagger_\uparrow(\mathbf{x}+\mathbf{R}/2)\psi_\uparrow(\mathbf{x}+\mathbf{R}'/2) &\to \psi^\dagger_\uparrow(\mathbf{x}+\mathbf{R}/2)\psi_\uparrow(\mathbf{x}+\mathbf{R}'/2)\, \overbrace{e^{-i\int_{\mathbf{x}+\mathbf{R}/2}^{\mathbf{x}+\mathbf{R}'/2}\mathbf{A}\cdot d\mathbf{l}}}^{e^{-i\mathbf{A}(\mathbf{x})\cdot(\mathbf{R}-\mathbf{R}')/2}}\\
\psi^\dagger_\downarrow(\mathbf{x}-\mathbf{R}/2)\psi_\downarrow(\mathbf{x}-\mathbf{R}'/2) &\to \psi^\dagger_\downarrow(\mathbf{x}-\mathbf{R}/2)\psi_\downarrow(\mathbf{x}-\mathbf{R}'/2)\, \overbrace{e^{-i\int_{\mathbf{x}-\mathbf{R}/2}^{\mathbf{x}-\mathbf{R}'/2}\mathbf{A}\cdot d\mathbf{l}}}^{e^{i\mathbf{A}(\mathbf{x})\cdot(\mathbf{R}-\mathbf{R}')/2}},
\end{aligned}
\tag{15.89}
$$

where the Peierls factors have been evaluated ignoring gradients in the vector potential. We notice that the two Peierls factors cancel, so there is no dependence of the pairing term on the external vector potential.

(a) We can now follow the methodology of Section 13.8, including the momentum dependence of the gap, throughout the calculation. We obtain

$$
Q_{ab} = \frac{4e^2}{\beta V}\sum_k \nabla_a\epsilon_{\mathbf{k}}\nabla_b\epsilon_{\mathbf{k}}\frac{\Delta^2_{\mathbf{k}}}{[(\omega_n)^2+\epsilon^2_{\mathbf{k}}+\Delta^2_{\mathbf{k}}]^2}.
\tag{15.90}
$$

Carrying out the integral over energy for each direction, and the summation over the Matsubara frequencies following the method of Section 14.8, then gives an angular-averaged version of (14.260):

$$
Q(T) = Q_0\left[1-\int_{-\infty}^{\infty} d\omega\left(-\frac{df(\omega)}{d\omega}\right)\int\frac{d\phi}{2\pi}\right.
\left.\mathrm{Re}\left(\frac{|\omega|}{\sqrt{(\omega-i\delta)^2-\Delta^2\cos^2 2\phi}}\right)\right],
\tag{15.91}
$$

where we have taken the real part of the integrand to eliminate terms where $|\omega| < |\Delta(\phi)|$.

We recognize the last term as the thermal average of the density of states, so that

$$
Q(T) = Q_0\left[1-\overline{\left(\frac{A(\omega)}{N(0)}\right)}\right],
$$

where (see (15.58))

$$
A(\omega) = \frac{2N(0)}{\pi}\,\mathrm{Re}\,K\left(\frac{\Delta}{\omega-i\delta}\right)
$$

and $K(x)$ is the elliptic integral (15.60).

(b) At low temperatures, the density of states is given by $A(\omega)/N(0) = (|\omega|/\Delta)$, so that the thermally averaged density of states

$$\overline{\left(\frac{A(\omega)}{N(0)}\right)} = \frac{k_B T}{\Delta} 2 \int_0^\infty \frac{x}{(e^x + 1)(e^{-x} + 1)} = \frac{k_B T}{\Delta} \ln 4 \tag{15.92}$$

grows linearly with temperature. Thus in a d-wave superconductor the inverse penetration depth $\frac{1}{\lambda_L^2} \propto Q(T)$ will exhibit a linear dependence on temperature at low temperatures, rather than the exponential dependence expected from a fully gapped s-wave superconductor:

$$1 - \frac{\lambda_L^2(0)}{\lambda_L^2(T)} \sim \frac{k_B T}{\Delta} \qquad (k_B T << \Delta).$$

(Note that in a dirty d-wave superconductor the density of states is constant at low temperatures, which leads to a quadratic temperature dependence of the inverse penetration depth at the lowest temperatures.)

15.5 Superfluid ^{3}He

15.5.1 Early history: theorists predict a new superfluid

As our second example of anisotropic pairing, we discuss the remarkable case of superfluid ^{3}He. As the 1950s came to an end and the wider significance of the BCS pairing instability was appreciated, the condensed-matter community began to realize that ^{3}He might form a BCS superfluid condensate, avoiding the mutual repulsion of the atoms by pairing in a higher angular momentum channel. Four independent groups (Lev Pitaevksii [6] at the Kapitza institute in Moscow; David Thouless at the Lawrence Radiation Laboratory, University of California, Berkeley [7]; Victor Emery and Andrew Sessler at the University of California, Berkeley [8]; and the Gang of Four, Keith Brueckner and Toshio Soda at the University of California, La Jolla, and Philip W. Anderson with Pierre Morel at Bell Laboratories, New Jersey [4] [9, 10]) came up with the idea of anisotropic pairing. Although these early papers examined both p- and d-wave pairs, each of them used *bare* nuclear interaction parameters as input to the BCS theory, and on the basis of these calculations came to the conclusion that the leading attractive channel was the $l = 2$, d-wave channel, predicting a d-wave superfluid condensate would develop in ^{3}He around $T_c = 50{-}150$ mK. The theory community would later be vindicated in their prediction of anistropic superfluidity in ^{3}He, but at a much lower temperature and with a p-wave rather than a d-wave symmetry.

During the 1960s the theory of anisotropic superfluidity developed rapidly, providing the framework for p-wave pairing that would ultimately be used to understand ^{3}He. In 1961 Morel and Anderson [10] introduced the ground state of what would later be identified

[4] Pierre Morel was officially a scientific attache at the French Embassy in New York City.

as the "A" phase, while in 1963 Roger Balian at the Centre d'Etude Nucléaires, Saclay, and Richard Werthamer at Bell Laboratories [11] discovered, an isotropic triplet paired ground state that would later be identified as the "B" phase. Gradually, towards the end of the 1960s, it became clear that the use of a bare interaction parameter as an input to BCS theory needed to be corrected for many-body effects, particularly with ladder diagram corrections to the pair scattering amplitude [12]. In a pioneering work, Walter Kohn at the University of California, San Diego, and Joaquin Luttinger at Columbia University, New York, [13] showed that, when many-body corrections to the Cooper channel interaction are considered, the sharpness of the Fermi surface guarantees that Fermi liquids are inevitably unstable to anisotropic pairing in some higher angular momentum channel. Using an input delta-function potential, Kohn and Luttinger derived an approximate asymptotic formula for T_c as a function of angular momentum l in ^{3}He, given by

$$T_c(l) \sim \epsilon_F \exp\left\{-\frac{\pi^2}{(k_F a)^2} l^4\right\}, \tag{15.93}$$

where l is the angular momentum of the pair, ϵ_F and k_F are the Fermi energy and momentum, respectively, and a is the diameter of the ^{3}He atom. Curiously, Kohn and Luttinger chose to illustrate this equation for $l = 2$, d-wave pairing, which for $k_F a \sim 2$ gives $T_c \sim 10^{-17}\epsilon_F$. Had they made the bold but uncontrolled insertion of $l = 1$, they would have obtained $T_c \sim 0.05\epsilon_F \sim 50\,\text{mK}$, surely an indication that p-wave pairing is a stronger candidate than d-wave! Then in 1967 D. Fay and A. Layzer, working at the Stevens Institute of Technology, New Jersey, made the critical observation [14] that in dilute neutral fluids many-body effects, which tend to ferromagnetically enhance interactions, will also generally lead to p-wave pairing.

It was not until 1972 that Douglas Osheroff, Robert Richardson, and David Lee at Cornell University finally discovered superfluidity in ^{3}He, developing at 2.65 mK [15] (see Figure 15.7). From the anomalies in the NMR response, this team was able to identify two phases: a high-temperature A phase and a low-temperature B phase in which most of the magnetic response disappeared. By carefully analyzing the detailed NMR measurements

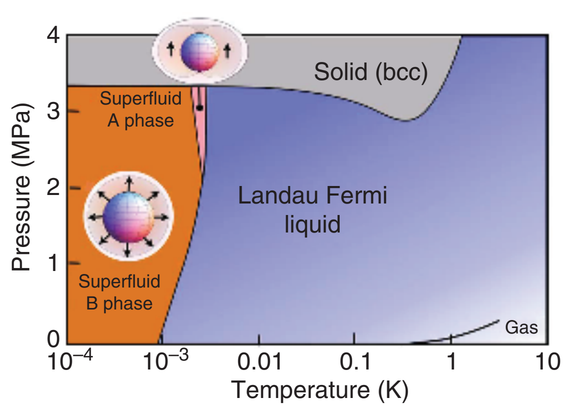


Fig. 15.7 Phase diagram of ^{3}He, showing the superfluid A and B phases, [22] with icons representing the gap anisotropy. Note that 0.1MPa = 1 atm. Adapted with permission from D. Vollhardt and P. Wölfle, *The Superfluid Phases of Helium 3*, Dover, 2013. Copyright 2013 by Dieter Vollhardt and Peter Wölfle.

carried out on these phases, Anthony Leggett, working at Sussex University [16], was able to show [17–19] that the pair symmetry of the A phase is triplet and probably corresponds to the Anderson–Morel state (now called the Anderson–Brinkman–Morel state). The pair symmetry of the B phase was later identified with the isotropic and fully gapped Balian–Werthamer state [20].

Curiously, although the early ^{3}He theorists predicted the wrong pair symmetry for ^{3}He, their efforts were not in vain, for d-wave pairing was realized seven years later in superconductors, with the discovery of the first anisotropic superconductor, $CeCuSi_2$, by Frank Steglich at Cologne University [21]. We now know many examples of d-wave superconductors, including the high-temperature cuprate superconductors.

15.5.2 Formulation of a model

The beauty of ^{3}He is that its isotropy provides us with a model system. The Fermi surface is perfectly spherical and in this case the pairing interaction between the quasiparticles depends only on the relative angle between the initial and final pair momenta $\mathbf{k}$ and $\mathbf{k}'$, i.e. $V_{\mathbf{k},\mathbf{k}'} = V(\cos\theta_{\mathbf{k},\mathbf{k}'})$. This implies that the pairing interaction can be decomposed as a multipole expansion involving Legendre polynomials:

$$V_{\mathbf{k},\mathbf{k}'} = \sum_l (2l+1) V_l P_l(\hat{\mathbf{k}} \cdot \hat{\mathbf{k}}'). \tag{15.94}$$

This is reminiscent of the multipole expansion of Fermi liquid interactions (6.38). Using the orthogonality relation $\int \frac{dc}{2} P_l(c) P_{l'}(c) = \delta_{l,l'}/(2l+1)$, the parameters V_l are given by

$$V_l = \int_{-1}^{1} \frac{d\cos\theta}{2} P_l(\cos\theta) V(\cos\theta) \qquad l \in \begin{cases} \text{even} & \text{(singlet)} \\ \text{odd} & \text{(triplet).} \end{cases} \tag{15.95}$$

These are the higher angular momentum analogues of the BCS s-wave interaction parameter. Now the parity of the Legendre polynomials alternates with l, $P_l = (-1)^l$ $(P_l(-x) = (-1)^l P_l(x))$, so the even l define singlet pair potentials while the odd l define triplet $(S=1)$ pair potentials.

Using the relationship $(2l+1)P_l(\hat{\mathbf{k}} \cdot \hat{\mathbf{k}}') = 4\pi \sum_{m=-l}^{l} Y^*_{lm}(\hat{\mathbf{k}}) Y_{lm}(\hat{\mathbf{k}}')$, we can factorize the anisotropic BCS interaction in the form

$$V_{\mathbf{k},\mathbf{k}'} = \sum_{l,m} V_l \, y^*_{lm}(\hat{\mathbf{k}}) y_{lm}(\hat{\mathbf{k}}'), \tag{15.96}$$

where we have used the notation $y_{lm} = \sqrt{4\pi} Y_{lm}$ to denote spherical harmonics normalized to give unit norm when averaged over the sphere $\int \frac{d\Omega}{4\pi} y^*_{lm} y_{lm} = \delta_{l,l'}\delta_{m,m'}$. This is the same kind of factorized interaction encountered in the previous section, and we can treat it in the same way. For ^{3}He, the hard-core repulsion between the atoms rules out an s-wave instability[5] and it is the p-wave $(l=1)$ triplet $(S=1)$ channel that takes over. Approximating $V_1 = -g/V$ and ignoring all other channels, then

[5] Curiously, in optical atom traps in which the atomic interactions among highly dilute fermions can be tuned through a Feshbach resonance, it is possible to produce an attractive s-wave interaction, so a conventional BCS instability does occur.

$$V_{\mathbf{k},\mathbf{k}'} = -\frac{g}{V}3\cos(\mathbf{k}\cdot\mathbf{k}') = -\frac{3g}{V}(\hat{k}_a\hat{k}'_a), \tag{15.97}$$

where $\hat{k}_a = k_a/k_F$ and the sum over the repeated index $a = 1,2,3$ is implied. The BCS Hamiltonian for a triplet superfluid is then [11]

$$\begin{aligned} H_{BCS} &= \sum_{\mathbf{k}\sigma}\epsilon_{\mathbf{k}}c^\dagger_{\mathbf{k}\sigma}c_{\mathbf{k}\sigma} - \frac{3g_0}{V}\sum_{\mathbf{k},\mathbf{k}'\in\frac{1}{2}\mathrm{BZ}}(\vec{\Psi}^\dagger_{\mathbf{k}}\hat{k}_\ell)\cdot(\hat{k}'_\ell\vec{\Psi}_{\mathbf{k}'}) \\ \vec{\Psi}_{\mathbf{k}} &= c_{-\mathbf{k}\alpha}\left(-i\sigma_2\vec{\sigma}\right)_{\alpha\beta}c_{\mathbf{k}\beta} \\ \vec{\Psi}^\dagger_{\mathbf{k}} &= c^\dagger_{\mathbf{k}\alpha}\left(\vec{\sigma}\,i\sigma_2\right)_{\alpha\beta}c^\dagger_{-\mathbf{k}\beta}. \end{aligned} \tag{15.98}$$

Notice that there are now three *triplet* channels ($\vec{\Psi}_{\mathbf{k}} \equiv \Psi^a_{\mathbf{k}}$, $a = 1,2,3$) and three *orbital* channels ($\hat{k}_l$, $l = x,y,z$) in which the pairing takes place. The summation over momentum in the interaction takes place over one-half the Brillouin zone.

15.5.3 Gap equation

If we carry out a Hubbard–Stratonovich transformation, we get

$$H_{MFT} = \sum_{\mathbf{k}\sigma}\epsilon_{\mathbf{k}}c^\dagger_{\mathbf{k}\sigma}c_{\mathbf{k}\sigma} + \sum_{\mathbf{k}\in\frac{1}{2}BZ}\left[\vec{\Psi}^\dagger_{\mathbf{k}}\cdot(\vec{\Delta}_l)\,\hat{k}_l + \mathrm{H.c.}\right] + \frac{V}{3g_0}(\vec{\Delta}^*_l\cdot\vec{\Delta}_l). \tag{15.99}$$

The three vectors $\vec{\Delta}_l$ ($l = x,y,z$) define a three-dimensional matrix $\Delta^a_l \equiv (\vec{\Delta}_l)^a$ which links the spin and orbital degrees of freedom. If we denote $\vec{\Delta}_{\mathbf{k}} = \sum_{l=x,y,z}\vec{\Delta}_l\hat{k}_l$, then, since $\int\frac{d\Omega_{\hat{k}}}{4\pi}\hat{k}_l\hat{k}_m = \frac{1}{3}\delta_{lm}$, it follows that

$$\Delta^a_l = (\vec{\Delta}_l)^a = 3\int\frac{d\Omega_{\hat{k}}}{4\pi}(\vec{\Delta}_{\mathbf{k}})^a\hat{k}_l. \tag{15.100}$$

Thus we can write

$$\frac{V}{3g_0}(\vec{\Delta}^*_l\cdot\vec{\Delta}_l) = \frac{3V}{g_0}\int\frac{d\Omega_{\hat{k}}}{4\pi}\frac{d\Omega_{\hat{k}'}}{4\pi}\vec{\Delta}_{\mathbf{k}}\cdot\vec{\Delta}_{\mathbf{k}'}(\hat{k}\cdot\hat{k}') \equiv -\int_{\hat{k},\hat{k}'}\vec{\Delta}^*_{\mathbf{k}}V^{-1}_{\mathbf{k},\mathbf{k}'}\vec{\Delta}_{\mathbf{k}'}, \tag{15.101}$$

where we have identified $V^{-1}_{\mathbf{k},\mathbf{k}'} \equiv -\frac{V}{g_0}(3\hat{k}\cdot\hat{k}')$ and denoted $\int_{\hat{k}} = \int\frac{d\Omega_{\hat{k}}}{4\pi}$. The mean-field Hamiltonian is then

$$H_{MFT} = \sum_{\mathbf{k}\sigma}\epsilon_{\mathbf{k}}c^\dagger_{\mathbf{k}\sigma}c_{\mathbf{k}\sigma} + \sum_{\mathbf{k}\in\frac{1}{2}BZ}\left(\vec{\Psi}^\dagger_{\mathbf{k}}\cdot\vec{\Delta}_{\mathbf{k}} + \mathrm{H.c.}\right) + \frac{3V}{g_0}\int\frac{d\Omega_{\hat{k}}}{4\pi}\frac{d\Omega_{\hat{k}'}}{4\pi}\vec{\Delta}_{\mathbf{k}}\cdot\vec{\Delta}_{\mathbf{k}'}(\hat{k}\cdot\hat{k}'). \tag{15.102}$$

Now, to diagonalize this mean-field theory we need to cast it into spinors. Triplet pairing mixes up and down electrons, which obliges us to use a four-component spinor called a *Balian–Werthamer spinor* [11] after its inventors:

$$\psi_{\mathbf{k}} \equiv \begin{pmatrix} c_{\mathbf{k}} \\ i\sigma_2 c^{\dagger}_{-\mathbf{k}} \end{pmatrix} \equiv \begin{pmatrix} c_{\mathbf{k}\uparrow} \\ c_{\mathbf{k}\downarrow} \\ c^{\dagger}_{-\mathbf{k}\downarrow} \\ -c^{\dagger}_{-\mathbf{k}\uparrow} \end{pmatrix}. \qquad \text{Balian–Werthamer spinor} \tag{15.103}$$

The upper two entries are the destruction operators for particles of momentum $\mathbf{k}$, while the lower two,

$$\begin{pmatrix} a_{\mathbf{k}\uparrow} \\ a_{\mathbf{k}\downarrow} \end{pmatrix} \equiv \begin{pmatrix} c^{\dagger}_{-\mathbf{k}\downarrow} \\ -c^{\dagger}_{-\mathbf{k}\uparrow} \end{pmatrix}, \tag{15.104}$$

are the destruction operators for *holes* of momentum $\mathbf{k}$. Hole-destruction operators are the time reversal (denoted by the operator θ) of the corresponding particle-creation operators, and the minus sign in the lower entry appears on time reversal of a down-spin state, $a^{\dagger}_{\mathbf{k}\downarrow} = \theta c_{\mathbf{k}\downarrow}\theta^{-1} = -c_{-\mathbf{k}\uparrow}$.[6] Notice how the $i\sigma_2$ that appears in the triplet pair operators is now neatly absorbed into the spinor. Moreoever, the BW spinor obeys canonical anticommutation rules:

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

Of course, we have doubled the number of components in the spinor, so we must now restrict the momentum to one-half of momentum space, $\mathbf{k} \in \frac{1}{2}BZ$. The payoff is that we now have a rotationally invariant representation in which the spin operator is defined in terms of block-diagonal Pauli matrices:

$$\vec{\sigma}_4 \equiv \underline{1} \otimes \vec{\sigma} = \left(\begin{array}{c|c} \vec{\sigma} & \\ \hline & \vec{\sigma} \end{array}\right), \tag{15.105}$$

while the Nambu matrices are now block matrices:

$$\vec{\tau}_4 \equiv \vec{\tau} \otimes \underline{1} = \left\{ \left(\begin{array}{c|c} & \underline{1} \\ \hline \underline{1} & \end{array}\right), \left(\begin{array}{c|c} & -i\underline{1} \\ \hline i\underline{1} & \end{array}\right), \left(\begin{array}{c|c} \underline{1} & \\ \hline & -\underline{1} \end{array}\right) \right\}. \tag{15.106}$$

In this notation, the BCS Hamiltonian can be succinctly rewritten as

$$\begin{aligned} H_{MFT} &= \sum_{\mathbf{k}\in\frac{1}{2}BZ} \psi^{\dagger}_{\mathbf{k}} h_{\mathbf{k}} \psi_{\mathbf{k}} + \frac{3V}{g_0} \int \frac{d\Omega_{\hat{k}}}{4\pi}\frac{d\Omega_{\hat{k}'}}{4\pi} \vec{\Delta}_{\mathbf{k}} \cdot \vec{\Delta}_{\mathbf{k}'} (\hat{k}\cdot\hat{k}') \\ h_{\mathbf{k}} &= \left(\begin{array}{c|c} \epsilon_{\mathbf{k}} & \vec{\Delta}_{\mathbf{k}}\cdot\vec{\sigma} \\ \hline \vec{\Delta}^{*}_{\mathbf{k}}\cdot\vec{\sigma} & -\epsilon_{\mathbf{k}} \end{array}\right) \equiv \epsilon_{\mathbf{k}}\tau_3 + (\vec{\Delta}_{\mathbf{k}}\cdot\vec{\sigma})\tau_+ + (\vec{\Delta}^{*}_{\mathbf{k}}\cdot\vec{\sigma})\tau_-, \end{aligned} \tag{15.107}$$

where $\tau_{\pm} = \frac{1}{2}(\tau_1 \pm i\tau_2)$. It is common to denote the direction of the gap function in spin space by the complex *d-vector* $\vec{d}_{\mathbf{k}}$,

$$\vec{\Delta}_{\mathbf{k}} = \Delta\vec{d}_{\mathbf{k}}, \tag{15.108}$$

which is normalized so that its angular average over the Fermi surface is unity:

$$\int \frac{d\Omega_{\mathbf{k}}}{4\pi} |\vec{d}_{\mathbf{k}}|^2 = 1. \tag{15.109}$$

[6] You can also verify that the diagonal and off-diagonal matrix elements of the spin operator are the same for particles and for holes, so that $h^{\dagger}_{\mathbf{k}}\vec{\sigma}h_{\mathbf{k}} = c_{-\mathbf{k}}(i\sigma_2)\vec{\sigma}(-i\sigma_2)c_{-\mathbf{k}} = c^{\dagger}_{-\mathbf{k}}\vec{\sigma}c_{-\mathbf{k}}$, where the last step follows because $\vec{\sigma}^T = -\sigma_2\vec{\sigma}\sigma_2$.

The d-vector is an emergent property of the Fermi surface, and the textures it gives rise to in momentum space define the state of the condensate.

If we take the determinant of $\omega - h_{\mathbf{k}}$ by multiplying out its two-dimensional block diagonals, we find

$$\begin{aligned}\det(\omega - h_{\mathbf{k}}) &= \det\left[(\omega^2 - \epsilon_{\mathbf{k}}^2)\underline{1} - (\vec{\Delta}_{\mathbf{k}}^* \cdot \vec{\sigma})(\vec{\Delta}_{\mathbf{k}} \cdot \vec{\sigma})\right] \\ &= \det\left[(\omega^2 - \epsilon_{\mathbf{k}}^2)\underline{1} - \Delta^2(|\vec{d}_{\mathbf{k}}|^2 + i\vec{d}_{\mathbf{k}}^* \times \vec{d}_{\mathbf{k}} \cdot \vec{\sigma})\right] \\ &= \det\left[(\omega^2 - \epsilon_{\mathbf{k}}^2)\underline{1} - \Delta^2(|\vec{d}_{\mathbf{k}}|^2 + 2\vec{d}_{1\mathbf{k}} \times \vec{d}_{2\mathbf{k}} \cdot \vec{\sigma})\right],\end{aligned} \qquad (15.110)$$

where we have used the identity $\sigma^a\sigma^b = \delta^{ab} + i\epsilon^{abc}\sigma^c$ on the second line and decomposed $\vec{d}_{\mathbf{k}} = \vec{d}_{1\mathbf{k}} - i\vec{d}_{2\mathbf{k}}$ into its real and imaginary parts on the last line. The quasiparticle energies determined by pairing matrix $h_{\mathbf{k}}$ are then

$$E_{\mathbf{k}\pm} = \sqrt{\epsilon_{\mathbf{k}}^2 + \Delta^2(|\vec{d}_{\mathbf{k}}|^2 \pm 2|\vec{d}_{1\mathbf{k}} \times \vec{d}_{2\mathbf{k}}|)}.$$

There are in fact two superfluid phases of ^{3}He, and, in both, $\vec{d}_{1\mathbf{k}}$ and $\vec{d}_{2\mathbf{k}}$ are parallel, and the gap functions take the form

$$\vec{\Delta}_{\mathbf{k}} = \Delta \times \begin{cases} \hat{k}_x\hat{\mathbf{x}} + \hat{k}_y\hat{\mathbf{y}} + \hat{k}_z\hat{\mathbf{z}} & \text{BW or B phase} \\ \sqrt{\frac{3}{2}}(\hat{k}_x + i k_y)\hat{\mathbf{z}}\,. & \text{ABM or A phase} \end{cases} \qquad (15.111)$$

The BW or B phase is named after Balian and Werhammer. In this phase the d-vector points radially outwards from the Fermi sea, forming a topological "hedgehog" configuration (see Figure 15.8(a)) with a uniform gap and quasiparticle energy given simply by

$$E_{\mathbf{k}} = \sqrt{\epsilon_{\mathbf{k}}^2 + \Delta^2}. \qquad \text{B phase}$$

The B phase, with a full gap, dominates the phase diagram. The ABM or A-phase, named after its discoverers, Anderson, Brinkman, and Morel, develops in a small sliver of the phase diagram under pressures of about 2 MPa (see Figure 15.7(b)). This phase involves pairing in a single triplet orbital channel with a uniform ("z") direction of the d-vector; now the magnitude of the gap is momentum-dependent:

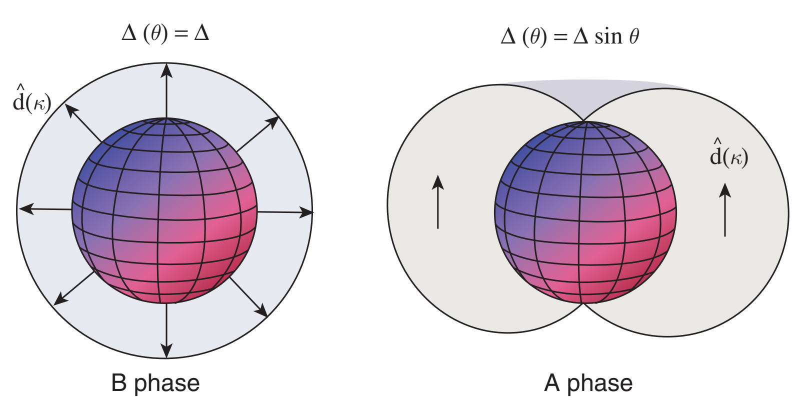


Fig. 15.8 Showing the gap structure and d-vector orientation for the B and A phases of superfluid ^{3}He.

$$\vec{\Delta}_{\mathbf{k}} = \sqrt{\frac{3}{2}}\Delta \sin\theta e^{i\phi}\hat{\mathbf{z}}. \qquad \text{A phase}$$

This function vanishes at the poles, giving rise to a quasiparticle excitation spectrum

$$E_{\mathbf{k}} = \sqrt{\epsilon_{\mathbf{k}}^2 + \frac{3}{2}\Delta^2 \sin^2\theta}. \qquad \text{A phase}$$

The derivation of the mean-field equations for these two solutions is simplified by the observation that, for both of them, the potential energy term is

$$\frac{3V}{g_0}\int \frac{d\Omega_{\hat{k}}}{4\pi}\frac{d\Omega_{\hat{k}'}}{4\pi}\vec{\Delta}_{\mathbf{k}}\cdot\vec{\Delta}_{\mathbf{k}'}(\hat{k}\cdot\hat{k}') = \frac{V}{g_0}\Delta^2.$$

The free energy of the mean-field theory then takes precisely the same form as in BCS theory:

$$F_{MFT} = -2T\sum_{\mathbf{k}}\ln\left(2\cosh\frac{\beta E_{\mathbf{k}}}{2}\right) + \frac{V}{g_0}\Delta^2.$$

If we differentiate with respect to Δ^2 we obtain the gap equation:

$$\frac{1}{g_0 N(0)} = \int_{-1}^{1}\frac{d\cos\theta}{2}\int_{-\omega_D}^{\omega_D} d\epsilon \frac{\Delta(\theta)^2/\Delta^2}{\sqrt{\epsilon^2+\Delta(\theta)^2}}\tanh\left[\frac{\sqrt{\epsilon^2+\Delta(\theta)^2}}{2}\right].$$

According to this analysis, the A and B phases have identical mean-field transition temperatures. However, at lower temperatures the B phase wins out because its fully gapped Fermi surface gives rise to a lower free energy.

Example 15.6 Consider a single triplet Cooper pair described by the state

$$|\Psi\rangle = \frac{1}{\sqrt{2}}\left(\hat{d}\cdot\vec{\Psi}^{\dagger}_{\mathbf{k}}\right)|0\rangle = \frac{1}{\sqrt{2}}\hat{d}\cdot\left(c^{\dagger}_{\mathbf{k}}\vec{\sigma}\, i\sigma_2 c^{\dagger}_{-\mathbf{k}}\right)|0\rangle,$$

where $\hat{d}$ is a real unit vector.

(a) Show that

$$\vec{S}|\Psi\rangle = \frac{i}{\sqrt{2}}(\hat{d}\times\vec{\Psi}^{\dagger}_{\mathbf{k}})|0\rangle$$

and use this to prove that the spin of the state is $S = 1$, i.e.

$$S^2|\Psi\rangle = 2|\Psi\rangle, \tag{15.112}$$

while the component of the spin in the direction of the d-vector vanishes:

$$(\hat{\mathbf{d}}\cdot\vec{S})|\Psi\rangle = 0 \tag{15.113}$$

and the expectation value of the magnetic moment is zero, i.e. $\langle\Psi|\vec{S}|\Psi\rangle = 0$.

(b) Show that the expectation value is

$$\langle\Psi|S^aS^b|\Psi\rangle = \delta^{ab} - \hat{d}^a\hat{d}^b, \tag{15.114}$$

so that $\langle S^2\rangle = S(S+1) = 2$, corresponding to a spin-quadrupole with a fluctuating moment in the plane perpendicular to the d-vector.

Solution

(a) The effective spin operator for this state only involves momenta $\pm\mathbf{k}$, so we may use $\vec{S} = \frac{1}{2}[c^\dagger_{\mathbf{k}}\vec{\sigma}c_{\mathbf{k}} + c^\dagger_{-\mathbf{k}}\vec{\sigma}c_{-\mathbf{k}}]$. To determine the action of the spin operator on the triplet pair, we need to commute it past the triplet pair operator onto the vacuum. The commutator is

$$\begin{aligned}\left[S^a, (\vec{\Psi}^\dagger_{\mathbf{k}})^b\right] &= \left[\left(c^\dagger_{\mathbf{k}}\sigma^a c_{\mathbf{k}} + c^\dagger_{-\mathbf{k}}\sigma^a c_{-\mathbf{k}}\right), \left(c^\dagger_{\mathbf{k}}\sigma^b i\sigma_2 c^\dagger_{-\mathbf{k}}\right)\right] \\ &= c^\dagger_{\mathbf{k}}\left(\sigma^a\sigma^b i\sigma_2 + \sigma^b i\sigma_2(\sigma^a)^T\right)c^\dagger_{-\mathbf{k}},\end{aligned}$$

where the first and second terms derive from the positive and negative momentum components of the spin operator. Using $\sigma_2(\sigma^a)^T = -\sigma^a\sigma_2$ we obtain

$$\left[S^a, (\vec{\Psi}^\dagger_{\mathbf{k}})^b\right] = \frac{1}{2}c^\dagger_{\mathbf{k}}\left[\sigma^a, \sigma^b\right]i\sigma_2 c^\dagger_{-\mathbf{k}} = i\epsilon_{abc}c^\dagger_{\mathbf{k}}\sigma^c i\sigma_2 c^\dagger_{-\mathbf{k}} \tag{15.115}$$

or

$$\left[S^a, \hat{d}\cdot\left(c^\dagger_{\mathbf{k}}\vec{\sigma}i\sigma_2 c^\dagger_{-\mathbf{k}}\right)\right] = i\epsilon_{abc}d^b\left(c^\dagger_{\mathbf{k}}\sigma^c i\sigma_2 c^\dagger_{-\mathbf{k}}\right) = i(\hat{d}\times\vec{\Psi}^\dagger_{\mathbf{k}})^a, \tag{15.116}$$

and hence

$$\vec{S}|\Psi\rangle = \frac{1}{\sqrt{2}}[\vec{S}, (\hat{d}\cdot\vec{\Psi}^\dagger_{\mathbf{k}})]|0\rangle = \frac{i}{\sqrt{2}}\left(\hat{d}\times\vec{\Psi}^\dagger_{\mathbf{k}}\right)|0\rangle. \tag{15.117}$$

Using (15.115), we have

$$S^a(\vec{\Psi}^\dagger_{\mathbf{k}})^b|0\rangle = i\epsilon_{abc}(\vec{\Psi}^\dagger_{\mathbf{k}})^c|0\rangle, \tag{15.118}$$

so that

$$\begin{aligned}S^2(\vec{\Psi}^\dagger_{\mathbf{k}})^b|0\rangle &= S^aS^a(\vec{\Psi}^\dagger_{\mathbf{k}})^b|0\rangle \\ &= i\epsilon_{abc}S_a(\vec{\Psi}^\dagger_{\mathbf{k}})^c|0\rangle \\ &= \overbrace{i\epsilon_{abc}i\epsilon_{acd}}^{2\delta_{bd}}(\vec{\Psi}^\dagger_{\mathbf{k}})^d|0\rangle = 2(\vec{\Psi}^\dagger_{\mathbf{k}})^b|0\rangle,\end{aligned} \tag{15.119}$$

so, writing this in vector notation,

$$S^2\vec{\Psi}^\dagger_{\mathbf{k}}|0\rangle = 2\vec{\Psi}^\dagger_{\mathbf{k}}|0\rangle. \tag{15.120}$$

Hence $S^2|\Psi\rangle = S^2(\hat{d}\cdot\vec{\Psi}^\dagger_{\mathbf{k}})|0\rangle = 2|\Psi\rangle$, corresponding to a spin of 1.

If we evaluate the expectation value of the moment, we get

$$\langle\Psi|\vec{S}|\Psi\rangle = \frac{1}{2}\langle 0|(\hat{d}^*\cdot\vec{\Psi}_{\mathbf{k}})(\hat{d}\times\vec{\Psi}^\dagger_{\mathbf{k}})|0\rangle = i\hat{d}\times\hat{d}^*. \tag{15.121}$$

In our case $\hat{d}$ is real, so that $\langle \vec{S} \rangle = 0$. Note, however, that if $\hat{d} = \hat{d}_1 + i\hat{d}_2$ is complex, then $\langle \vec{S} \rangle = 2\hat{d}_1 \times \hat{d}_2$, so that if $\hat{d}_1$ and $\hat{d}_2$ are not parallel, the Cooper pair state carries a net magnetic moment.

(b) Taking the result (15.117), we have

$$
\begin{aligned}
\langle \Psi | S^a S^b | \Psi \rangle &= \frac{1}{2}\epsilon_{apq}\epsilon_{brs} d^p d^r \overbrace{\langle 0 | \left(\vec{\Psi}_{\mathbf{k}}\right)^q \left(\vec{\Psi}^\dagger_{\mathbf{k}}\right)^s |0\rangle}^{2\delta^{qs}} = \epsilon_{apq}\epsilon_{brq} \\
&= \left(\delta^{ab}\delta^{pr} - \delta^{ar}\delta^{pb}\right) d^p d^r \\
&= \delta^{ab} - d^a d^b,
\end{aligned}
\tag{15.122}
$$

so the moment fluctuations of the pair lie in the plane perpendicular to the d-vector.

Example 15.7 Derive the BCS pair wavefunction for the B phase of ^{3}He.

Solution

By analogy with the case of singlet pairing, we expect the ground state to be a coherent state of a triplet pair,

$$
|\Psi\rangle = \exp\left[\Lambda^\dagger_T\right] |0\rangle, \tag{15.123}
$$

where

$$
\Lambda^\dagger_T = \frac{1}{2}\sum_{\mathbf{k}} \phi_{\mathbf{k}} (\hat{k} \cdot \vec{\Psi}^\dagger_{\mathbf{k}}) \tag{15.124}
$$

creates a triplet pair and $\phi_{\mathbf{k}} = \phi_{-\mathbf{k}}$ is an even function of momentum. The factor of $\frac{1}{2}$ is included as a normalization that takes account of the fact that $\Psi^\dagger_{\mathbf{k}}$ is only independent in one-half of momentum space.

Now the ground state is annihilated by the quasiparticle destruction operators. For the triplet B phase we write the quasiparticle-creation operators as

$$
a^\dagger_{\mathbf{k}} = \psi^\dagger_{\mathbf{k}} \cdot \begin{pmatrix} u_{\mathbf{k}} \\ v_{\mathbf{k}} \end{pmatrix} = c^\dagger_{\mathbf{k}\sigma} u_{\mathbf{k}\sigma} + \tilde{c}_{\mathbf{k}\sigma} v_{\mathbf{k}\sigma}, \tag{15.125}
$$

where $\tilde{c}_{\mathbf{k}\alpha} = c_{-\mathbf{k}\beta}[-i\sigma_2]_{\beta\alpha}$ and the $u_{\mathbf{k}\sigma}$ and $v_{\mathbf{k}\sigma}$ are two-component spinors. For the B phase, we can take the mean-field Hamilonian to be

$$
H_{MFT} = \sum_{\mathbf{k}\in\frac{1}{2}BZ} \psi^\dagger_{\mathbf{k}} h_{\mathbf{k}} \psi_{\mathbf{k}}, \qquad h_{\mathbf{k}} = \left(\begin{array}{c|c} \epsilon_{\mathbf{k}} & \Delta(\hat{k}\cdot\vec{\sigma}) \\ \hline \Delta(\hat{k}\cdot\vec{\sigma}) & -\epsilon_{\mathbf{k}} \end{array}\right). \tag{15.126}
$$

Now since $[H, a_{\mathbf{k}}] = E_{\mathbf{k}} a_{\mathbf{k}}$, it follows that

$$
\left(\begin{array}{c|c} \epsilon_{\mathbf{k}} & \Delta(\hat{k}\cdot\vec{\sigma}) \\ \hline \Delta(\hat{k}\cdot\vec{\sigma}) & -\epsilon_{\mathbf{k}} \end{array}\right) \begin{pmatrix} u_{\mathbf{k}} \\ v_{\mathbf{k}} \end{pmatrix} = E_{\mathbf{k}} \begin{pmatrix} u_{\mathbf{k}} \\ v_{\mathbf{k}} \end{pmatrix}. \tag{15.127}
$$

(Notice that, if we choose a spin quantization axis parallel to $\hat{k}$, then this eigenvalue equation is identical to singlet pairing.)

Now we must find the condensate that is annihilated by the quasiparticle operators:

$$a_{\mathbf{k}} = (u^\dagger_{\mathbf{k}}, v^\dagger_{\mathbf{k}}) \cdot \psi_{\mathbf{k}} = u^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} + v^\dagger_{\mathbf{k}\sigma} \tilde{c}^\dagger_{\mathbf{k}\sigma}. \tag{15.128}$$

To commute the quasiparticle operator with the pair creation operator, we note that

$$[a_{\mathbf{k}}, c^\dagger_{\mathbf{k}'\sigma}] = u^\dagger_{\mathbf{k}\sigma} \delta_{\mathbf{k},\mathbf{k}'}, \tag{15.129}$$

so that

$$\begin{aligned}
[a_{\mathbf{k}}, \Lambda^\dagger_T] &= \frac{1}{2}\left[a_{\mathbf{k}}, \sum_{\mathbf{k}'} \phi_{\mathbf{k}'} c^\dagger_{\mathbf{k}'} (\hat{k}' \cdot \vec{\sigma}) i\sigma_2 c^\dagger_{-\mathbf{k}'} \right] \\
&= \frac{1}{2}\phi_{\mathbf{k}} \left[u^\dagger_{\mathbf{k}} (\hat{k} \cdot \vec{\sigma}) i\sigma_2 c^\dagger_{-\mathbf{k}} + c^\dagger_{-\mathbf{k}} (\hat{k} \cdot \vec{\sigma}) i\sigma_2 (u^\dagger_{\mathbf{k}})^T \right] \\
&= \frac{1}{2}\phi_{\mathbf{k}} \left[u^\dagger_{\mathbf{k}} (\hat{k} \cdot \vec{\sigma}) i\sigma_2 c^\dagger_{-\mathbf{k}} + u^\dagger_{\mathbf{k}} \overbrace{-i\sigma_2 (\hat{k} \cdot \vec{\sigma}^T)}^{(\hat{k}\cdot\vec{\sigma})i\sigma_2} c^\dagger_{-\mathbf{k}} \right] \\
&= \phi_{\mathbf{k}} \left[u^\dagger_{\mathbf{k}} (\hat{k} \cdot \vec{\sigma}) \tilde{c}^\dagger_{-\mathbf{k}} \right],
\end{aligned} \tag{15.130}$$

where we have used $\sigma_2 \vec{\sigma}^T = -\vec{\sigma}\sigma_2$ and the fact that $\phi_{\mathbf{k}} = \phi_{-\mathbf{k}}$. Now by (15.127),

$$u^\dagger_{\mathbf{k}} (\hat{k} \cdot \vec{\sigma}) = \frac{(E_{\mathbf{k}} + \epsilon_{\mathbf{k}})}{\Delta} v^\dagger_{\mathbf{k}}, \tag{15.131}$$

so that

$$\frac{|u_{\mathbf{k}}|}{|v_{\mathbf{k}}|} = \frac{(E_{\mathbf{k}} + \epsilon_{\mathbf{k}})}{\Delta}, \tag{15.132}$$

enabling the commutator of the quasiparticle operator with the pair creation operator to be written in the compact form

$$[\alpha_{\mathbf{k}}, \Lambda^\dagger_T] = \frac{|u_{\mathbf{k}}|}{|v_{\mathbf{k}}|} \phi_{\mathbf{k}} (v^\dagger_{\mathbf{k}} \tilde{c}^\dagger_{-\mathbf{k}}). \tag{15.133}$$

As in the case of singlet pairing, if we choose

$$\phi_{\mathbf{k}} = -\frac{|v_{\mathbf{k}}|}{|u_{\mathbf{k}}|} \tag{15.134}$$

then

$$[\alpha_{\mathbf{k}}, \Lambda^\dagger_T] = -v^\dagger_{\mathbf{k}} \cdot \tilde{c}^\dagger_{-\mathbf{k}}, \tag{15.135}$$

and since $\tilde{c}_{\mathbf{k}}$ commutes with $\Lambda^\dagger_T$, it follows that

$$[\alpha_{\mathbf{k}}, (\Lambda^\dagger_T)^n] = -n(\Lambda^\dagger_T)^{n-1} v^\dagger_{\mathbf{k}} \tilde{c}_{\mathbf{k}}, \tag{15.136}$$

so that

$$[\alpha_{\mathbf{k}}, \exp[\Lambda^\dagger_T]] = -\exp[\Lambda^\dagger_T] v^\dagger_{\mathbf{k}} \tilde{c}_{\mathbf{k}}. \tag{15.137}$$

This means that

$$\alpha_{\mathbf{k}} \exp[\Lambda^\dagger_T] = \exp[\Lambda^\dagger_T]\alpha_{\mathbf{k}} - \exp[\Lambda^\dagger_T] v^\dagger_{\mathbf{k}} \tilde{c}_{\mathbf{k}} = \exp[\Lambda^\dagger_T] u^\dagger_{\mathbf{k}} \cdot c_{\mathbf{k}}, \tag{15.138}$$

so that $\alpha_{\mathbf{k}}$ annihilates the coherent state:

$$\alpha_{\mathbf{k}} \exp[\Lambda_T^\dagger]|0\rangle = \exp[\Lambda_T^\dagger] u_{\mathbf{k}}^\dagger \cdot c_{\mathbf{k}}|0\rangle = 0, \tag{15.139}$$

proving that

$$|\Psi\rangle = \exp\left[-\frac{1}{2}\sum \frac{|v_{\mathbf{k}}|}{|u_{\mathbf{k}}|}(\hat{k}\cdot\vec{\Psi}_{\mathbf{k}}^\dagger)\right]|0\rangle \tag{15.140}$$

is the ground state.

Note that we have to be careful in reducing this to the usual multiplicative BCS form, for the square of the triplet pair operator is *not* zero. If one splits the sum over momentum space into two parts, $k_z > 0$ and $k_z < 0$, then the Cooper pair operator can be written as

$$\begin{aligned}\Lambda_T^\dagger &= \sum_{k_z>0} \phi_{\mathbf{k}} c_{\mathbf{k}}^\dagger \left(\frac{\hat{k}\cdot\vec{\sigma}+1}{2}\right)\tilde{c}_{-\mathbf{k}} + \sum_{k_z<0} \phi_{\mathbf{k}} c_{\mathbf{k}}^\dagger \left(\frac{\hat{k}\cdot\vec{\sigma}-1}{2}\right)\tilde{c}_{-\mathbf{k}} \\ &= \sum_{\mathbf{k}} \phi_{\mathbf{k}} c_{\mathbf{k}}^\dagger \left(\frac{\hat{k}\cdot\vec{\sigma}+\mathrm{sgn}(k_z)}{2}\right)\tilde{c}_{-\mathbf{k}}.\end{aligned} \tag{15.141}$$

The additional singlet term that has been added and subtracted from the upper and lower halves of momentum space cancel with each other. Now the terms inside the pair operators are projection operators, and the squares of these operators do vanish. We can now expand the coherent triplet paired state as a BCS product, as follows:

$$|\Psi\rangle = \prod_{\mathbf{k}} \left(|u_{\mathbf{k}}| - |v_{\mathbf{k}}| c_{\mathbf{k}}^\dagger \left(\frac{\hat{k}\cdot\vec{\sigma}+\mathrm{sgn}(k_z)}{2}\right)\tilde{c}_{-\mathbf{k}}\right)|0\rangle. \tag{15.142}$$

Example 15.8

(a) Show that the Nambu Green's function for ^{3}HeB is given by

$$\mathcal{G}(k) = [i\omega_n - \epsilon_{\mathbf{k}}\tau_3 - (\vec{\Delta}_{\mathbf{k}}\cdot\vec{\sigma})\tau_1]^{-1} = \frac{i\omega_n + \epsilon_{\mathbf{k}}\tau_3 + (\vec{\Delta}_{\mathbf{k}}\cdot\vec{\sigma})\tau_1}{(i\omega_n)^2 - E_{\mathbf{k}}^2}.$$

(b) Calculate the magnetic susceptibility of the B phase of ^{3}He. Show that the ground-state condensate has a finite Pauli susceptibility equal to 2/3 of the normal state.

Solution

(a) As in the case of singlet pairing, we can write the propagator as $G(\mathbf{k}) = -\frac{1}{\partial_\tau + h_{\mathbf{k}}}$. Let us start with the imaginary-time propagator, which we will write

$$\mathcal{G}(\mathbf{k},\tau) = -\langle T\psi_{\mathbf{k}}(\tau)\psi_{\mathbf{k}}^\dagger(0)\rangle \tag{15.143}$$

or, written out explicitly, $\mathcal{G}_{\alpha\beta}(\mathbf{k},\tau) = -\langle T\psi_{\mathbf{k}\alpha}(\tau)\psi_{\mathbf{k}\beta}^\dagger(0)\rangle$, where $\psi_{\mathbf{k}\alpha}$ is a Balian–Werthamer spinor. The expectation values are to be evaluated with the mean-field Hamiltonian $H = \sum_{\mathbf{k}\in\frac{1}{2}BZ} \psi_{\mathbf{k}}^\dagger h_{\mathbf{k}} \psi_{\mathbf{k}}$, where

$$h_{\mathbf{k}} = \epsilon_{\mathbf{k}}\tau_3 + (\vec{\Delta}_{\mathbf{k}} \cdot \vec{\sigma})\tau_1. \tag{15.144}$$

When we take account of the time-ordering, the equation of motion for $\mathcal{G}$ is

$$\begin{aligned}\partial_\tau \mathcal{G}(\mathbf{k},\tau) &= -\delta(\tau)\langle\{\psi_{\mathbf{k}}, \psi^\dagger_{\mathbf{k}}\}\rangle - \langle T(\partial_\tau \psi_{\mathbf{k}}(\tau))\psi^\dagger_{\mathbf{k}}(0)\rangle \\ &= -\delta(\tau)\underline{1} - \langle T[H, \psi_{\mathbf{k}}(\tau)]\psi^\dagger_{\mathbf{k}}(0)\rangle \\ &= -\delta(\tau)\underline{1} - h_{\mathbf{k}}\mathcal{G}(\mathbf{k},\tau),\end{aligned} \tag{15.145}$$

where we have used $\psi_{\mathbf{k}}(\tau) = e^{H\tau}\psi_{\mathbf{k}}e^{-H\tau}$ and $\partial_\tau\psi_{\mathbf{k}}(\tau) = [H, \psi_{\mathbf{k}}(\tau)] = -h_{\mathbf{k}}\psi_{\mathbf{k}}$. It follows that

$$(\partial_\tau + h_{\mathbf{k}})\mathcal{G}(\mathbf{k},\tau) = -\delta(\tau)\underline{1} \tag{15.146}$$

or $\mathcal{G}(\mathbf{k},\tau) = -1/[\partial_\tau + h_{\mathbf{k}}]$. Fourier transforming this expression in time ($\mathcal{G}(\mathbf{k},\tau) \to \mathcal{G}(\mathbf{k}, i\omega_n)$, $\partial_\tau \to -i\omega_n$), it follows that $(-i\omega_n + h_{\mathbf{k}})\mathcal{G}(k) = -1$, or

$$G(\mathbf{k}, i\omega_n) = \frac{1}{i\omega_n - \epsilon_{\mathbf{k}}\tau_3 - (\vec{\Delta}_{\mathbf{k}} \cdot \vec{\sigma})\tau_1} = \frac{i\omega_n + \epsilon_{\mathbf{k}}\tau_3 + (\vec{\Delta}_{\mathbf{k}} \cdot \vec{\sigma})\tau_1}{(i\omega_n)^2 - E^2_{\mathbf{k}}}, \tag{15.147}$$

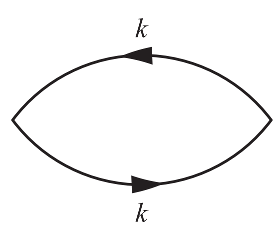
where, for ^{3}He-B, we can take $\Delta_{\mathbf{k}} = \Delta\hat{k}$, so that $(\vec{\Delta}_{\mathbf{k}} \cdot \vec{\sigma})^2 = \Delta^2$.

(b) In a magnetic field, the free energy becomes

$$F = -\frac{T}{2}\sum_k \mathrm{Tr}\ln[-\mathcal{G}^{-1}(k) - \mu_N\vec{\sigma} \cdot \vec{B}] + \text{field-independent terms}, \tag{15.148}$$

where the factor of $\frac{1}{2}$ derives from expanding the summation over one-half the Brillouin zone to the entire momentum space and μ_N is the nuclear moment of the ^{3}He-atom. We can either differentiate this twice with respect to the field or write the spin susceptibility as a mean-field polarization bubble, to obtain

$$\chi^{ab} = -\frac{\partial^2 F}{\partial B_a \partial B_b} = a$$



$$b \quad = -\frac{T\mu_N^2}{2}\sum_k \mathrm{Tr}\left[\sigma^a \mathcal{G}(k)\sigma^b\mathcal{G}(k)\right]. \tag{15.149}$$

Inserting (15.147), we obtain

$$\chi^{ab} = -\frac{T\mu_N^2}{2}\sum_k \mathrm{Tr}\left[\sigma^a \frac{i\omega_n + \epsilon_{\mathbf{k}}\tau_3 + (\vec{\Delta}_{\mathbf{k}} \cdot \vec{\sigma})\tau_1}{(i\omega_n)^2 - E^2_{\mathbf{k}}}\sigma^b \frac{i\omega_n + \epsilon_{\mathbf{k}}\tau_3 + (\vec{\Delta}_{\mathbf{k}} \cdot \vec{\sigma})\tau_1}{(i\omega_n)^2 - E^2_{\mathbf{k}}}\right]. \tag{15.150}$$

Now we can carry out the traces over the Nambu and Pauli matrices separately. Carrying out the trace over the Nambu components, we obtain

$$\chi^{ab} = -T\mu_N^2\sum_k \frac{1}{[(i\omega_n)^2 - E^2_{\mathbf{k}}]^2}\left([(i\omega_n)^2 + \epsilon^2_{\mathbf{k}}]\mathrm{Tr}[\sigma^a\sigma^b] + \left[\sigma^a(\vec{\Delta}_{\mathbf{k}} \cdot \vec{\sigma})\sigma^b(\vec{\Delta}_{\mathbf{k}} \cdot \vec{\sigma})\right]\right).$$

Now $\mathrm{Tr}[\sigma^a\sigma^b] = 2\delta^{ab}$. To calculate $\mathrm{Tr}[\sigma^a\sigma^b\sigma^c\sigma^d]$, one can cyclically anticommute σ^a around the trace (using $\sigma^a\sigma^b = 2\delta^{ab} - \sigma^b\sigma^a$), picking up the remainders, to obtain

$$\mathrm{Tr}[\sigma^a\sigma^b\sigma^c\sigma^d] = 2\left(\delta^{ab}\delta^{cd} - \delta^{ac}\delta^{bd} + \delta^{ad}\delta^{bc}\right),$$

so that

$$\mathrm{Tr}[\sigma^a(\vec{\Delta}_{\mathbf{k}}\cdot\vec{\sigma})\sigma^b(\vec{\Delta}_{\mathbf{k}}\cdot\vec{\sigma})] = 2[2\Delta^a_{\mathbf{k}}\Delta^b_{\mathbf{k}} - \delta^{ab}\Delta_{\mathbf{k}}\cdot\Delta_{\mathbf{k}}] = 2\Delta^2[2\hat{k}^a\hat{k}^b - \delta^{ab}], \quad (15.151)$$

so the susceptibility can be rewritten

$$\begin{aligned}\chi^{ab} &= -2T\mu_N^2\sum_k \frac{1}{[(i\omega_n)^2 - E_{\mathbf{k}}^2]^2}\left([(i\omega_n)^2 + \epsilon_{\mathbf{k}}^2]\delta^{ab} + \Delta^2[2\hat{k}^a\hat{k}^b - \delta^{ab}]\right)\\ &= -2T\mu_N^2\sum_k \frac{1}{[(i\omega_n)^2 - E_{\mathbf{k}}^2]^2}\left([(i\omega_n)^2 + \epsilon_{\mathbf{k}}^2 + \Delta^2]\delta^{ab} + 2\Delta^2[\hat{k}^a\hat{k}^b - \delta^{ab}]\right).\end{aligned} \quad (15.152)$$

After the momentum sums, $\hat{k}^a\hat{k}^b \rightarrow \frac{1}{3}\delta^{ab}$ so the susceptibility is isotropic, $\chi^{ab} = \chi(T)\delta^{ab}$, where

$$\chi = -2T\mu_N^2\sum_k \frac{1}{[(i\omega_n)^2 - E_{\mathbf{k}}^2]^2}\left([(i\omega_n)^2 + E_{\mathbf{k}}^2] - \frac{4}{3}\Delta^2\right). \quad (15.153)$$

The first term is recognized as the Pauli susceptibility of a singlet BCS superconductor, which drops exponentially to zero as $T \rightarrow 0$, while the second term must be interpreted as an additional contribution derived from the polarizability of the triplet condensate. The evaluation of the Matsubara sums follows the same lines as for a singlet superconductor. We obtain

$$\begin{aligned}\chi &= -2\mu_N^2\sum_{\mathbf{k}}\oint_{z=\pm E_{\mathbf{k}}}\frac{dz}{2\pi i}f(z)\frac{1}{(z-E_{\mathbf{k}})^2(z+E_{\mathbf{k}})^2}\left(z^2 + E_{\mathbf{k}}^2 - \frac{4}{3}\Delta^2\right)\\ &= -2\mu_N^2\sum_{\mathbf{k}}\left\{\frac{\partial}{\partial z}\left[f(z)\frac{1}{(z+E_{\mathbf{k}})^2}\left(z^2 + E_{\mathbf{k}}^2 - \frac{4}{3}\Delta^2\right)\right]_{z=E_{\mathbf{k}}} + (E_{\mathbf{k}} \rightarrow -E_{\mathbf{k}})\right\}\\ &= 2\mu_N^2\sum_{\mathbf{k}}\left\{-f'(E_{\mathbf{k}})\left(1 - \frac{2\Delta^2}{3E_{\mathbf{k}}^2}\right) + (1 - 2f(E_{\mathbf{k}}))\frac{\Delta^2}{3E_{\mathbf{k}}^3}\right\}.\end{aligned} \quad (15.154)$$

At zero temperature, the first term vanishes. The second term becomes

$$\begin{aligned}\chi(T=0) &= 2\mu_N^2 N(0)\int_{-\infty}^{\infty} d\epsilon\left(\frac{\Delta^2}{3[\epsilon^2 + \Delta^2]^{3/2}}\right)\\ &= 2\mu_N^2 N(0)\left[\frac{\epsilon}{3\sqrt{\epsilon^2 + \Delta^2}}\right]_{-\infty}^{\infty} = \frac{2}{3}\times 2\mu_N^2 N(0),\end{aligned} \quad (15.155)$$

so the zero-temperature susceptibility is 2/3 of the normal-state Pauli susceptibility. This intrinsic susceptibility of the condensate is present because the triplet pairs become slightly spin-polarized in a magnetic field.

We can actually do a little better than this, however, by noticing that, at a finite temperature (denoting $E = \sqrt{\epsilon^2 + \Delta^2}$),

$$\begin{aligned} \frac{2}{3} &= \frac{1}{3}\int_{-\infty}^{\infty} d\epsilon \frac{d}{d\epsilon}\left[\frac{\epsilon}{\sqrt{\epsilon^2+\Delta^2}}[1-2f(E)]\right] \\ &= \frac{1}{3}\int_{-\infty}^{\infty} d\epsilon \frac{d}{d\epsilon}\left[\frac{\Delta^3}{E^2}[1-2f(E)] - 2f'(E)\left(1-\frac{\Delta^2}{E^2}\right)\right], \end{aligned} \tag{15.156}$$

which we recognize as the argument of the second part of the integral in (15.154). We can thus rewrite the susceptibility as

$$\chi(T) = \frac{1}{3}\chi_S(T) + \frac{2}{3}\chi_P,$$

where $\chi_P = 2\mu_N^2 N(0)$ is the Pauli susceptibility of the normal state and

$$\chi_S(T) = 2\mu_N^2 N(0)\int_{-\infty}^{\infty} d\epsilon[-f'(\sqrt{\epsilon^2+\Delta^2})] = 2\mu_N^2 N(0) Y\left[\frac{\Delta}{2T}\right], \tag{15.157}$$

where

$$Y[x] = \frac{1}{2}\int_{-\infty}^{\infty} \frac{du}{\cosh^2[\sqrt{u^2+x^2}]} \tag{15.158}$$

is called the *Yoshida function*, after its inventor, Kei Yoshida. The final expression for the susceptibility of the B phase is then

$$\chi_B(T) = \chi_P\left[\frac{2}{3} + \frac{1}{3}Y[\Delta/2T]\right]. \tag{15.159}$$

Exercises

Exercise 15.1 The standard two-component Nambu spinor approach does not allow a rotationally invariant treatment of the electron spin and the Zeeman coupling of fermions to a magnetic field. This drawback can be overcome by switching to a four-component Balian–Werthamer spinor, denoted by

$$\psi_{\mathbf{k}} = \begin{pmatrix} c_{\mathbf{k}}^{\dagger} \\ -i\sigma_2 (c_{\mathbf{k}}^{\dagger})^T \end{pmatrix} = \begin{pmatrix} c_{\mathbf{k}\uparrow} \\ -c_{\mathbf{k}\downarrow} \\ c_{-\mathbf{k}\downarrow}^{\dagger} \\ c_{-\mathbf{k}\uparrow}^{\dagger} \end{pmatrix}. \tag{15.160}$$

(a) Show, using this notation, that the total electron spin can be written

$$\vec{S} = \frac{1}{4}\sum_{\mathbf{k}} \psi_{\mathbf{k}}^{\dagger} \vec{\sigma}_{(4)} \psi_{\mathbf{k}}, \tag{15.161}$$

where

$$\vec{\sigma}_4 = \begin{pmatrix} \vec{\sigma} & 0 \\ 0 & \vec{\sigma} \end{pmatrix} \tag{15.162}$$

is the four-component Pauli matrix. (You may find it useful to use the relationship $\vec{\sigma}^T = i\sigma_2\vec{\sigma}i\sigma_2$.) In practical usage, the subscript 4 is normally dropped.

(b) Show that, in a Zeeman field, the BCS Hamiltonian

$$H_{MFT} = \sum_{\mathbf{k}\sigma} c^\dagger_{\mathbf{k}\alpha}[\epsilon_{\mathbf{k}}\delta_{\alpha\beta} - \vec{\sigma}_{\alpha\beta}\cdot\vec{B}]c_{\mathbf{k}\beta} + \sum_{\mathbf{k}}\left[\bar{\Delta}c_{-\mathbf{k}\downarrow}c_{\mathbf{k}\uparrow} + c^\dagger_{\mathbf{k}\uparrow}c^\dagger_{-\mathbf{k}\downarrow}\Delta\right] + \frac{V}{g_0}\bar{\Delta}\Delta \tag{15.163}$$

can be rewritten using Balian–Werthamer spinors in the compact form

$$H_{MFT} = \frac{1}{2}\sum_{\mathbf{k}}\psi^\dagger_{\mathbf{k}}\left[\underline{h}_{\mathbf{k}} - \vec{\sigma}_4\cdot\vec{B}\right]\psi_{\mathbf{k}} + \frac{V}{g_0}\bar{\Delta}\Delta, \tag{15.164}$$

where $\underline{h}_{\mathbf{k}} = \epsilon_{\mathbf{k}}\tau_1 + \Delta_1\tau_1 + \Delta_2\tau_2$ as before, but the $\vec{\tau}$ now refer to the four-dimensional Nambu matrices

$$\vec{\tau} = \left(\begin{bmatrix} 0 & \underline{1} \\ \underline{1} & 0 \end{bmatrix}, \begin{bmatrix} 0 & -i\underline{1} \\ i\underline{1} & 0 \end{bmatrix}, \begin{bmatrix} \underline{1} & 0 \\ 0 & -\underline{1} \end{bmatrix}\right). \tag{15.165}$$

(c) Show that the quasiparticle energies in a field are given by $\pm E_{\mathbf{k}} - \sigma B$.

Exercise 15.2 Pauli limited type II superconductors.

The BCS Hamiltonian introduced in describes a *Pauli limited superconductor*, in which the Zeeman coupling of the paired electrons with the magnetic field dominates over the orbital coupling to the magnetic field. In the flux lattice of a Pauli limited type II superconductor, the magnetic field penetrates the condensate and can be considered to be approximately uniform.

(a) Assuming that the orbital coupling of the electron to the magnetic field is negligible, use the Balian–Werthamer approach developed in the previous problem to formulate BCS theory in a uniform Zeeman field, as a path integral. Show that the free energy can be written

$$\begin{aligned} F &= -\frac{T}{2}\sum_{\mathbf{k}}\mathrm{Tr}\ln[\partial_\tau + h_{\mathbf{k}} - \vec{\sigma}_4\cdot\vec{B}] + \frac{V}{g_0}\bar{\Delta}\Delta \\ &= -\frac{T}{2}\sum_{\mathbf{k},i\omega_n,\sigma}\ln\left[E^2_{\mathbf{k}} - (i\omega_n - \sigma B)^2\right] + \frac{V}{g_0}\bar{\Delta}\Delta \\ &= -T\sum_{\mathbf{k},\sigma}\ln\left[2\cosh\frac{\beta(E_{\mathbf{k}} - \sigma B)}{2}\right] + \frac{V}{g_0}\bar{\Delta}\Delta. \end{aligned} \tag{15.166}$$

(b) Show that the gap equation for a Pauli limited superconductor becomes

$$\frac{1}{g_0} = \frac{1}{2}\sum_{\mathbf{k},\sigma}\tanh\left(\frac{\beta(E_{\mathbf{k}} - \sigma B)}{2}\right)\frac{1}{2E_{\mathbf{k}}}.$$

Use this expression to show that the upper critical field is given by $g\mu_B B_{c2}/2 = \Delta/2$, where Δ is the zero-temperature value of the gap.

(c) Pauli limited superconductors usually undergo a first-order transition to the flux state at a higher field than the one just estimated. Why is this?

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