Physics 502 - Problem Set #6

(Dated: December 6, 2023)

1. Size of the Cooper pair

We calculate ρ^2, the expectation value of r^2 with the Cooper pair wave function $\Psi = \sum_{\mathbf{k}} g_{\mathbf{k}} e^{i\mathbf{kr}}$. The denominator reads

$$\int d^3r |\Psi(\mathbf{r})|^2 = \int d^3r \sum_{\mathbf{k},\mathbf{k}'} g_{\mathbf{k}} g^*_{\mathbf{k}'} e^{i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{r}} = \sum_{\mathbf{k},\mathbf{k}'} g_{\mathbf{k}} g^*_{\mathbf{k}'} \delta_{\mathbf{k},\mathbf{k}'} = \sum_{\mathbf{k}} |g_{\mathbf{k}}|^2.$$

The numerator is similar with an extra factor of r^2

$$\int d^3r r^2 |\Psi(\mathbf{r})|^2 = \int d^3r r^2 \sum_{\mathbf{k},\mathbf{k}'} g_{\mathbf{k}} g^*_{\mathbf{k}'} e^{i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{r}} = \frac{1}{i}\frac{1}{-i} \int d^3r \sum_{\mathbf{k},\mathbf{k}'} g_{\mathbf{k}} g^*_{\mathbf{k}'} \nabla_{\mathbf{k}} \nabla_{\mathbf{k}'} e^{i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{r}}$$

$$= \int d^3r \sum_{\mathbf{k},\mathbf{k}'} (\nabla_{\mathbf{k}} g_{\mathbf{k}})(\nabla_{\mathbf{k}'} g^*_{\mathbf{k}'}) e^{i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{r}} = \sum_{\mathbf{k},\mathbf{k}'} (\nabla_{\mathbf{k}} g_{\mathbf{k}})(\nabla_{\mathbf{k}'} g^*_{\mathbf{k}'}) \delta_{\mathbf{k},\mathbf{k}'} = \sum_{\mathbf{k}} |\nabla_{\mathbf{k}} g_{\mathbf{k}}|^2.$$

In the last line we integrated by parts and neglected the surface term. To proceed from here one can convert the momentum sums to energy integrals. The denominator gives

$$\sum_{\mathbf{k}} |g_{\mathbf{k}}|^2 \approx \int d\epsilon g^2(\epsilon) = \int_{2\epsilon_F}^{2\epsilon_F+\hbar\omega_D} d\epsilon \frac{1}{(\epsilon + \Delta - 2\epsilon_F)^2} = \left(\frac{1}{\Delta} - \frac{1}{\Delta + \hbar\omega_D}\right).$$

In order to calculate the numerator we apply the same method and approximate the gradients as follows

$$\nabla_{\mathbf{k}} = \nabla_{\mathbf{k}} \epsilon_{\mathbf{k}} \frac{d}{d\epsilon} \approx \hbar v_F \frac{d}{d\epsilon}.$$

We therefore have:

$$\sum_{\mathbf{k}} |\nabla_{\mathbf{k}} g_{\mathbf{k}}|^2 = \hbar^2 v_F^2 \int_{2\epsilon_F}^{2\epsilon_F+\hbar\omega_D} d\epsilon \left| \frac{d}{d\epsilon} \left(\frac{1}{\epsilon + \Delta - 2\epsilon_F} \right) \right|^2 =$$

$$\hbar^2 v_F^2 \int_{2\epsilon_F}^{2\epsilon_F+\hbar\omega_D} d\epsilon \frac{1}{(\epsilon + \Delta - 2\epsilon_F)^4} = \frac{1}{3}\hbar^2 v_F^2 \left(\frac{1}{\Delta^3} - \frac{1}{(\Delta + \hbar\omega_D)^3} \right).$$

Putting everything together and neglecting Δ with respect to $\hbar\omega_D$ we find:

$$\rho \approx \frac{\hbar v_F}{\sqrt{3}\Delta}.$$

Plugging in numerical values for typical elemental superconductors ($v_F \simeq 10^6$m/s and $\Delta \simeq$ 1meV) we get $\rho \approx 4 \times 10^3$ Å.

2. *d*-wave superconductivity in high T_c cuprates

a. In order to diagonalize the Hamiltonian we first Fourier transform. This gives:

$$H = \sum_{\mathbf{k},\sigma}[-2t(\cos k_x + \cos k_y) - \mu]c^\dagger_{\mathbf{k},\sigma}c_{\mathbf{k},\sigma} + \Delta\sum_{\mathbf{k}}(\cos k_x - \cos k_y)[c_{\mathbf{k},\uparrow}c_{-\mathbf{k},\downarrow} + \text{h.c.}].$$

The gap function is now proportional to $(\cos k_x - \cos k_y)$, a function that changes sign upon $\pi/2$ rotation ($k_x \to k_y$ and $k_y \to -k_x$). Had we defined the pairing with a positive sign on each bond, the Fourier transformed function would be proportional to $(\cos k_x + \cos k_y)$. This function has the full symmetry of the lattice and is known as *s*-wave.

To find the spectrum we need to diagonalize the Hamiltonian via the Bogoliubov-Vallatin transformation. This can be done easily if we introduce a Nambu spinor

$$\Psi_{\mathbf{k}} = \begin{pmatrix} c_{\mathbf{k}} \\ c^\dagger_{-\mathbf{k}} \end{pmatrix}.$$

With this definition the Hamiltonian can be written as $H = \sum_{\mathbf{k}} \Psi^\dagger_{\mathbf{k}} h_{\mathbf{k}} \Psi_{\mathbf{k}}$ and the matrix $h_{\mathbf{k}}$ is given by

$$h_{\mathbf{k}} = \begin{pmatrix} \epsilon_{\mathbf{k}} - \mu & \Delta_{\mathbf{k}} \\ \Delta_{\mathbf{k}} & -\epsilon_{\mathbf{k}} + \mu \end{pmatrix}.$$

The spectrum is given by the eigenvalues of the matrix $\pm E_{\mathbf{k}}$ with $E_{\mathbf{k}} = \sqrt{(\epsilon_{\mathbf{k}} - \mu)^2 + \Delta^2_{\mathbf{k}}}$.

b. The gap function vanshies along two lines,

$$\Delta_{\mathbf{k}} = 0 \quad \Rightarrow \quad \cos k_x = \cos k_y \quad \Rightarrow \quad k_x = \pm k_y$$

The lines intersect the underlying Fermi surface at four points. To find them we require $\epsilon_{\mathbf{k}} = 0$ as well as the condition above

$$\cos k_x + \cos k_y = -\frac{\mu}{2t}$$

$$2\cos k_x = -\frac{\mu}{2t} \quad \Rightarrow k_x = \text{ArcCos}\left(-\frac{\mu}{4t}\right) = \pm k_y$$

At half filling $\mu = 0$ and the gap nodes are located at $(\pm\pi/2, \pm\pi/2)$; see figure 1.

c. Let us define new momenta $k_1 = (k_x + k_y)/\sqrt{2} - \pi$ and $k_2 = (k_x - k_y)/\sqrt{2}$. [These are momenta defined relative to the $(\pi/2, \pi/2)$ nodal point and rotated by 45^0.] We now expand $\epsilon_{\mathbf{k}}$ and $\Delta_{\mathbf{k}}$ to leading order near the node,

$$\epsilon_{\mathbf{k}} \simeq \mathbf{k} \cdot \nabla_{\mathbf{k}} \epsilon_{\mathbf{k}}|_{(\pi/2,\pi/2)} = \sqrt{2}tk_1,$$

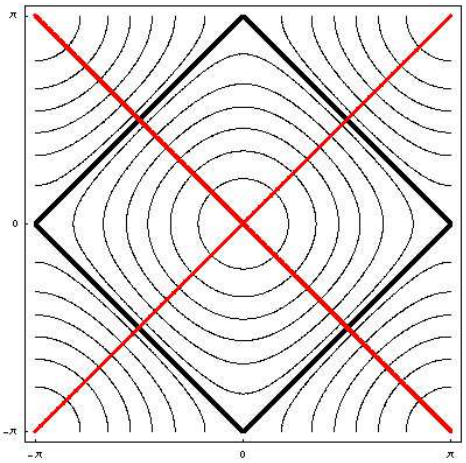

FIG. 1: The energy dispersion $\epsilon_{\mathbf{k}}$ in the Brillouin zone with the diamond shape Fermi surface at half filling denoted by a thick line. The nodal directions (diagonal red lines) intersect the Fermi surface at four points $(\pm\pi/2, \pm\pi/2)$.

$$\Delta_{\mathbf{k}} \simeq \mathbf{k} \cdot \nabla_{\mathbf{k}} \Delta_{\mathbf{k}}|_{(\pi/2,\pi/2)} = \sqrt{2}\Delta k_2.$$

The velocities are therefore $\hbar v_F = \sqrt{2}ta$ and $\hbar v_\Delta = \sqrt{2}\Delta a$ (where we have added the constants a and $\hbar$ that were implicitly set to 1).

d. The density of states is given by:

$$\rho(\epsilon) = \frac{2}{V}\sum_{\mathbf{k}} \delta(E_{\mathbf{k}} - \epsilon) \approx 2\int \frac{d^2k}{(2\pi)^2}\delta(\sqrt{(v_F k_1)^2 + (v_\Delta k_2)^2} - \epsilon) =$$

$$\frac{2}{v_F v_\Delta}\int \frac{d(v_F k_1)d(v_\Delta k_2)}{(2\pi)^2}\delta(\sqrt{(v_F k_1)^2 + (v_\Delta k_2)^2} - \epsilon) = \frac{2}{(2\pi)^2 v_F v_\Delta}\int 2\pi Q dQ \delta(Q - \epsilon) = \frac{\epsilon}{\pi v_F v_\Delta},$$

where we have introduced scaled coordinates $Q_1 = v_F k_1$ and $Q_2 = v_\Delta k_2$.

Using the above density of states we can calculate the low-temperature specific heat

$$c_v = \frac{\partial U}{\partial T} = \frac{1}{k_B T^2}\frac{\partial U}{\partial \beta} = \frac{1}{k_B T^2}\frac{\partial}{\partial \beta}\int_0^\infty d\epsilon \epsilon g(\epsilon)\frac{1}{e^{\beta\epsilon}+1}$$

$$= \frac{1}{k_B T^2}\frac{1}{\pi v_F v_\Delta}\int_0^\infty d\epsilon \epsilon^2 \frac{\epsilon e^{\beta\epsilon}}{(e^{\beta\epsilon}+1)^2} = \frac{1}{\beta^4}\frac{1}{k_B T^2}\frac{1}{\pi v_F v_\Delta}\int_0^\infty dx x^3 \frac{e^x}{(e^x+1)^2}.$$

This gives $c_v \propto T^2$. The result is valid when $k_B T \ll \Delta$; for temperatures approaching T_c one must include the T-dependence of the gap function Δ into account when calculating the specific heat.