TFY4245/FY8917 Solid State Physics, Advanced Course
Problemset 5

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SUGGESTED SOLUTION

Problem 1

(a) Consider the zero-temperature limit, so that $f_{\boldsymbol{k}} = \theta(k_F - k)$, i.e. a Heaviside-step function. Due to the spin-degeneracy, the spin sum gives a factor 2. Taking the continuum limit of $\boldsymbol{k}$ in the summation gives us an integral:

$$\chi_0(\boldsymbol{q}) = \frac{2}{V}\frac{1}{(2\pi)^3/V}\int d\boldsymbol{k}\frac{\theta(k_F-k)-\theta(k_F-|\boldsymbol{k}-\boldsymbol{q}|)}{\frac{\hbar^2}{2m}[k^2-(\boldsymbol{k}-\boldsymbol{q})^2]}$$
$$= \frac{m}{2\pi^3\hbar^2}\int d\boldsymbol{k}\frac{\theta(k_F-k)}{2\boldsymbol{k}\cdot\boldsymbol{q}-q^2} - \frac{m}{2\pi^3\hbar^2}\int d\boldsymbol{p}\frac{\theta(k_F-p)}{(\boldsymbol{p}+\boldsymbol{q})^2-p^2} \tag{1}$$

where in the second term we introduced the new variable $\boldsymbol{p} \equiv \boldsymbol{k}-\boldsymbol{q}$. If we now simply rename the variable $\boldsymbol{p}$ to $\boldsymbol{k}$, we obtain

$$\chi_0(\boldsymbol{q}) = -\frac{m}{2\pi^3\hbar^2}\int d\boldsymbol{k}\theta(k_F-k)\Big(\frac{1}{q^2+2\boldsymbol{k}\cdot\boldsymbol{q}}+\frac{1}{q^2-2\boldsymbol{k}\cdot\boldsymbol{q}}\Big). \tag{2}$$

Perform now the first integral:

$$\int d\boldsymbol{k}\theta(k_F-k)\frac{1}{q^2+2\boldsymbol{k}\cdot\boldsymbol{q}} = 2\pi\int_0^{k_F}dk\,k^2\int_0^{\pi}d\phi\sin\phi\frac{1}{q^2+2kq\cos\phi}$$
$$= \frac{\pi}{q}\int_0^{k_F}dk\,k\ln\Big|\frac{q/(2k)+1}{q/(2k)-1}\Big|. \tag{3}$$

The second integral is obtained by $\boldsymbol{q}\to-\boldsymbol{q}$, so that

$$\int d\boldsymbol{k}\theta(k_F-k)\frac{1}{q^2-2\boldsymbol{k}\cdot\boldsymbol{q}} = -\frac{\pi}{q}\int_0^{k_F}dk\,k\ln\Big|\frac{-q/(2k)+1}{-q/(2k)-1}\Big|$$
$$= \frac{\pi}{q}\int_0^{k_F}dk\,k\ln\Big|\frac{q/(2k)+1}{q/(2k)-1}\Big|. \tag{4}$$

In total, we therefore have

$$\chi_0(\boldsymbol{q}) = -\frac{m}{\pi^2\hbar^2}\frac{1}{q}\int_0^{k_F}dk\,k\ln\Big|\frac{q/(2k)+1}{q/(2k)-1}\Big|$$
$$= -\frac{m}{\pi^2\hbar^2}\frac{1}{q}\Big[\frac{k^2}{2}\ln\Big|\frac{q/(2k)+1}{q/(2k)-1}\Big| - \int dk\,k^2\Big(\frac{1}{q+2k}+\frac{1}{q-2k}\Big)\Big]_0^{k_F}$$
$$= -\frac{m}{\pi^2\hbar^2}\frac{1}{q}\Big[\frac{k^2}{2}\ln\Big|\frac{q/(2k)+1}{q/(2k)-1}\Big| - \int dk\Big(-q/2+q^2/4\Big(\big(\frac{1}{q+2k}+\frac{1}{q-2k}\Big)\Big)\Big]_0^{k_F}$$
$$= -\frac{m}{\pi^2\hbar^2}\frac{1}{q}\Big[\Big(\frac{k^2}{2}-\frac{q^2}{8}\Big)\ln\Big|\frac{q/(2k)+1}{q/(2k)-1}\Big| + \frac{qk}{2}\Big]_0^{k_F}$$
$$= -\frac{m}{\pi^2\hbar^2}\frac{1}{q}\Big[\Big(\frac{k_F^2}{2}-\frac{q^2}{8}\Big)\ln\Big|\frac{q/(2k_F)+1}{q/(2k_F)-1}\Big| + \frac{qk_F}{2}\Big]. \tag{5}$$

(b) The dielectric function is obtained from

$$\varepsilon_r(\boldsymbol{q},\omega) = 1 - \frac{e^2}{\varepsilon_0 q^2}\chi_0(\boldsymbol{q},\omega) \tag{6}$$

which yields

$$\varepsilon_r(\boldsymbol{q},0) = 1 + \frac{e^2}{\varepsilon_0 q^2}\frac{m}{\pi^2\hbar^2 q}\Big[\frac{qk_F}{2} + \Big(\frac{k_F^2}{2} - \frac{q^2}{8}\Big)\ln\Big|\frac{q/(2k_F)+1}{q/(2k_F)-1}\Big|\Big]. \tag{7}$$

We see that $\varepsilon_r \to \infty$ when $q \to 0$. This is physically reasonable for a metal. We know that the permittivity is a material property that affects the Coulomb force between two point charges in the material. In particular, the relative permittivity is the factor by which the electric field between the charges is decreased relative to vacuum.

In metals, we have electrons that can move freely in response to the electric field and thus completely screen the external field. This means that the ratio of the electric field outside the material and inside the material is infinite. In other words, since the Coulomb-force between charges is screened in metals, the permittivity is infinite.

(c) A metal with free electrons is expected to be able to fully screen any added test charge. Thus, we expect the displaced charge δQ to equal exactly opposite of the added charge en_{a0}. We compute

$$\delta Q = e\delta n = e\int d^3r\,\delta n(\boldsymbol{r}) = \lim_{\boldsymbol{q}\to 0} e\Big[\frac{1}{\varepsilon_r(q)} - 1\Big]n_a(\boldsymbol{q}) = -en_{a0}, \tag{8}$$

which is thus physically reasonable.

Problem 2

Let us denote the perturbation term

$$H' = \sum_{\boldsymbol{kq}} M_{\boldsymbol{q}}(a^\dagger_{-\boldsymbol{q}} + a_{\boldsymbol{q}})c^\dagger_{\boldsymbol{k}+\boldsymbol{q}}c_{\boldsymbol{k}} \tag{9}$$

The eigenstate of the unperturbed Hamiltonian is denoted $|\Phi\rangle$ and describes a free electron gas plus a free magnon gas without any coupling between the two.

The first order correction in perturbation theory is then

$$E_1 = \langle\Phi|H'|\Phi\rangle. \tag{10}$$

This term has to be zero. The reason is that H' is linear in the magnon operators. Thus, the state $H'|\Phi\rangle$ will always differ from $|\Phi\rangle$ with either one extra or one missing phonon, and the overlap between the states is zero.

Let us then turn to the second order correction. The general expression is

$$E_2 = \sum_{m\neq\Phi}\frac{\langle m|H'|\Phi\rangle\langle m|H'|\Phi\rangle^*}{E_\Phi - E_m} \tag{11}$$

where $|m\rangle$ is an excited state of the unperturbed Hamiltonian and E_m its corresponding energy eigenvalue whereas E_Φ is the energy eigenvalue of the state $|\Phi\rangle$. Using that $H' = (H')^\dagger$, we can rewrite the above as

$$\begin{aligned} E_2 &= \sum_{m\neq\Phi} \frac{\langle m|H'|\Phi\rangle\langle\Phi|H'|m\rangle}{E_\Phi - E_m} \\ &= \langle\Phi| \sum_{m\neq\Phi} \frac{1}{E_\Phi - E_m} \sum_{\boldsymbol{kq}} M_{\boldsymbol{q}}(a^\dagger_{-\boldsymbol{q}} + a_{\boldsymbol{q}})c^\dagger_{\boldsymbol{k}+\boldsymbol{q}}c_{\boldsymbol{k}}|m\rangle \sum_{\boldsymbol{k}'\boldsymbol{q}'} \langle m|M_{\boldsymbol{q}'}(a^\dagger_{-\boldsymbol{q}'} + a_{\boldsymbol{q}'})c^\dagger_{\boldsymbol{k}'+\boldsymbol{q}'}c_{\boldsymbol{k}'}|\Phi\rangle \end{aligned} \tag{12}$$

We rewrite this expression by using the formula in the lecture notes in the section on Peierls instability:

$$\sum_{m\neq n} \frac{\langle n|H'|m\rangle\langle m|H'|n\rangle}{E_n^0 - E_m^0} = \langle n|H'(E_n^0 - H_0)^{-1}H'|n\rangle \tag{13}$$

upon defining the operator $(E_n^0 - H_0)^{-1}$ whose eigenstates are $|m\rangle$ with eigenvalues $1/(E_n^0 - E_m^0)$ for $n \neq m$ and eigenvalue zero if $n = m$. It then follows that in order for the matrix elements to be non-zero, we need the electron and magnon operators to cancel each others excitations. This happens when $\boldsymbol{q}' = -\boldsymbol{q}$ and when $\boldsymbol{k} + \boldsymbol{q} = \boldsymbol{k}'$, as can be verified by matching annihilation and creation operators for the electrons and magnons. This leaves us with

$$\begin{aligned} E_2 = \sum_{\boldsymbol{kq}} |M_{\boldsymbol{q}}|^2 \Big[&\frac{1}{\varepsilon_{\boldsymbol{k}} - \varepsilon_{\boldsymbol{k}-\boldsymbol{q}} + \hbar\omega_{-\boldsymbol{q}}} \langle\Phi|a^\dagger_{-\boldsymbol{q}}c^\dagger_{\boldsymbol{k}}c_{\boldsymbol{k}-\boldsymbol{q}}a_{-\boldsymbol{q}}c^\dagger_{\boldsymbol{k}-\boldsymbol{q}}c_{\boldsymbol{k}}|\Phi\rangle \\ &+ \frac{1}{\varepsilon_{\boldsymbol{k}} - \varepsilon_{\boldsymbol{k}-\boldsymbol{q}} - \hbar\omega_{\boldsymbol{q}}} \langle\Phi|a_{\boldsymbol{q}}c^\dagger_{\boldsymbol{k}}c_{\boldsymbol{k}-\boldsymbol{q}}a^\dagger_{\boldsymbol{q}}c^\dagger_{\boldsymbol{k}-\boldsymbol{q}}c_{\boldsymbol{k}}|\Phi\rangle \Big] \end{aligned} \tag{14}$$

where we relabeled $\boldsymbol{k} \to \boldsymbol{k} - \boldsymbol{q}$ in the summation. This relabeling can be done since we are performing a summation over all possible momenta $\boldsymbol{k}$ anyway. The energy terms in the denominator are obtained as follows. We know that $E_\Phi = \sum_{\boldsymbol{k}} \varepsilon_{\boldsymbol{k}} n_F(\boldsymbol{k}) + \sum_{\boldsymbol{q}} \hbar\omega_{\boldsymbol{q}} n_B(\boldsymbol{q})$. Now, the state $|m\rangle$ which contributes in the sum has to differ from Φ in the following ways: it has an extra electron with momentum $\boldsymbol{k} - \boldsymbol{q}$, a missing electron with momentum $\boldsymbol{k}$ and *either* a missing phonon with $-\boldsymbol{q}$ or an extra phonon with $\boldsymbol{q}$. Thus, we have

$$E_\Phi - E_m = -(\varepsilon_{\boldsymbol{k}-\boldsymbol{q}} - \varepsilon_{\boldsymbol{k}} - \hbar\omega_{-\boldsymbol{q}}) = \varepsilon_{\boldsymbol{k}} - \varepsilon_{\boldsymbol{k}-\boldsymbol{q}} + \hbar\omega_{-\boldsymbol{q}} \tag{15}$$

in one term and

$$E_\Phi - E_m = -(\varepsilon_{\boldsymbol{k}-\boldsymbol{q}} - \varepsilon_{\boldsymbol{k}} + \hbar\omega_{\boldsymbol{q}}) = \varepsilon_{\boldsymbol{k}} - \varepsilon_{\boldsymbol{k}-\boldsymbol{q}} - \hbar\omega_{\boldsymbol{q}} \tag{16}$$

in the other.

We see that what enters are combinations of creation and annihilation operators that form number operators of the type $b^\dagger b$ (after a commutation of operators for the magnons). The expectation value of such number operators in the state $|\Phi\rangle$ is the Fermi-Dirac distribution n_F for electrons and Bose-Einstein distribution n_B for magnons. Thus, we obtain the final result:

$$E_2 = \sum_{\boldsymbol{kq}} |M_{\boldsymbol{q}}|^2 n_F(\boldsymbol{k})[1 - n_F(\boldsymbol{k}-\boldsymbol{q})] \Big[\frac{n_B(-\boldsymbol{q})}{\varepsilon_{\boldsymbol{k}} - \varepsilon_{\boldsymbol{k}-\boldsymbol{q}} + \hbar\omega_{-\boldsymbol{q}}} + \frac{n_B(\boldsymbol{q}) + 1}{\varepsilon_{\boldsymbol{k}} - \varepsilon_{\boldsymbol{k}-\boldsymbol{q}} - \hbar\omega_{\boldsymbol{q}}} \Big]. \tag{17}$$

You might ask: but what if for instance the electron state $\boldsymbol{k} - \boldsymbol{q}$ is already present in $|\Phi\rangle$? Due to the Pauli principle, $|m\rangle$ cannot then differ from $|\Phi\rangle$ by having an additional electron in the same state. However, this is accounted for in the above expression due to the expectation values. Namely, we see that if $n_F(\boldsymbol{k} - \boldsymbol{q}) = 1$, the contribution from that momentum value vanishes in E_2 since the process is not possible.