Condensed Matter Theory problem set 9

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Problem 23: Plasma oscillations

The Coulomb interaction potential between two electrons has the form $v_{\boldsymbol q} = 4\pi e^2/q^2$. Two electrons in a metal additionally feel the screening effect of the other surrounding electrons, and the density response function is given by $\chi^R_{nn}(\boldsymbol q,\omega) = \Pi^R(\boldsymbol q,\omega)/\epsilon(\boldsymbol q,\omega)$ in terms of the dielectric function $\epsilon(\boldsymbol q,\omega) = 1 - v_{\boldsymbol q}\Pi^R(\boldsymbol q,\omega)$. Finding the exact polarization function $\Pi^R(\boldsymbol q,\omega)$ is a difficult problem, so we shall use the *random-phase approximation* (previous exercise). The *dynamical structure factor* at zero temperature,

$$S(\boldsymbol q,\omega) = -\frac{1}{n}\,\mathrm{Im}\left[\chi^R_{nn}(\boldsymbol q,\omega)\right] = -\frac{1}{nv_{\boldsymbol q}}\,\mathrm{Im}\left[\frac{1}{\epsilon(\boldsymbol q,\omega)}\right], \tag{1}$$

describes the excitations of the electron gas and is depicted in Fig. 1. There is a sharp excitation at small momentum and high frequency, the so-called plasma excitation. Compute its frequency ω_{pl} by finding the zero of $\epsilon(\boldsymbol q,\omega)$ for $q \to 0$ and $\omega > 0$, and compare with Fig. 1 at the given coupling.

[*Hint*: One may compute $\Pi^R(\boldsymbol q,\omega)$ to order $\mathcal{O}(q^2)$: shift $\boldsymbol k \mapsto \boldsymbol k - \boldsymbol q/2$ and expand denominator for $(\boldsymbol k\cdot\boldsymbol q/m)^2 \ll \omega^2$, then shift $\boldsymbol k$ in each term separately such that the Fermi functions appear in the form $f(\xi_{\boldsymbol k})$. Write the result as $1/\epsilon(\boldsymbol q,\omega) = \omega^2/\big((\omega+i0)^2 - \omega_{\mathrm{pl}}^2\big)$ with a pole at the plasma frequency ω_{pl}.]

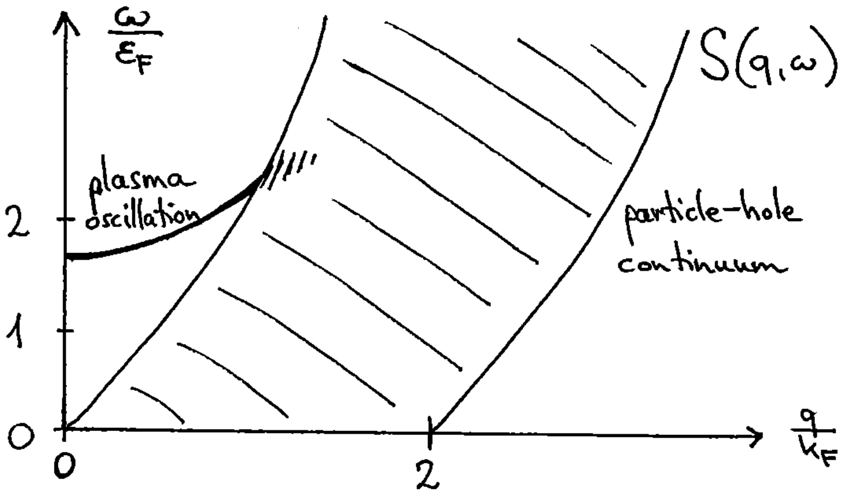

Figure 1: Dynamical structure factor $S(\boldsymbol q,\omega)$ at dimensionless coupling $4\pi e^2 g(0)/k_F^2 = 2$.

Problem 24: Fröhlich transformation

A system of spinless electrons coupled to phonons is described by the Hamiltonian

$$\mathcal{H} = \underbrace{\sum_k \epsilon_k c_k^\dagger c_k + \sum_q \omega_q b_q^\dagger b_q}_{\mathcal{H}_0} + \underbrace{\sum_{kq} M_q (b_{-q}^\dagger + b_q) c_{k+q}^\dagger c_k}_{\mathcal{H}_1} \tag{2}$$

with electron-phonon coupling $M_q = M_{-q}^*$ und phonon energy $\omega_q = \omega_{-q}$. $\mathcal{H}$ can be diagonalized by a canonical transformation $\tilde{\mathcal{H}} = e^{-S}\mathcal{H}e^{S}$ which decouples electronic quasiparticles (polarons) from phononic degrees of freedom.

(a) Which form must S have such that the canonical transformation eliminates the electron-phonon coupling $\mathcal{H}_1$ to leading order, *i.e.*,

$$[\mathcal{H}_0, S] + \mathcal{H}_1 = 0\ ? \tag{3}$$

Start with the (anti-hermitean) *ansatz*

$$S = -\sum_{kq} \left[\alpha_{kq}\, c_{k+q}^\dagger c_k b_q - \text{h.c.} \right] \tag{4}$$

and determine the coefficients α_{kq}.

(b) Compute the electron-electron interaction induced by the phonons,

$$\hat{V} = \frac{1}{2}[\mathcal{H}_1, S] \tag{5}$$

(the commutator yields further terms which do not interest us here).

[*Note*: As an intermediate step one can derive the identities

$$[c_{k'}^\dagger c_{k'}, c_{k+q}^\dagger c_k] = (\delta_{k',k+q} - \delta_{k',k})\, c_{k+q}^\dagger c_k$$
$$[b_{q'}^\dagger b_{q'}, b_q] = -\delta_{q',q}\, b_q$$

from the canonical commutation relations.]

Problem 25: Hartree-Fock equations

Consider the N-electron system described by the Hamiltonian

$$\mathcal{H} = \sum_i \left[\frac{\mathbf{p}_i^2}{2m} + U_{\text{ion}}(\mathbf{r}_i) \right] + \frac{1}{2} \sum_{i \neq j} \frac{e^2}{|\mathbf{r}_i - \mathbf{r}_j|}. \tag{6}$$

(a) Let $\psi_1, \ldots, \psi_N$ be mutually orthogonal single-particle states with spin $\sigma_i \in \{\uparrow, \downarrow\}$. Show that the expectation value of $\mathcal{H}$ with the Slater determinant state

$$\langle \mathbf{r}_1, \ldots, \mathbf{r}_N | \Psi \rangle = \Psi(\mathbf{r}_1, \ldots, \mathbf{r}_N) = \sum_P (-1)^P \psi_{P(1)}(\mathbf{r}_1, \sigma_1) \ldots \psi_{P(N)}(\mathbf{r}_N, \sigma_N) \tag{7}$$

is given by

$$\begin{aligned} \langle \Psi | \mathcal{H} | \Psi \rangle = &\sum_i \int d\mathbf{r}\, \psi_i^*(\mathbf{r}) \left(-\frac{\hbar^2 \nabla^2}{2m} + U_{\text{ion}}(\mathbf{r}) \right) \psi_i(\mathbf{r}) \\ &+ \frac{1}{2} \sum_{i \neq j} \int d\mathbf{r} \int d\mathbf{r}' \frac{e^2}{|\mathbf{r} - \mathbf{r}'|} |\psi_i(\mathbf{r})|^2 |\psi_j(\mathbf{r}')|^2 \\ &- \frac{1}{2} \sum_{i \neq j} \int d\mathbf{r} \int d\mathbf{r}' \frac{e^2}{|\mathbf{r} - \mathbf{r}'|} \delta_{\sigma_i \sigma_j} \psi_i^*(\mathbf{r}) \psi_i(\mathbf{r}') \psi_j^*(\mathbf{r}') \psi_j(\mathbf{r}) \,. \end{aligned} \tag{8}$$

(b) Vary $\langle \Psi | \mathcal{H} | \Psi \rangle - \sum_i E_i \left(\int d\mathbf{r} |\psi_i|^2 - 1 \right)$ with respect to ψ_i^*, where E_i are Lagrange multipliers to ensure normalization, and derive the Hartree-Fock equation

$$\begin{aligned} E_i \psi_i(\mathbf{r}) = &\left[\left(-\frac{\hbar^2 \nabla^2}{2m} + U_{\text{ion}}(\mathbf{r}) \right) \psi_i(\mathbf{r}) + \sum_j \int d\mathbf{r}' \frac{e^2}{|\mathbf{r} - \mathbf{r}'|} |\psi_j(\mathbf{r}')|^2 \right] \psi_i(\mathbf{r}) \\ &- \sum_j \int d\mathbf{r}' \frac{e^2}{|\mathbf{r} - \mathbf{r}'|} \psi_i(\mathbf{r}') \psi_j^*(\mathbf{r}') \psi_j(\mathbf{r}) \delta_{\sigma_i \sigma_j} \,. \end{aligned} \tag{9}$$