Theoretische Festkörperphysik
Sommersemester 2012

Übungsblatt 6

(Ausgabe: 25.05.12, Besprechung: Freitag, 01.06.12)

Exercise 1 – Effective Mass in the Hartree-Fock approximation

In the last exercise (sheet 5, problem 2), you calculated the exchange energy in the Slater approximation, \( \Delta E_{\text{ex}}^k \). Since in the same approximation, the Hartree electron density is exactly compensated by the (homogeneous) ionic background charge, the effective single particle energy in the Hartree-Fock approximation is given by

\[
\epsilon_k = \frac{\hbar^2 k^2}{2m} + \Delta E_{\text{ex}}^k = \frac{\hbar^2 k^2}{2m} - \frac{2e^2}{\pi} k_F F \left( \frac{k}{k_F} \right),
\]

with \( F(x) = \frac{1}{2} + \frac{1-x^2}{2x} \ln \left| \frac{1+x}{1-x} \right| \). Show that at \( k = 0 \) there is a band minimum and that the effective mass \( m^* \) is given by

\[
\frac{m}{m^*} = \frac{1}{1 + 0.22(r_S/a_0)},
\]

so that \( \epsilon_k \approx \frac{\hbar^2 k^2}{2m^*} \).

Exercise 2 – General Kubo Formula

In the lecture, we considered an external perturbation that linearly couples to the density in the Hamiltonian, and calculated the linear response to the density of the system. Now we want to generalize this to an arbitrary external force \( F(r,t) \) that linearly couples to the observable \( \hat{B}(r) \) (density operator, current operator, etc.), i.e.

\[
\hat{H}_{\text{ext}} = \int d^3r \, \hat{B}(r) F(r,t).
\]

The correction to the expectation value of observable \( \hat{A}(r) \) to linear order in the external force is then given by

\[
\delta A(r,t) = \int d^3r' dt' \, \chi_{AB}(r - r', t - t') F(r', t').
\]
Analogous to the lecture, show that the corresponding linear response function is given by

\[ \chi_{AB}(\mathbf{r} - \mathbf{r'}, t - t') = -i \frac{\theta(t - t')}{\hbar} \langle [\hat{A}_f(\mathbf{r}, t), \hat{B}_I(\mathbf{r}', t')] \rangle, \]

where \( \hat{A}_f, \hat{B}_I \) denote operators in the interaction picture.

**Exercise 3 – Linear Response Theory and Dissipation**

We consider a system described by the Hamiltonian \( \hat{H}_0 \) and switch on a time-dependent perturbation \( \hat{B} F(t) \) at \( t = 0 \), so that the total Hamiltonian reads \( \hat{H} = \hat{H}_0 + \theta(t) \hat{B} F(t) \). The operator \( \hat{B} \) is hermitian and its expectation value is assumed to vanish in thermal equilibrium, i.e. \( \langle \hat{B} \rangle_0 = \text{Tr}[\rho_0 \hat{B}] = 0 \) with the equilibrium density matrix \( \rho_0 = Z^{-1} e^{-\beta \hat{H}_0} \).

(a) Show that the average energy absorbed by the system per unit time is given by the expression

\[ \frac{\partial}{\partial t} \langle \hat{H} \rangle = \dot{F}(t) \int_0^\infty dt' \chi(t - t') F(t'), \]

with the linear response function \( \chi(t - t') = -i \frac{\theta(t - t')}{\hbar} \langle [\hat{B}_I(t), \hat{B}_I(t')] \rangle_0 \).

*Remark:* \( \langle [\hat{B}_I(t), \hat{B}_I(t')] \rangle_0 = \langle [\hat{B}_I(t - t'), \hat{B}_I(0)] \rangle_0 \).

(b) Let us introduce the Fourier transformations \( \chi(\omega) = \int dt (t-t') \chi(t-t') e^{i\omega(t-t')}, f(\omega) = \int dt f(t) e^{i\omega t} \) and their corresponding back transformations and note that \( \chi^*(\omega) = \chi(-\omega), f^*(\omega) = f(-\omega) \). Calculate the total dissipated energy and thus verify that

\[ \Delta E = \int_0^\infty dt \frac{\partial}{\partial t} \langle \hat{H} \rangle = -\int_0^\infty \frac{d\omega}{2\pi} \omega |F(\omega)|^2 \text{Im} \chi(\omega). \]

*Remark:* \( \int_{-\infty}^{+\infty} dt e^{i\omega t} = 2\pi \delta(\omega) \)

(c) The fluctuation-dissipation theorem

\[ -2\hbar \text{Im} \chi(\omega) = (1 - e^{-\beta \hbar \omega}) S(\omega) \]

relates the linear response function \( \chi(\omega) \) to the corresponding correlation function

\[ S(\omega) = \int_{-\infty}^{\infty} dt e^{i\omega t} \langle \hat{B}_I(t) \hat{B}_I(0) \rangle_0. \]

Proof this relation by explicitly evaluating it using the eigenstates of the Hamiltonian \( \hat{H}_0 \) as the basis: \( \hat{H}_0 |n\rangle = E_n |n\rangle \) and with the matrix elements of \( \hat{B} \) given as \( \langle m | \hat{B} | n \rangle = B_{mn} \).