Problem set: Screening and Peierls instability

9.1. The dielectric function

Consider an electron system which is subject to a small external potential $\Phi^\text{ext}(r)$ generated by an external charge density $\rho^\text{ext}(r)$. This perturbation induces an electronic charge density $\rho^\text{ind}(r)$ and a corresponding potential $\Phi^\text{ind}(r)$. Recall from electrodynamics, that when using Fourier-transformed quantities like $\rho^\text{ind}(q) = \int d^3r e^{-iqr} \rho^\text{ind}(r)$, a potential is related to the generating charge density by the Poisson equation as $q^2 \Phi(q) = 4\pi \rho(q)$. For small external potentials the following approximate relation holds (linear response):

$$
\rho^\text{ind}(q) = \rho^\text{tot}(q) \Phi^\text{tot}(q),
$$

where $\Phi^\text{tot} = \Phi^\text{ext} + \Phi^\text{ind}$ is the total potential felt by the electrons. Eqs. (1) define the static dielectric function $\epsilon(q)$ and the static susceptibility $\chi(q)$.

(a) Derive a relationship between $\epsilon(q)$ and $\chi(q)$.

(b) Obtain an expression for the static susceptibility in terms of the electronic properties for a free electron gas. Start with the expression for the charge density

$$
\rho(r) = -2e \sum_k f_k |\tilde{\psi}_k(r)|^2,
$$

where $f_k = f(E_k) = 1/(1 + e^{(E_k - E_F)/(k_B T)})$ is the Fermi function. The electronic wave function in the presence of the perturbation $H_1 = -e\Phi^\text{tot}(r)$ is given in first-order perturbation theory by

$$
\tilde{\psi}_k(r) = \psi_k(r) + \sum_{k' \neq k} \psi_{k'}(r) \frac{\langle \psi_{k'} | H_1 | \psi_k \rangle}{E_k - E_{k'}}.
$$

Evaluate the matrix elements for a free electron gas, and show that the static susceptibility can be expressed as

$$
\chi(q, T) = 2e^2 \int \frac{d^3k}{(2\pi)^3} \frac{f_k - f_{k+q}}{E_k - E_{k+q}}
$$
(c) Show that for $|q| \to 0$ and $T \to 0$, the susceptibility approaches the limit

$$\chi \to -e^2 g(E_F)$$  \hspace{1cm} (5)

where $g(E_F)$ is the electronic density of states at the Fermi energy.

Hint: Calculate first the limit $|q| \to 0$ and then use the relation $\partial f/\partial E \approx -\delta(E - E_F)$ for $T \to 0$.

9.2. Linear response of the one-dimensional electron gas

Consider free electrons in one dimension with dispersion relation $E_k = \frac{k^2}{2m}$. Similarly to Eq. (4), the static susceptibility in one dimension is given by

$$\chi(q, T) = 2e^2 \int \frac{dk}{2\pi} \frac{f_k - f_{k+q}}{E_k - E_{k+q}}$$  \hspace{1cm} (6)

(a) Calculate $\chi(q, T)$ for $T = 0$, where the Fermi function is just a step function. Verify explicitly that for $q \to 0$, $\chi(q) \to -e^2 g(E_F)$.

(b) Plot the ratio $\chi(q, T)/\chi(0)$ for $T = 0$ as function of the reduced variable $x = q/(2k_F)$ with $k_F$ the Fermi wavevector ($E_F = \frac{k_F^2}{2m}$). What is the behavior at $x = 1$?

(c) Replace the quadratic dispersion relation $E_k = \frac{k^2}{2m}$ by a linearized one of the form

$$\tilde{E}_k - E_F = c(|k| - k_F)$$  \hspace{1cm} (7)

Determine $c$ by the requirement that both dispersion relations should have the same derivative at $k_F$.

With this linearized dispersion relation, calculate $\chi(q, T)$ for $q = 2k_F$ for temperatures $T \ll E_F/k_B$ and show that it diverges logarithmically for $T \to 0^+$.

Hint: Use the relations $\tilde{E}_{k+2k_F} - E_F = -(\tilde{E}_k - E_F)$ and the asymptotic behavior $\int_0^y \ln\frac{\ln x}{x} \approx \ln y + C$ for $y \gg 1$, with $C \approx \ln(2.68)$.

(d) Calculate and plot $\chi(q, T)$ for arbitrary $q$ for the set of temperatures given by $E_F/(k_B T) = 4, 16, 64, 256$ by numerically integrating Eq. (6).

9.3. Coupled electronic bands (optional)

Consider the following model Hamiltonian of two electronic coupled bands in one dimension

$$H = \sum_k \left\{ \epsilon_k (c^\dagger_{1k} c_{1k} - c^\dagger_{2k} c_{2k}) + \Delta (c^\dagger_{1k} c_{2k} + c^\dagger_{2k} c_{1k}) \right\}$$  \hspace{1cm} (8)
where the (positive real) quantity $\Delta$ describes a $k$-independent coupling energy.

Consider new fermionic operators defined by

$$
\gamma_{1k} = u_k c_{1k} - v_k c_{2k}; \quad \gamma_{2k} = v_k c_{1k} + u_k c_{2k}
$$

with real numbers $u_k$ and $v_k$.

(a) Derive a relation between $u_k$ and $v_k$, for which the new operators obey the standard fermionic anticommutation relations $[\gamma_{ik}, \gamma_{jl}]^+ = \delta_{ij} \delta_{kl}$ and $[\gamma_{ik}, \gamma_{jl}]^+ = [\gamma_{ik}^\dagger, \gamma_{jl}^\dagger]^+ = 0$.

(b) Diagonalize the Hamiltonian by expressing $H$ in terms of the new fermionic operators. Under which condition do the off-diagonal couplings vanish? Derive an expression for the effective band energies of the new operators.

(c) For a linear dispersion $\epsilon_k = \hbar \nu_F k$, show that the energy spectrum shows a gap of size $2\Delta$.

Note: The model Hamiltonian appears in the mean-field description of the low-temperature Peierls-distorted linear chain.