

Aspects of Electron-Phonon Systems

Exercise 6.1 Self-consistent treatment of the phonon dispersion

The coupling of the electrons to a longitudinal phonon field is described by

$$\hat{H} = \hat{H}_{el} + \hat{H}_{ph} + \hat{H}_{el-ph} \quad (1)$$

where \hat{H}_{el} is the Hamilton operator of the (interacting) electrons, \hat{H}_{ph} the free-phonon Hamilton operator

$$\hat{H}_{ph} = \frac{1}{2} \sum_{\vec{q}} \left(\hat{P}_{-\vec{q}} \hat{P}_{\vec{q}} + \Omega_{\vec{q}}^2 \hat{Q}_{-\vec{q}} \hat{Q}_{\vec{q}} \right) \quad (2)$$

and \hat{H}_{el-ph} describes the electron-phonon interaction

$$\hat{H}_{el-ph} = \sum_{\vec{q}} v_{\vec{q}} \hat{\rho}_{\vec{q}}^{\dagger} \hat{Q}_{\vec{q}}. \quad (3)$$

An example for the bare phonon frequency $\Omega_{\vec{q}}$ and the interaction parameter $v_{\vec{q}}$ is given in the next exercise. Furthermore, $\hat{\rho}_{\vec{q}}^{\dagger} = \sum_{\vec{k}\sigma} \hat{c}_{\vec{k}+\vec{q}\sigma}^{\dagger} \hat{c}_{\vec{k}\sigma}$ is the electron density fluctuation operator.

- a) Show that the equation of motion of the phonon oscillator amplitude $\hat{Q}_{\vec{q}}$ is

$$\ddot{\hat{Q}}_{\vec{q}}(t) + \Omega_{\vec{q}}^2 \hat{Q}_{\vec{q}}(t) = -v_{-\vec{q}} \hat{\rho}_{\vec{q}}(t). \quad (4)$$

- b) Assume the existence of a sound wave of some frequency $\omega_{\vec{q}}$ to relate $\langle \hat{\rho}_{\vec{q}} \rangle$ to $\langle \hat{Q}_{\vec{q}} \rangle$ (in linear response). Show that the self-consistency equation for the phonon dispersion reads

$$\omega_{\vec{q}}^2 = \Omega_{\vec{q}}^2 + |\vec{v}_{\vec{q}}|^2 \chi(\vec{q}, \omega_{\vec{q}}) \quad (5)$$

where $\chi(\vec{q}, \omega)$ is the density-density response function to an *external* charge density potential and thus related to the dielectric function by

$$\varepsilon(\vec{q}, \omega)^{-1} = 1 + \frac{4\pi e^2}{q^2} \chi(\vec{q}, \omega). \quad (6)$$

- c) In general, the phonon dispersion $\omega_{\vec{q}}$ will be a complex quantity. Let us introduce the real and imaginary parts of the phonon dispersion

$$\omega_{\vec{q}} = \omega_1 - i\omega_2 \quad (7)$$

and assume $\omega_2 \ll \omega_1$. Show that in a metal we have for $\omega_1 \ll qv_F$

$$\omega_1^2 = \Omega_{\vec{q}}^2 - \frac{q^2}{4\pi e^2} |\vec{v}_{\vec{q}}|^2 \left[1 - \frac{1}{\varepsilon(\vec{q}, 0)} \right] \quad (\text{shift}), \quad (8)$$

$$\frac{\omega_2}{\omega_1} = \frac{q^2}{8\pi e^2} \frac{|\vec{v}_{\vec{q}}|^2}{\omega_1^2} \left[-\text{Im} \frac{1}{\varepsilon(\vec{q}, \omega_1)} \right] \quad (\text{damping}). \quad (9)$$

Exercise 6.2 Phonon energy shift and damping in the Jellium model

To obtain an order-of-magnitude estimate for Eqs. (8) and (9) we consider the Jellium model where the periodic character of the ion potential is neglected (see chapter 3.1). For this model the bare phonon frequency reduces to the appropriate ionic plasma frequency

$$\Omega_{\vec{q}}^2 \equiv \Omega_p^2 = \frac{4\pi n_i (Ze)^2}{M} \quad (10)$$

where n_i is the density of ions with ion valency Z and mass M . The phonon-electron coupling is given by

$$v_{\vec{q}} = -i\vec{q} \frac{4\pi Ze^2}{q^2} \sqrt{\frac{n_i}{M}}. \quad (11)$$

a) Show that

$$\omega_1^2 = \frac{\Omega_p^2}{\varepsilon(\vec{q}, 0)}. \quad (12)$$

In particular,

$$\omega_1 = s_{ph}q \quad (13)$$

for $q \rightarrow 0$. What is the phonon sound velocity?

Hint: Use $\varepsilon(\vec{q}, 0) = 1 + \frac{\omega_p^2}{s^2 q^2}$ for $\vec{q} \rightarrow 0$ where the electron plasma frequency is $\omega_p^2 = 4\pi n_0 e^2 / m$ and the sound velocity s is given in weak coupling approximation by $v_F / \sqrt{3}$.

b) Show that the damping is given by

$$\frac{\omega_2}{\omega_1} = \frac{\varepsilon_2(\vec{q}, \omega_1)}{2\varepsilon(\vec{q}, 0)} \quad (14)$$

which reduces in the long wavelength limit to

$$\frac{\omega_2}{\omega_1} = \frac{\pi}{12} \sqrt{\frac{m}{M}} Z \frac{p_F}{ms} \quad (15)$$

Why is the damping small?

c) Derive Eqs. (10) and (11).