SFI5711 - Solid State Physics (2020) List of exercises #6

1. Size of a Cooper pair

The typical energy spread of two electrons near the Fermi level forming a Cooper pair is given by the gap Δ .

- (a) (3 points) Use Heisenberg's uncertainty principle, $\delta p \, \delta x \approx \hbar$, to estimate the size of a Cooper pair as function of T_c and of the electronic density n.
- (b) (2 points) Find the values of T_c and n for Al (consult Ashcroft & Mermin) and use the expression you found in the previous item to estimate the Cooper pair size.

2. Superconducting gap near T_c

(10 points) The gap equation at an arbitrary temperature is given by

$$1 = V_0 \rho_F \int_0^{\hbar\omega_D} \frac{\mathrm{d}\varepsilon}{\sqrt{\varepsilon^2 + \Delta^2}} \tanh\left(\frac{\sqrt{\varepsilon^2 + \Delta^2}}{2k_B T}\right)$$

Consider a temperature below but very close to T_c , i.e. $T = T_c (1 - t)$, with $t \ll 1$. For consistency, the gap Δ also has to be small, i.e. $\Delta \ll k_B T_c$. Expand the gap equation for both t and Δ and show that the gap function vanishes as T approaches T_c according to the power-law

$$\frac{\Delta\left(T\right)}{\Delta\left(T=0\right)} \approx 1.74 \sqrt{1-\frac{T}{T_c}}.$$

3. BCS ground state energy

From the BCS solution, we found that the ground state energy at zero temperature (per electron) is given by

$$E_0 = \frac{1}{N} \sum_{\mathbf{k}} \left(\xi_{\mathbf{k}} - E_{\mathbf{k}} + \Delta_{\mathbf{k}} \left\langle c_{\mathbf{k}\uparrow}^{\dagger} c_{-\mathbf{k}\downarrow}^{\dagger} \right\rangle \right)$$

- (a) (3 points) Determine the difference between the superconducting and normal state energies $\delta E_0 \equiv E_0 E_0 (\Delta = 0)$ as function of Δ . (*Hint*: the integration is restricted to $|\xi| < \hbar \omega_D$. Recall that $\hbar \omega_D \gg \Delta$).
- (b) (3 points) By minimizing the energy found in the previous item, show that one recovers the formula for Δ at zero temperature found in class. (*Hint*: use the weak-coupling approximation $\rho_F V_0 \ll 1$).
- (c) (4 points) Show that the thermodynamic critical field H_c necessary to kill superconductivity is given by

$$\frac{H_c}{\Delta \left(T=0\right)} = 2\sqrt{\pi \rho_F},$$

where ρ_F is the density of states at the Fermi level. (*Hint:* the magnetic energy density is given by $H_c^2/(8\pi)$).

4. d-wave superconductivity in the cuprates

In the family of high-temperature superconductors known as the cuprates (such as La₂CuO₄ and YBa₂Cu₃O₇), the superconducting gap $\Delta_{\mathbf{k}}$ changes as function of the momentum \mathbf{k} . In a very simplified model, we can consider a *two-dimensional* parabolic band $\xi_{\mathbf{k}} = \frac{\hbar^2 k^2}{2m} - \mu$ and a gap function of the form

$$\Delta_{\mathbf{k}} = \Delta_0 \cos 2\varphi,$$

where φ is the azimuthal angle. This gap vanishes and changes sign in the so-called nodal points, located at $\varphi = \pi/4$ and its multiples.

(a) (3 points) What is the orbital angular momentum of the d-wave Cooper pair? What is its spin state, singlet or triplet? (*Hint*: compare the gap function with spherical harmonics).

(b) (5 points) The density of states for the d-wave superconductor is defined as

$$\rho\left(E\right) = \int \frac{d^2k}{\left(2\pi\right)^2} \,\delta\left(E - \sqrt{\xi_{\mathbf{k}}^2 + \Delta_{\mathbf{k}}^2}\right).$$

Obtain the low-energy $(E \ll \Delta)$ expression for the density of states, and show that it vanishes linearly with E. Why is the spectrum not gapped, like in the s-wave case $\Delta_{\mathbf{k}} = \Delta_0$?

(c) (3 points) The behavior of the density of states at low energies is manifested in the low-temperature behavior of the specific heat. In fact, the specific heat inside the superconducting state is given by

$$C = 2k_B \int_0^\infty dE \,\rho\left(E\right) \left(\frac{E}{2k_B T}\right)^2 \cosh^{-2}\left(\frac{E}{2k_B T}\right).$$

First, use the expression for $\rho(E)$ we found in class for the s-wave superconductor $\Delta_{\mathbf{k}} = \Delta_0$ to obtain the low-temperature $(k_B T \ll \Delta_0)$ behavior of the specific heat. (*Hint*: you only need to evaluate the integral in the limit $k_B T \ll \Delta_0$).

(d) (4 points) Now, use the expression you found in item (b) for the density of states at low energies to determine the specific heat behavior at low temperatures $(k_B T \ll \Delta_0)$ inside of a d-wave superconductor. How does it compare to your result for the s-wave superconductor?

5. s^{+-} superconductivity in the iron pnictides

The other known family of high-temperature superconductors, the iron pnictides (such as LaFeAsO and BaFe₂As₂), are multi-band compounds. In this case, the superconducting gap can have different signs on different bands. Let us consider a very simplified model, with two parabolic two-dimensional bands: a hole-like band $\xi_{1,\mathbf{k}}$, with density of states ρ_1 , and an electron-like band $\xi_{2,\mathbf{k}}$, with density of states ρ_2 . The gap equations form a 2 × 2 system of equations

$$\Delta_{\lambda} = -\frac{1}{N} \sum_{\lambda'=1}^{2} V_{\lambda\lambda'} \Delta_{\lambda'} \sum_{\mathbf{k}} \frac{1}{2E_{\lambda',\mathbf{k}}} \tanh\left(\frac{E_{\lambda',\mathbf{k}}}{2k_B T}\right),$$

where $\lambda, \lambda' = 1, 2$ are band indices. The momentum integration is limited to $|\xi_{\lambda',\mathbf{k}}| < W$, where W is some energy scale associated with the pairing mechanism, which replaces the Debye energy $\hbar\omega_D$. The interaction potential $V_{\lambda\lambda'}$ and the gap functions Δ_{λ} do not depend on the momentum, i.e. we are considering s-wave states.

(a) (5 points) Consider that the only non-vanishing interaction is the inter-band interaction V_{12} , i.e. $V_{11} = V_{22} = 0$. Show that T_c is given by

$$T_c = 1.13 \frac{W}{k_B} \exp\left(-\frac{1}{|V_{12}|\sqrt{\rho_1 \rho_2}}\right).$$

(b) (5 points) Show that, if V_{12} is an attractive interaction, the signs of the two gap functions Δ_1 and Δ_2 are the same (the so-called s^{++} state), whereas if V_{12} is a repulsive interaction, their signs are different (known as the s^{+-} state). Determine the absolute value of the ratio between the two gap functions Δ_1/Δ_2 immediately below T_c in both cases. Does this ratio depend on whether the superconducting state is s^{+-} or s^{++} ?

6. Magnetic instability of the one-dimensional electron gas

(10 points) The criterion for a Stoner instability at the wave vector \mathbf{q} is $\chi(\mathbf{q}) U = 1$. Here, $\chi(\mathbf{q})$ is the Lindhard function:

$$\chi\left(\mathbf{q}\right) = \frac{1}{v} \sum_{\mathbf{k}} \frac{f\left(\varepsilon_{\mathbf{k}+\mathbf{q}}\right) - f\left(\varepsilon_{\mathbf{k}}\right)}{\varepsilon_{\mathbf{k}} - \varepsilon_{\mathbf{k}+\mathbf{q}}}$$

v is the volume and f(x) is the Fermi-Dirac distribution function. For the one-dimensional electron gas, where $\varepsilon_{\mathbf{k}} = \hbar^2 k^2 / (2m)$, show that

$$\chi\left(\mathbf{q}\right) = \frac{m}{\pi\hbar^{2}q}\ln\left(\frac{2k_{F}+q}{2k_{F}-q}\right).$$

Plot this function and verify that it diverges at $q = \pm 2k_F$. Therefore, the 1D electron gas in unstable towards a magnetically ordered state whose magnetization has a $2k_F$ modulation.

7. Stoner continuum

The metallic (itinerant) ferromagnet has two types of excitations: spin waves and the particle-hole spin-flip pair. In the latter, an electron at the Fermi level ε_F is excited from the spin-up band $\varepsilon_{\mathbf{k}\uparrow}$ to the spin-down band $\varepsilon_{\mathbf{k}\downarrow}$. Measuring all energies with respect to the bottom of the spin-up band, we have $\varepsilon_{\mathbf{k}\uparrow} = \hbar^2 k^2 / (2m)$ and

$$\varepsilon_{\mathbf{k}\downarrow} = \frac{\hbar^2 k^2}{2m} + \Delta,$$

where $\Delta = 4UM > 0$ is the gap. Consider that this process involves a change in energy of $\hbar\omega$ and a change in momentum of \mathbf{q} , i.e. $\varepsilon_{\mathbf{k}_2\downarrow} - \varepsilon_{\mathbf{k}_1\uparrow} = \hbar\omega$ and $\mathbf{k}_2 - \mathbf{k}_1 = \mathbf{q}$.

- (a) (7 points) The region in the $(\hbar\omega, q)$ plane where this type of excitation is allowed is called the Stoner continuum. Find the equations $\hbar\omega(q)$ describing the boundaries of the Stoner continuum. (*Hint:* in the boundaries the vectors \mathbf{k}_1 and \mathbf{k}_2 are either parallel or anti-parallel).
- (b) (3 points) Using the previous result, sketch the Stoner continuum in the $(\hbar\omega, q)$ plane. What happens (qualitatively) to the spin-wave excitations when they meet the Stoner continuum? (Recall that the spin waves dispersion is $\omega \propto q^2$ for small q)

8. Spin-waves for an anisotropic ferromagnet

Consider the anisotropic Heisenberg ferromagnet:

$$H = -\sum_{\langle ij\rangle} \left[J_z \hat{S}_i^z \hat{S}_j^z + J \left(\hat{S}_i^x \hat{S}_j^x + \hat{S}_i^y \hat{S}_j^y \right) \right]$$

where $J_z > J > 0$. This Hamiltonian interpolates between the Heisenberg model ($J = J_z$, studied in class) and the Ising model (J = 0).

(a) (8 points) Repeat the Holstein-Primakoff calculation we did for the isotropic case, which assumes that the ordered state corresponds to all spins pointing to the $\hat{\mathbf{z}}$ direction. Show that the spin-wave dispersion in the anisotropic case is given by

$$\hbar\omega_{\mathbf{k}} = 2Sz\left(J_z - J\gamma_{\mathbf{k}}\right),$$

where z and $\gamma_{\mathbf{k}}$ are the same as in the isotropic case.

(b) (2 points) Show that $\omega_{\mathbf{k}\to 0}$ remain finite in the anisotropic case. The spin-wave excitation spectrum is said to be gapped, since there is a minimum energy necessary to excite spin waves. Why is it different than the isotropic case, where $\omega_{\mathbf{k}\to 0}$ goes to zero?

9. Spin-wave dispersion for an antiferromagnet

Apply the Holstein-Primakoff transformation to an antiferromagnet in a hyper-cubic lattice. This lattice can be subdivided into two other hyper-cubic sub-lattices A and B. In the Néel state, all the spins in A point up and all the spins in B point down. The Heisenberg Hamiltonian is thus

$$H = J \sum_{\langle i,j \rangle} \left[\hat{S}_{A,i}^{z} \hat{S}_{B,j}^{z} + \frac{1}{2} \left(\hat{S}_{A,i}^{+} \hat{S}_{B,j}^{-} + \hat{S}_{A,i}^{-} \hat{S}_{B,j}^{+} \right) \right]$$

where J > 0, *i* is a site of sublattice *A*, and *j* is a site of sublattice *B*. By definition, *i* and *j* are nearest-neighbors of the original lattice, i.e. $\mathbf{R}_j = \mathbf{R}_i + \boldsymbol{\delta}$.

(a) (5 points) Use the Holstein-Primakoff transformation

$$\begin{split} \hat{S}_{A,i}^{z} &= S - c_{i}^{\dagger}c_{i}, \quad \hat{S}_{B,j}^{z} = -S + d_{j}^{\dagger}d_{j}, \\ \hat{S}_{A,i}^{+} &= \sqrt{2S} \left(1 - \frac{c_{i}^{\dagger}c_{i}}{2S} \right)^{1/2} c_{i}, \quad \hat{S}_{B,j}^{+} = \sqrt{2S} d_{j}^{\dagger} \left(1 - \frac{d_{j}^{\dagger}d_{j}}{2S} \right)^{1/2}, \\ \hat{S}_{A,i}^{-} \sqrt{2S} c_{i}^{\dagger} \left(1 - \frac{c_{i}^{\dagger}c_{i}}{2S} \right)^{1/2}, \quad \hat{S}_{B,j}^{-} = \sqrt{2S} \left(1 - \frac{d_{j}^{\dagger}d_{j}}{2S} \right)^{1/2} d_{j}, \end{split}$$

in the large-S limit to show that the Hamiltonian can be recast in the form

$$H = JSz \sum_{\mathbf{k}} \left[\gamma_{\mathbf{k}} \left(c_{\mathbf{k}} d_{-\mathbf{k}} + d_{-\mathbf{k}}^{\dagger} c_{\mathbf{k}}^{\dagger} \right) + \left(c_{\mathbf{k}}^{\dagger} c_{\mathbf{k}} + d_{-\mathbf{k}}^{\dagger} d_{-\mathbf{k}} \right) \right], \tag{1}$$

where $c_{\mathbf{k}}^{\dagger}$ and $d_{\mathbf{k}}^{\dagger}$ are the appropriate Fourier-transformed bosonic operators and $\gamma_{\mathbf{k}}$ is the same as in the ferromagnetic case.

(b) (5 points) The bosonic Hamiltonian (1) can be solved via a Bogliubov transformation

$$c_{\mathbf{k}} = u_{\mathbf{k}}\alpha_{\mathbf{k}} - v_{\mathbf{k}}\beta_{\mathbf{k}}^{\dagger},$$
$$d_{-\mathbf{k}} = u_{\mathbf{k}}\beta_{\mathbf{k}} - v_{\mathbf{k}}\alpha_{\mathbf{k}}^{\dagger}.$$

Show that

$$H = \sum_{\mathbf{k}} \hbar \omega_{\mathbf{k}} \left(\alpha_{\mathbf{k}}^{\dagger} \alpha_{\mathbf{k}} + \beta_{\mathbf{k}}^{\dagger} \beta_{\mathbf{k}} \right),$$

with the spin-wave dispersion

$$\hbar\omega_{\mathbf{k}} = JSz\sqrt{1-\gamma_{\mathbf{k}}^2}.$$

Show that $\omega_{\mathbf{k}} \propto k$ for small k.

(c) (5 points) The deviation of the staggered magnetization \overline{M} from the saturation value S is given by

$$\Delta \bar{M} = \left\langle \sum_{i} \left(\hat{S}_{A,i}^{z} - S \right) - \sum_{j} \left(\hat{S}_{B,j}^{z} + S \right) \right\rangle = -\sum_{\mathbf{k}} \left(\left\langle c_{\mathbf{k}}^{\dagger} c_{\mathbf{k}} \right\rangle + \left\langle d_{-\mathbf{k}}^{\dagger} d_{-\mathbf{k}} \right\rangle \right).$$

Express $c_{\mathbf{k}}^{\dagger}c_{\mathbf{k}}$ and $d_{\mathbf{k}}^{\dagger}d_{\mathbf{k}}$ in terms of the Bogoliubov operators $\alpha_{\mathbf{k}}$ and $\beta_{\mathbf{k}}$. Using the fact that in the ground state there are no spin waves, i.e., $\left\langle \alpha_{\mathbf{k}}^{\dagger}\alpha_{\mathbf{k}}\right\rangle = \left\langle \beta_{\mathbf{k}}^{\dagger}\beta_{\mathbf{k}}\right\rangle = 0$, show that

$$\Delta \bar{M} = -\sum_{\mathbf{k}} \left(\frac{1}{\sqrt{1 - \gamma_{\mathbf{k}}^2}} - 1 \right).$$

Show that $\Delta \overline{M}$ diverges for the one-dimensional case. For simplicity, use the small k expansion. What does the divergence of $\Delta \overline{M}$ imply?