PHZ 7427 Spring 2011 – Homework 4

Due by 5:00 p.m. on Wednesday, April 13. After that, the assignment may be submitted for 75% credit until the start of class on Monday, April 18.

Answer all parts of the question. Please write neatly and include your name on the front page of your answers. You must also clearly identify all your collaborators on this assignment. To gain maximum credit you should explain your reasoning and show all working.

Electron-phonon interactions. The interaction of electrons and longitudinal phonons within a solid can be described by the Hamiltonian

$$\begin{aligned} H &= H_0 + H_{\mathrm{e-ph}}, \\ H_0 &= \sum_{\mathbf{k}} \varepsilon_{\mathbf{k}} c_{\mathbf{k}}^\dagger c_{\mathbf{k}} + \sum_{\mathbf{q}} \hbar\omega_{\mathbf{q}} a_{\mathbf{q}}^\dagger a_{\mathbf{q}}, \\ H_{\mathrm{e-ph}} &= \frac{1}{\sqrt{V}} \sum_{\mathbf{k},\mathbf{q}} M_{\mathbf{q}} \alpha_{\mathbf{k}+\mathbf{q},\mathbf{q}} c_{\mathbf{k}+\mathbf{q}}^\dagger c_{\mathbf{k}} \left(a_{\mathbf{q}} + a_{-\mathbf{q}}^\dagger \right). \end{aligned}$$

Since the problem is independent of spin, we can drop the σ index For simplicity, we have neglected the possibility of Umklapp scattering, and set the electronic overlap factor $\alpha_{\mathbf{k}+\mathbf{q},\mathbf{k}} \equiv \langle \mathbf{k}+\mathbf{q} | e^{i\mathbf{q}\cdot\mathbf{r}} | \mathbf{k} \rangle$ to unity (the exact value for plane-wave single-particle states).

(a) Consider a many-body state $|\Psi\rangle$ characterized by a set of electronic occupation numbers $\{n_{\mathbf{k}}\}$ and a set of phonon occupation numbers $\{N_{\mathbf{q}}\}$. Through second order in the electron-phonon coupling, the total energy of this state is

$$E = E_0 + \langle \Psi | H_{\mathrm{e-ph}} | \Psi \rangle + \langle \Psi | H_{\mathrm{e-ph}} (E_0 - H_0)^{-1} H_{\mathrm{e-ph}} | \Psi \rangle,$$

where $E_0 = \langle \Psi | H_0 | \Psi \rangle$. Show that this energy equals

$$E = E_0 + \frac{1}{V} \sum_{\mathbf{k},\mathbf{q}} |M_{\mathbf{q}}|^2 n_{\mathbf{k}} (1 - n_{\mathbf{k}+\mathbf{q}}) \left(\frac{N_{\mathbf{q}}}{\varepsilon_{\mathbf{k}} - \varepsilon_{\mathbf{k}+\mathbf{q}} + \hbar\omega_{\mathbf{q}}} + \frac{N_{-\mathbf{q}} + 1}{\varepsilon_{\mathbf{k}} - \varepsilon_{\mathbf{k}+\mathbf{q}} - \hbar\omega_{-\mathbf{q}}} \right).$$

(b) Show that in the grand canonical ensemble specified by the Boltzmann distribution $e^{-\beta H_0}$, the expectation value of the total energy is

$$\langle E \rangle = \langle E_0 \rangle + \frac{1}{V} \sum_{\mathbf{k},\mathbf{q}} |M_{\mathbf{q}}|^2 \langle n_{\mathbf{k}} \rangle (1 - \langle n_{\mathbf{k}+\mathbf{q}} \rangle) \left(\frac{\langle N_{\mathbf{q}} \rangle}{\varepsilon_{\mathbf{k}} - \varepsilon_{\mathbf{k}+\mathbf{q}} + \hbar\omega_{\mathbf{q}}} + \frac{\langle N_{-\mathbf{q}} \rangle + 1}{\varepsilon_{\mathbf{k}} - \varepsilon_{\mathbf{k}+\mathbf{q}} - \hbar\omega_{-\mathbf{q}}} \right).$$

(c) Using the properties $\omega_{\mathbf{q}} = c_s |\mathbf{q}|$, $M_{\mathbf{q}} = M_{-\mathbf{q}}$, and $\langle N_{\mathbf{q}} \rangle = \langle N_{-\mathbf{q}} \rangle$ (for all $\mathbf{q}$), show that the expectation value from part (b) can be rewritten

$$\langle E \rangle = \langle E_0 \rangle + \frac{1}{V} \sum_{\mathbf{k},\mathbf{q}} |M_{\mathbf{q}}|^2 \langle n_{\mathbf{k}} \rangle \left[\frac{2(\varepsilon_{\mathbf{k}} - \varepsilon_{\mathbf{k}+\mathbf{q}}) \langle N_{\mathbf{q}} \rangle}{(\varepsilon_{\mathbf{k}} - \varepsilon_{\mathbf{k}+\mathbf{q}})^2 - (\hbar\omega_{\mathbf{q}})^2} + \frac{1 - \langle n_{\mathbf{k}+\mathbf{q}} \rangle}{\varepsilon_{\mathbf{k}} - \varepsilon_{\mathbf{k}+\mathbf{q}} - \hbar\omega_{\mathbf{q}}} \right].$$

(d) Based on the result of part (c), calculate the renormalized phonon energy defined by

$$\hbar\tilde{\omega}_{\mathbf{q}} = \frac{\partial \langle E \rangle}{\partial \langle N_{\mathbf{q}} \rangle}.$$

Show that if $\hbar\omega_{\mathbf{q}} \ll |\varepsilon_{\mathbf{k}} - \varepsilon_{\mathbf{k}+\mathbf{q}}|$,

$$\tilde{\omega}_{\mathbf{q}} \simeq \omega_{\mathbf{q}} + \frac{2|M_{\mathbf{q}}|^2}{\hbar V} \sum_{\mathbf{k}} \frac{\langle n_{\mathbf{k}} \rangle}{\varepsilon_{\mathbf{k}} - \varepsilon_{\mathbf{k}+\mathbf{q}}}.$$

(e) By considering situations where $\mathbf{k}$ lies close to a point $\mathbf{k}_0$ on the (spherical) Fermi surface and $\mathbf{k}+\mathbf{q}$ lies close to the opposite point $-\mathbf{k}_0$, show by summing over $\mathbf{k}$ that $\partial\tilde{\omega}_{\mathbf{q}}/\partial\mathbf{q}$ is logarithmically divergent at $|\mathbf{q}| = 2k_F$. This consequence of electron-phonon coupling is called the *Kohn anomaly*.

(f) Based on the result of part (c), calculate the renormalized electron energy defined by

$$\tilde{\varepsilon}_{\mathbf{k}} = \frac{\partial\langle E \rangle}{\partial\langle n_{\mathbf{k}} \rangle}.$$

You should be able to cast $\tilde{\varepsilon}_{\mathbf{k}} - \varepsilon_{\mathbf{k}}$ as a sum over $\mathbf{q}$ of three terms: term (1) containing $\langle n_{\mathbf{k}+\mathbf{q}} \rangle$ as the only single-particle expectation value; term (2) containing just $\langle N_{\mathbf{q}} \rangle$; and term (3) containing no single-particle expectation value.

(g) Show that term (1) defined in part (f) leads to a decrease in the effective Fermi velocity from v_{k_F} to $\tilde{v}_{k_F} = (1-\alpha)v_{k_F}$, which can be interpreted as an enhancement in the effective electron mass from m to $m_1^* = m/(1-\alpha)$. Provide an expression for α.