Solid State Theory II: Ex 2 **(SS 2015)** **Prof. Krüger**

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Problem 5: Hartree-Fock approximation **(3 points)**

The Hamilton operator of interacting electrons in a potential $V(\vec{r})$ has the form

$$\hat{H} = \sum_{j=1}^{N} \left(\frac{\hat{p}_j^2}{2m} + V(\vec{r}_j) \right) + \frac{1}{2} \sum_{j \neq j'} \frac{e^2}{4\pi\varepsilon_0} \frac{1}{|\vec{r}_j - \vec{r}_j|} .$$

In the occupation number representation (basis: $\psi_l(\vec{r}, \vec{s}) = \psi_l(\vec{x})$), the Hamilton operator is given by

$$\hat{H} = \sum_{i,l} A_{il} \hat{c}_i^+ \hat{c}_l + \sum_{i,j,l,m} \frac{1}{2} B_{ijlm} \hat{c}_i^+ \hat{c}_j^+ \hat{c}_l \hat{c}_m .$$

a) Which relation exists between B_{ijlm} and B_{jiml}?

b) In the Hartree-Fock approach, $\hat{H}$ is approximated by the effective Hamilton operator

$$\hat{H}_{\text{eff}} = \hat{H}_{\text{HF}} + W \qquad \text{with} \qquad \hat{H}_{\text{HF}} = \sum_{i,l} D_{il} \hat{c}_i^+ \hat{c}_l .$$

The term W does not contain any creation or annihilation operators. The approximation is realized by the following substitution of the product of four operators:

$$\begin{aligned} \hat{c}_i^+ \hat{c}_j^+ \hat{c}_l \hat{c}_m \approx\ & \hat{c}_i^+ c_m \langle \hat{c}_j^+ c_l \rangle_0 + \hat{c}_j^+ \hat{c}_l \langle \hat{c}_i^+ \hat{c}_m \rangle_0 \\ -\ & \langle \hat{c}_i^+ \hat{c}_m \rangle_0 \langle \hat{c}_j^+ \hat{c}_l \rangle_0 \\ -\ & \hat{c}_i^+ \hat{c}_l \langle \hat{c}_j^+ c_m \rangle_0 - \hat{c}_j^+ \hat{c}_m \langle \hat{c}_i^+ \hat{c}_l \rangle_0 \\ +\ & \langle \hat{c}_i^+ \hat{c}_l \rangle_0 \langle \hat{c}_j^+ \hat{c}_m \rangle_0 . \end{aligned}$$

The expectation values $\langle\ \rangle_0$ are calculated with the eigenfunctions of the effective Hamilton operator. Then:

$$\langle \hat{c}_i^+ c_m \rangle_0 = n_m \cdot \delta_{i,m} .$$

i) Calculate D_{il} and W. Represent your result in terms of A_{il}, B_{ijjl}, B_{ijlj} and n_j.
Hint: Use an appropriate substitution for the variables in the summation.

ii) The coefficients D_{il} of the operator $\hat{H}_{\text{HF}}$ can be written as

$$D_{il} = \int \psi_i^*(\vec{x})\, \hat{O}(\vec{r})\, \psi_l(\vec{x})\, d^3x .$$

The functions $\psi_l(\vec{x})$ are chosen to be eigenfunctions of $\hat{O}$

$$\hat{O}\, \psi_l(\vec{x}) = \lambda_l\, \psi_l(\vec{x}) .$$

This leads to

$$D_{il} = \lambda_l\, \delta_{i,l} .$$

Compare this eigenvalue problem for $\hat{O}$ with the Hartree-Fock equation in the position-spin representation (see last semester).

Problem 6: Dielectric function of the electron gas (4 points)

The dielectric function of the three-dimensional electron gas has the form (Random phase approximation and $T = 0$)

$$\varepsilon(\vec{q}, \omega) = 1 - \frac{e^2}{\varepsilon_0 \Omega} \frac{2}{q^2} \sum_{\substack{\vec{k} \\ |\vec{k}| \le k_F}} \left(\frac{1}{E(\vec{k}) - E(\vec{k} + \vec{q}) + \hbar \omega} + \frac{1}{E(\vec{k}) - E(\vec{k} + \vec{q}) - \hbar \omega} \right).$$

We consider the static limit $\omega = 0$.

a) Calculate $\varepsilon(\vec{q}, 0)$. To this end, substitute the sum over $\vec{k}$ by an integral.

b) Consider the case $q \ll 2 k_F$ and take terms up to the order $\frac{1}{q^2}$ into account. Calculate the screened potential in this case

$$\tilde{V}_{\text{eff}}(\vec{q}) = \frac{\tilde{V}_{\text{el}}(\vec{q})}{\varepsilon(\vec{q})} \qquad \text{with} \qquad \tilde{V}_{\text{el}}(\vec{q}) = -\frac{e^2}{\varepsilon_0 \Omega} \frac{1}{q^2}.$$

Use $\tilde{V}_{\text{eff}}(\vec{q})$ to determine the screened potential $V_{\text{eff}}(\vec{r})$ in real space.

c) Discuss the behaviour of $\varepsilon(\vec{q}, 0)$ in the limit $q \to \infty$?

d) Plot $\varepsilon(\vec{q}, 0)$.

Hint:

$$\int x \ln \left| \frac{a x + b}{a x - b} \right| = \frac{b}{a} x + \frac{1}{2} \left(x^2 - \frac{b^2}{a^2} \right) \ln \left| \frac{a x + b}{a x - b} \right|.$$

Problem 7: Lorentz oscillator (3 points)

In a classical model for the screening in a solid, we assume that an external field

$$\vec{E}(t) = \vec{E}_0 \cdot e^{-i \omega t}$$

shifts the electrons in a solid by $\vec{r}(t)$. A "restoring force" $-m \omega_0^2 \vec{r}(t)$ and the friction force $-2 m \gamma \dot{\vec{r}}(t)$ are acting in addition to the field $\vec{E}$ on the electron. The displacement induces a dipol moment, which leads to a polarisation $\vec{P} = -e \cdot n \vec{r}(t)$ with the electron density n.

a) Solve Newton's equation of motion for this system.

b) Use

$$\varepsilon_0 \varepsilon(\omega) \vec{E}(\omega) = \varepsilon_0 \vec{E}(\omega) + \vec{P}(\omega)$$

to calculate the dielectric function.

Use the plasma frequency

$$\omega_p^2 = \frac{e^2}{\varepsilon_0} \frac{n}{m}$$

to represent your result.

c) Decompose $\varepsilon(\omega)$ into the real part $\varepsilon_1(\omega)$ and the imaginary part $\varepsilon_2(\omega)$. Plot both functions.