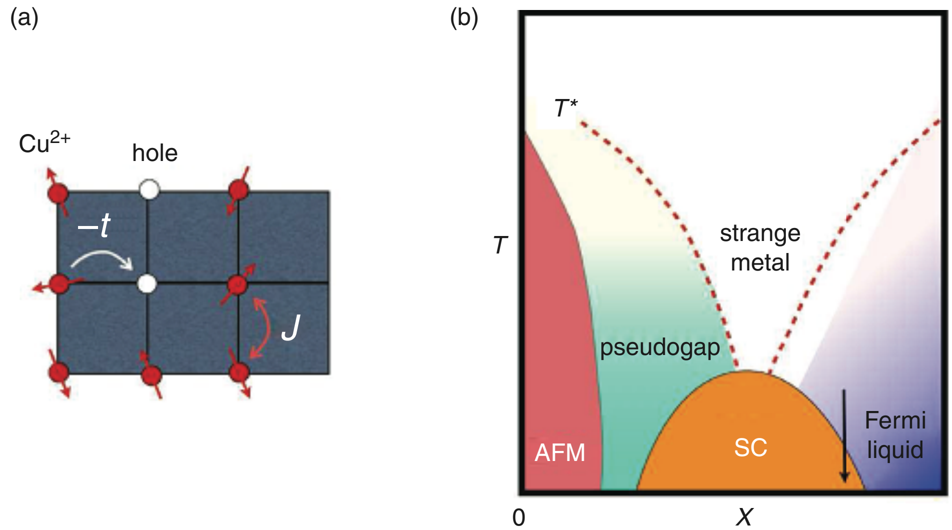

Fig. 15.4

(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

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

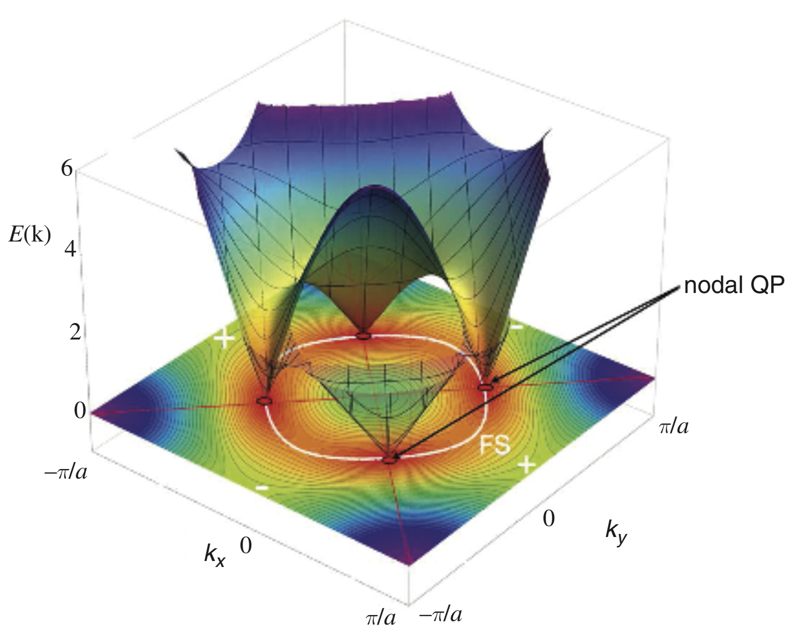

Fig. 15.5 Energy dispersion for a two-dimensional d-wave superconductor with a $d_{x^2-y^2}$ gap function. The upper part of the plot shows a cut-away three-dimensional plot of the dispersion, showing the banana-shaped quasiparticle cones of quasiparticle excitations around the nodes. In the lower contour 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

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

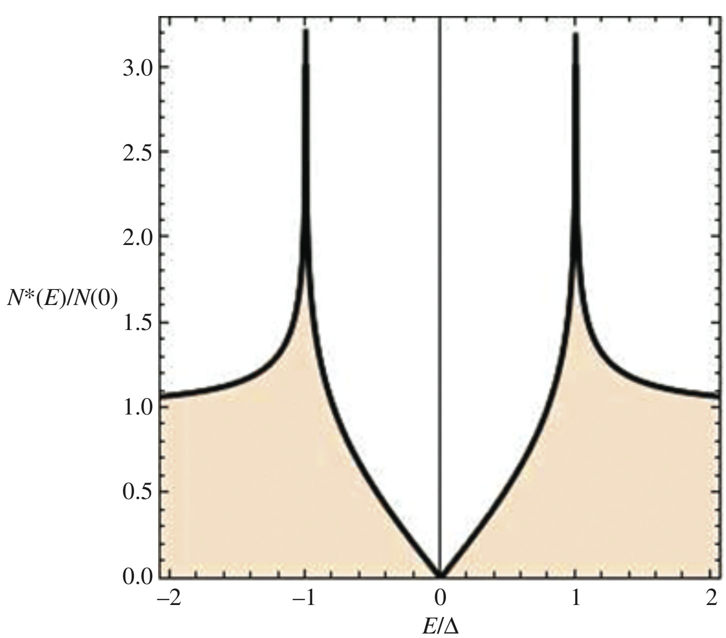

Fig. 15.6 Density of states $N^*(E)/N(0))$ for a d-wave superconductor.

[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

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

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

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

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

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

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

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

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

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

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):

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

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))

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

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.