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Condensed Matter Theory 1 — Exercise 11

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To be discussed on: *Thursday 2024/01/25*

1. Hartree-Fock effective mass near $k = 0$

In the lecture, the Hartree-Fock approximation for free electrons was discussed. In this approximation, the single-particle energy is given by $\varepsilon_{\boldsymbol{k}}^{\mathrm{HF}} = \frac{\hbar^2 k^2}{2m} + \varepsilon_{\boldsymbol{k}}^{\mathrm{ex}}$ with the exchange correction

$$\varepsilon_{\boldsymbol{k}}^{\mathrm{ex}} = -\frac{2e^2}{\pi} k_F F(k/k_F), \tag{1}$$

where F is the Lindhard function

$$F(x) = \frac{1}{2} + \frac{1-x^2}{4x} \ln\left(\frac{1+x}{1-x}\right) . \tag{2}$$

For the limit of small k, show that the energy is still parabolic, $\varepsilon_{\boldsymbol{k}}^{\mathrm{HF}} \approx \frac{\hbar^2 k^2}{2m^*}$, and that the effective mass is given by

$$m^*_{k\to 0} \approx \frac{m}{1 + 0.22(r_s/a)} . \tag{3}$$

As in the lecture, $r_s = [3/(4\pi n)]^{1/3}$ is the radius of a sphere with volume $1/n$ and $a = \hbar^2/(me^2)$ is the Bohr radius.
Hints: $k_F = (3\pi^2 n)^{1/3}$ *and* $\ln(1-x) = -\sum_n x^n/n$ *and* $\ln(1+x) = -\sum_n (-x)^n/n$.

2. Magnetic Friedel oscillations

In the lecture, it was derived that the Lindhard theory of screening leads to Friedel ($2k_F$-)oscillations in the Coulomb potential. The goal of this exercise is to show that similar oscillations exist in the magnetization far from magnetic impurities. Therefore, we will first determine the perturbative corrections to the free electron wavefunction in the presence of a magnetic impurity and, in a second step, use this result to compute the magnetization which requires careful treatment of the Lindhard function.
Consider a spin-$\frac{1}{2}$ Fermi gas with the Hamiltonian $\hat{H}_0$ and its eigenstates $|\boldsymbol{k},\sigma\rangle_0$:

$$\hat{H}_0 |\boldsymbol{k},\sigma\rangle_0 = \frac{\hbar^2 k^2}{2m} |\boldsymbol{k},\sigma\rangle_0 = \epsilon_{\boldsymbol{k}}^{(0)} |\boldsymbol{k},\sigma\rangle_0 , \quad \langle \boldsymbol{r}|\boldsymbol{k},\sigma\rangle_0 = \Psi^{(0)}_{\boldsymbol{k},\sigma}(\boldsymbol{r}) = \frac{e^{i\boldsymbol{k}\cdot\boldsymbol{r}}}{\sqrt{V}}\psi_\sigma, \quad \psi_\uparrow = \begin{pmatrix}1\\0\end{pmatrix}, \quad \psi_\downarrow = \begin{pmatrix}0\\1\end{pmatrix} \tag{4}$$

where V is the volume. Additionally, consider a magnetic impurity

$$V(\boldsymbol{r}) = -\frac{g\mu_B}{2}\boldsymbol{\sigma}\cdot\boldsymbol{B}(\boldsymbol{r}) \tag{5}$$

which we will treat in the following as a small perturbation, assuming that B is smalll. For simplicity, set $\boldsymbol{B}(\boldsymbol{r}) = B\hat{z}\delta(\boldsymbol{r})$ such that the number of spin-$\uparrow$ and spin-$\downarrow$ fermions is separately conserved and they can be treated as two independent Fermi seas.

a) Determine the correction to the eigenfunctions in lowest order perturbation theory in B: $|\boldsymbol{k},\sigma\rangle = |\boldsymbol{k},\sigma\rangle_0 + |\boldsymbol{k},\sigma\rangle_1$. Show that the result is

$$\Psi^{(1)}_{\boldsymbol{k},\sigma}(\boldsymbol{r}) = \langle \boldsymbol{r}|\boldsymbol{k},\sigma\rangle_1 = -\frac{g\mu_B B}{2V^{3/2}} \sum_{\boldsymbol{p}\neq\boldsymbol{k}} \frac{e^{i\boldsymbol{p}\cdot\boldsymbol{r}}}{\epsilon^{(0)}_{\boldsymbol{k}} - \epsilon^{(0)}_{\boldsymbol{p}}} \sigma\psi_\sigma \tag{6}$$

with $\sigma = 1$ and -1 for $\sigma = \uparrow$ and $\downarrow$, respectively.

b) Calculate the energy difference $\Delta\epsilon_{\boldsymbol{k}} = \epsilon^{(1)}_{\boldsymbol{k},\sigma=1} - \epsilon^{(1)}_{\boldsymbol{k},\sigma=-1}$ between the spin-$\uparrow$ and spin-$\downarrow$ fermions and discuss its value in the limit of an infinitely large volume, $V \to \infty$.

The magnetization for a system with distribution function $f_{\boldsymbol{k}}$ is given by

$$\boldsymbol{M}(\boldsymbol{r}) = \frac{g\mu_B}{2} \sum_{\boldsymbol{k},\sigma,\sigma'} f(\boldsymbol{k}) \Psi^\dagger_{\boldsymbol{k},\sigma}(\boldsymbol{r}) \boldsymbol{\sigma}_{\sigma,\sigma'} \Psi_{\boldsymbol{k},\sigma'}(\boldsymbol{r}) \ , \tag{7}$$

where the tensor $\boldsymbol{\sigma}$ is the vector of Pauli matrices and indices σ and σ' denote the spin components of the wave functions Ψ and each Pauli matrix, respectively. In the following we will use the zero temperature equilibrium distribution $f^{(0)}_{\boldsymbol{k}} = \Theta(E_F - \epsilon_{\boldsymbol{k}})$, where $E_F = \hbar^2 k_F^2/(2m)$ is the Fermi energy.

c) Show that the magnetization is zero without a magnetic field, i.e. when $\Psi_{\boldsymbol{k},\sigma}(\boldsymbol{r}) = \Psi^{(0)}_{\boldsymbol{k},\sigma}(\boldsymbol{r})$.

To linear order in B, the response of the system to the perturbation results in a finite magnetization in z-direction:

$$M_z(\boldsymbol{r}) = \frac{g\mu_B}{2} \sum_{\boldsymbol{k},\sigma=\pm1} \sigma f^{(0)}_{\boldsymbol{k}} \left(\Psi^{(0)\dagger}_{\boldsymbol{k},\sigma}(\boldsymbol{r}) \Psi^{(1)}_{\boldsymbol{k},\sigma}(\boldsymbol{r}) + \Psi^{(1)\dagger}_{\boldsymbol{k},\sigma}(\boldsymbol{r}) \Psi^{(0)}_{\boldsymbol{k},\sigma}(\boldsymbol{r}) \right) \ . \tag{8}$$

d) Using the result in Eq. (6), show that Eq. (8) takes the form

$$M_z(\boldsymbol{r}) = \left(\frac{g\mu_B}{2}\right)^2 \nu(E_F) \frac{2k_F^2}{\pi^2 |\boldsymbol{r}|} g(2k_F|\boldsymbol{r}|) \ B \ , \tag{9}$$

where $\nu(E_F) = mk_F/(\hbar^2\pi^2)$ is the density of states at the Fermi energy and

$$g(a) = \int_0^\infty dx x \sin(ax) F(x) \ . \tag{10}$$

Here,

$$F(x) = \frac{1}{2} + \frac{1-x^2}{8x} \ln\left(\left(\frac{1+x}{1-x}\right)^2 \right) \tag{11}$$

denotes the *Lindhard function*, written in an alternative form where the square inside the logarithm takes care of the sign of the argument.

Hints: Choose the polar coordinates for $\boldsymbol{k}$ *relative to* $\mathbf{p}$ *and substitute* $\boldsymbol{k} = k_F\boldsymbol{y}$. *Choose the polar coordinates for* $\boldsymbol{p}$ *relative to* $\boldsymbol{r}$ *and substitute* $\boldsymbol{p} = 2k_F\boldsymbol{x}$.

Helpful integrals:

$\int_{-1}^{1} \frac{1}{q+2k\tau} d\tau = \frac{1}{2k} \ln\left|\frac{q+2k}{q-2k}\right|$

$\int_0^1 \frac{y}{2} \ln\left(\frac{x+y}{x-y}\right)^2 dy = 2xF(x)$

In the following, we investigate $M_z(\boldsymbol{r})$ in the limit of large distance from the impurity, $r \to \infty$, and find an approximate, explicit expression for the result in Eq. (9). Taking this limit requires a discussion of the behavior of $g(a \to \infty)$. The asymptotic value of the integral, Eq. (10), is dominated by the region $z \approx 1$ where the integrand is non-analytic. To show the non-analyticity more explicitly, one can rewrite $g(a)$ using partial integration as

$$g(a) = -\int_0^\infty dx \left(\frac{-x\cos(ax)}{a} + \frac{\sin(ax)}{a^2} \right) F'(x) \ . \tag{12}$$

e) Calculate the derivative of the Lindhard function which can be split into a smooth and a divergent part, $F'(x) = F'_{\text{smooth}}(x) + F'_{\text{div}}(x)$. Show that the divergent part takes is

$$F'_{\text{div}} = \frac{1}{2}\ln(|1-x|) \ , \tag{13}$$

i.e., there is a logarithmic singularity at $x = 1$. Use a computer program to visualize this non-analyticity, i.e., first, plot the Lindhard function to convince yourself that it is a smooth function and, next, plot $F'(x)$ together with F'_{smooth} and F'_{div}.

The logarithmic divergence around $x = 1$ determines the asymptotic behavior of $g(a)$ for $a \to \infty$. Therefore, Eq. (12) becomes

$$\begin{aligned} g(a) \underset{\varepsilon>0, a\to\infty}{\approx} & -\int_{1-\varepsilon}^{1+\varepsilon} dx \left(\frac{-x\cos(ax)}{a} + \frac{\sin(ax)}{a^2} \right) F'_{\text{div}}(x) \\ = & \int_{1-\varepsilon}^{1+\varepsilon} dx \frac{2\cos(ax) + ax\sin(ax)}{2a^3(x-1)} \ , \end{aligned} \tag{14}$$

where we have performed a partial integration from the first to the second line.

f) Since we focus on the limit $a \to \infty$, consider in Eq. (14) only the most slowly decaying terms in a and show that, with $\varepsilon a \to \infty$, the result becomes

$$g(a \to \infty) = \frac{\pi}{2}\frac{\cos(a)}{a^2} + \mathcal{O}\left(\frac{1}{a^3}\right) \ . \tag{15}$$

g) What is the asymptotic behavior $M_z(|\boldsymbol{r}| \to \infty)$?