8.231 Physics of Solids I — Fall 2017
Problem Set 3

Posted: Tuesday, Sep 19, 2017
Due: **Tuesday, Sep 26, 2017**

Readings (Optional)

- Simon, Steven H. *The Oxford Solid State Basics*, Chapter 9-11.

Note: Bonus problems are more challenging. It is fine you do not solve them. By solving them you can earn extra credits.

Problem 1

Pauli Paramagnetism

When the magnetic field is applied to electrons, the effects are two-fold:

- Orbital effect. Classically, the electrons will feel the Lorentz force and do cyclotron motion. Quantum-mechanically, the energy eigenstates form Landau levels.
- Spin effect. The internal spin degrees of freedom will have a Zeeman splitting.

In this problem, we neglect the orbital effect and focus on the spin effect. The Hamiltonian is then given as

$$H = \frac{\mathbf{p}^2}{2m} + g_e \mu_B \mathbf{B} \cdot \mathbf{S}, \tag{1}$$

where $g_e = 2$ is the Landé g-factor for the electron, $\mu_B \equiv e\hbar/(2m_e)$ is the Bohr magneton. $\mathbf{S}$ is the spin operator for the electrons whose eigenvalue are $\pm 1/2$.

(a) What are the good quantum numbers? What are the energy eigenvalues given good quantum numbers?

(b) What is the density of states $g(E)$?
(Hint: It is piecewise with different functional form when $-\mu_B B \leq E < \mu_B B$ and $\mu_B B \leq E$.)

(c) The magnetization of the system can be computed by

$$M = -\frac{1}{V}\left(\frac{\partial \Phi}{\partial B}\right)_{\mu}, \tag{2}$$

where $\Phi \equiv U - TS - \mu N$ is the grand potential of the system. First compute Φ at zero temperature *explicitly*. Then compute M using Eq. (2). Note that the chemical potential (i.e. Fermi energy) is fixed when the magnetic field varies.

(d) The magnetic susceptibility is defined as

$$\chi = \left.\frac{\partial M}{\partial H}\right|_{B\to 0}. \tag{3}$$

Compute χ. Express your result using the density of states at Fermi energy *without* the magnetic field $g(E_F)$. By considering everything in the very small B limit, can you obtain the same result without doing any calculation? Give your argument.

You should find $\chi > 0$, i.e., the induced magnetization is of the same direction as the external magnetic field. This is why this phenomenon is called "paramagnetism".

(e) (Bonus) Eq. (2) can actually be simplified to

$$M = -\frac{\mu_B}{V}\left(N_\uparrow - N_\downarrow\right), \tag{4}$$

where $N_\uparrow$ and $N_\downarrow$ are the number of electrons whose spin are parallel and anti-parallel with the magnetic field. (You can use this formula to check your calculation in (c).) Prove Eq. (4) at $T = 0$.

(Hint: This problem is not as trivial as it seems to be, since both $N_\uparrow$ and $N_\downarrow$ are functions of B implicitly and will in principle have non-vanishing B derivatives.)

Problem 2

Friedel Oscillations

In a translationally-invariant system, electron density $n(x) = n_0$ is uniform. This is no longer the case when a boundary or an impurity is present. A remarkable prediction of quantum theory of metals is that electron density shows a spatial oscillation that persists to far away from the boundary. This wave-like phenomenon is known as Friedel oscillations. See the beautiful scanning tunneling microscope images in Figure 1.

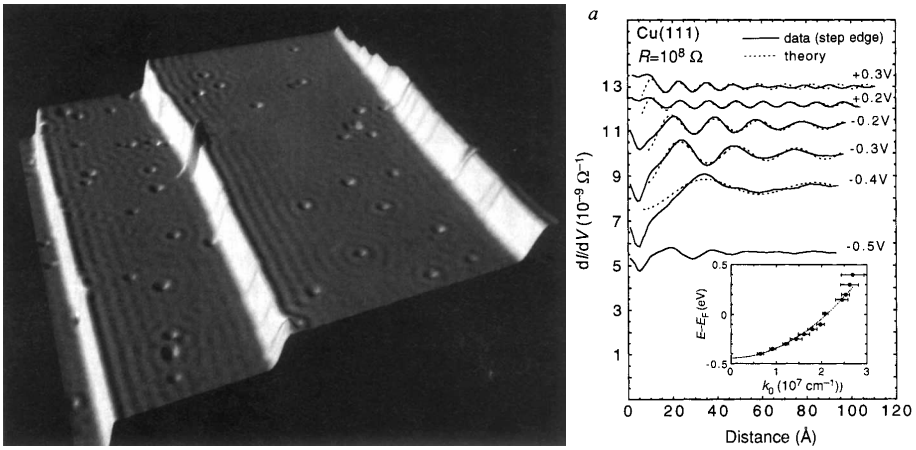

Figure 1: The scanning tunneling microscope image of local density of states of the Cu(111) surface. Taken from M. F. Crommie, C. P. Lutz, and D. M. Eigler, *Nature*, **363**, 524 (1993).

To understand the essential physics of Friedel oscillations, let us consider non-interacting electrons in an one-dimensional system with infinite hardwall boundary at $x = 0$ and $x = L$. The goal of this problem is to calculate the deviation of the electron density from average: $\rho(x) = n(x) - n_0$ due to the boundary effect.

(a) Solve the energy eigenstates $\psi_k(x)$, which are standing waves labeled by the good quantum number k. Specify what are the possible values of k.

(b) Assume there are N electrons and take into account spin degeneracy. Express the Fermi wavevector k_F for the highest occupied state with the average electron density n_0.

(c) The observed electron density can be computed by averaging over all the occupied states weighted by the Fermi-Dirac distribution n_F:

$$n(x) = \sum_k |\psi_k(x)|^2 n_F(E(k)), \tag{5}$$

where $E(k)$ is the energy eigenvalue for ψ_k. At zero temperature, compute $\rho(x) = n(x) - n_0$. Convert the summation in Eq. (5) into an integral by taking the limit $L \to \infty$, and evaluate the integral analytically. Your result should look similar to the right panel of Figure 1.

(d) With dimensional analysis and putting constant prefactors like 2 or π aside, reproduce (c) without doing any calculation.

(e) (Bonus) Compute Friedel oscillations at finite temperature $T \ll T_F$. Comment your result in the $T \to 0$ limit and $x \gg 1$ limit.

In order to perform the integral analytically, you may linearize the dispersion as $E(k) - E_F \simeq v_F(k - k_F)$, where $v_F = \hbar k_F/m$. You will also find this Fourier transform useful:

$$\int_{-\infty}^{\infty} dz \frac{e^{i\lambda z}}{1 + \cosh(bz)} = \frac{2\pi\lambda}{b^2} \frac{1}{\sinh(\pi\lambda/b)}. \tag{6}$$