Solid State Theory II: Ex 5 **(SS 2015)** **Prof. Krüger**
Date of issue: 16.06.2015 Deadline: 23.06.2015

Problem 14: Excited states **(3 points)**

Consider two electrons in a model system with the Hamilton operator

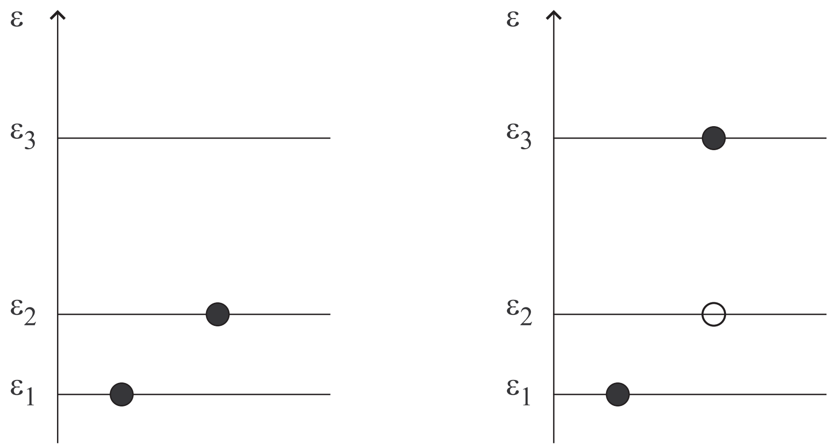
$$\hat{H} = \sum_{i,j} A_{ij}\, \hat{c}_i^\dagger\, \hat{c}_j + \frac{1}{2} \sum_{i,j,k,l} B_{ijkl}\, \hat{c}_i^\dagger\, \hat{c}_j^\dagger\, \hat{c}_k\, \hat{c}_l \ .$$

In the Hartree-Fock approximation, the total energy of the system is given by

$$E^{\mathrm{HF}} = \sum_i A_{ii} \cdot n_i + \frac{1}{2} \sum_{i,j} n_i\, n_j\, (B_{ijji} - B_{ijij})$$

with the occupation numbers n_i. The one-particle energies ε_i have the form

$$\varepsilon_i = A_{ii} + \sum_j n_j\, (B_{ijji} - B_{ijij}) \ .$$



ground state $n_1 = 1$, $n_2 = 1$ excited state $n_1 = 1$, $n_3 = 1$

a) Calculate the total energy E_0^{HF} and the one-particle energies ε_1, ε_2 and ε_3 for the ground state with

$$n_j = \begin{cases} 1 & \text{for} \quad j = 1 \quad \text{and} \quad j = 2 \\ 0 & \text{else} \end{cases} \ .$$

b) Consider an excited state ($2 \rightarrow 3$) with the occupation

$$n_j = \begin{cases} 1 & \text{for} \quad j = 1 \quad \text{and} \quad j = 3 \\ 0 & \text{else} \end{cases} \ .$$

i) Calculate the total energy $E_{\mathrm{ex}}^{\mathrm{HF}}$.

ii) Use the one-particle energies from a) together with E_0^{HF} to express the total energy in the form

$$E_{\mathrm{ex}}^{\mathrm{HF}} = E_0^{\mathrm{HF}} + \varepsilon_3 - \varepsilon_2 + I \ .$$

Determine the interaction I. Discuss your result.

Problem 15: Wannier exciton (3 points)

Consider a Wannier exciton in the state n, l with wave vector $\vec{K} = 0$, i. e. $\vec{k}_l = \vec{k}_v = \vec{k}$.

$$|\phi_{\mathrm{ex}}^{(n,\,l)}\rangle = \sum_{\vec{k}} g_{\vec{k},\,\vec{k}}^{(n,\,l)}\, \hat{c}_{\vec{k}}^{\dagger}\, \hat{d}_{\vec{k}}^{\dagger}\, |\phi_0\rangle \ .$$

$g_{\vec{k},\,\vec{k}}^{(n,\,l)}$ is the Fourier transform of a hydrogen-like wave function $G_{n,\,l}\,(\vec{r}_e,\,\vec{r}_h)$.

Optical transitions due to a vector potential $\vec{A}$ are described by the operator

$$\vec{A} \cdot \hat{\vec{p}} = \sum_{\vec{k}_l,\,\vec{k}_v} \hat{c}_{\vec{k}_l}^{\dagger}\, d_{\vec{k}_v}^{\dagger}\, D_{\vec{k}_l,\,\vec{k}_v}$$

with the matrix elements

$$D_{\vec{k}_l,\,\vec{k}_v} = \langle \psi_{l\,\vec{k}_l} | \frac{\hbar}{i}\, \vec{A} \cdot \vec{\nabla} | \psi_{v\,\vec{k}_v} \rangle$$

a) Calculate the probability

$$W = \left| \langle \phi_{\mathrm{ex}}^{(n,\,l)} | \vec{A} \cdot \vec{p} | \phi_0 \rangle \right|^2$$

for the transition from the ground state into an exciton state. First, consider dipole-allowed transitions with $D_{\vec{k},\,\vec{k}} \approx D^{(1)}$. $D^{(1)}$ is independent of $\vec{k}$. Relate W to the radial part $R_{n,\,l}$ of the wave function $G_{n,\,l}$ in real space. Which values of n and l lead to $W \neq 0$?

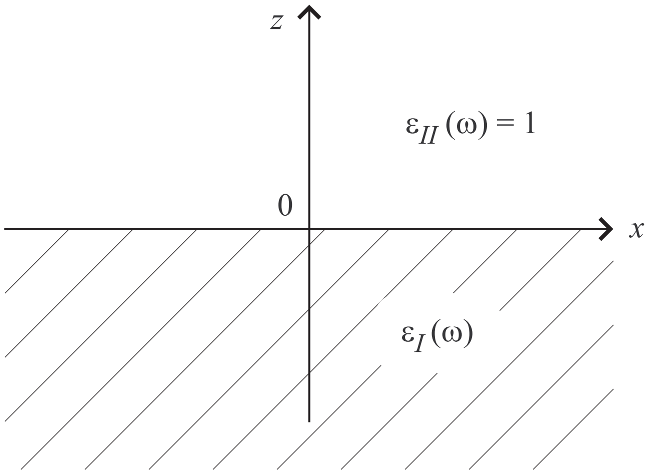
b) Consider now dipole-forbidden transitions with $D_{\vec{k},\,\vec{k}} \approx \vec{A}_0 \cdot \vec{k}\, D^{(2)}$. $\vec{A}_0$ gives the direction of $\vec{A}$ and the constant $D^{(2)}$ is independent of $\vec{k}$. Show that W is related to

$$\left| \frac{\partial\, R_{n,\,l}}{\partial\, r} \Big|_{\vec{r}=0} \right|^2 \ .$$

Which values of n and l give rise to these transitions?

Problem 16: Surface polariton (4 points)

In this problem, electromagnetic waves at the interface of a medium I with a dielectric function $\varepsilon_I(\omega)$ and the vacuum with $\varepsilon_{II}(\omega) = \varepsilon_{\text{vac}} = 1$ are considered. Medium I is located in the half space $z < 0$ and vacuum is in the region $z > 0$.



Consider a wave which is localized at the surface and propagates in x direction.

$$\vec{E}(\vec{r}, t) = \begin{cases} \vec{E}_I \quad e^{i k x} e^{\alpha_I z} e^{-i \omega t} & \text{for} \quad z \leq 0 \\ \vec{E}_{II} \quad e^{i k x} e^{-\alpha_{II} z} e^{-i \omega t} & \text{for} \quad z \geq 0 \, . \end{cases}$$

and

$$\vec{E}_I = E_1 \left(i k, \, 0, \, \frac{k^2}{\alpha_I} \right) \qquad \text{and} \qquad \vec{E}_{II} = E_2 \left(i k, \, 0, \, -\frac{k^2}{\alpha_{II}} \right) .$$

The constants α_I and α_{II} depend on k and ω but not on $\vec{r}$.

a) Calculate rot rot $\vec{E}(\vec{r}, t)$.

b) Use the wave equation rot rot $\vec{E}(\vec{r}, t) + \mu_0 \ddot{\vec{D}}(\vec{r}, t) = 0$ and the fact that the tangential (normal) component of $\vec{E}$ ($\vec{D}$) are continuous functions to derive the dependence of $\varepsilon_I(\omega) = \varepsilon(\omega)$ on k and ω.

c) The dielectric function of a simple metal is given by

$$\varepsilon(\omega) = 1 - \frac{\omega_p^2}{\omega^2}$$

with the plasma frequency ω_p. Use your result from a) to calculate the possible frequencies $\omega(k)$ of the electric field $\vec{E}(\vec{r}, t)$. Plot $\omega(k)$!

d) Is it possible to excite surface plasmon polaritons (in air) with light $\omega = c k$?