Problem 11: $\boldsymbol{F}$-sum rule **(4 points)**

In problem 8, perturbation theory (PT) has been employed to calculate the wave function $u_{n\,\vec{k}+\vec{q}}$. Here, PT should be used to determine the energy $E_{n\,\vec{k}\pm\vec{q}}$ from $E_{n'\,\vec{k}}$ (for all n').

a) Use *second* order perturbation theory to show that

$$E_{n\,\vec{k}+\vec{q}} - 2\,E_{n\,\vec{k}} + E_{n\,\vec{k}-\vec{q}} = \lambda \left(1 - \sum_{n'\neq n} F_{n,n'}(\vec{k})\right)$$

with the oscillator strength

$$F_{n,n'}(\vec{k}) = \frac{2}{m}\,\frac{|\vec{e}_q \cdot \langle u_{n\,\vec{k}}|\hat{\vec{p}}|u_{n'\,\vec{k}}\rangle|^2}{E_{n'\,\vec{k}} - E_{n\,\vec{k}}} .$$

Determine λ.

Hint: Use $\hat{U}$ from problem 8 with $\vec{q}$ and $-\vec{q}$ as perturbation to calculate $E_{n\,\vec{k}+\vec{q}}$ and $E_{n\,\vec{k}-\vec{q}}$, respectively.

b) The intraband part of the dielectric function is given by

$$\varepsilon(\vec{q},\omega) = 1 - \sum_{n\,\vec{k}} f(E_{n\,\vec{k}})\,\frac{E_{n\,\vec{k}+\vec{q}} - 2\,E_{n\,\vec{k}} + E_{n,\vec{k}-\vec{q}}}{(E_{n\,\vec{k}} - E_{n\,\vec{k}+\vec{q}} + \hbar\,(\omega + i\,\eta))\,(E_{n\,\vec{k}-\vec{q}} - E_{n\,\vec{k}} + \hbar\,(\omega + i\,\eta))} \cdot \frac{e^2 \cdot 2}{\varepsilon_0\,\Omega\,q^2}.$$

Use your result from a) together with the result from the lecture for $\varepsilon(\vec{q},\omega)$ to prove the F-sum rule in the limit $\vec{q} \to 0$

$$\sum_{n'\neq n} F_{n,n'}(\vec{k}) = 1 - m\,\vec{e}_{\vec{q}} \cdot \overline{\overline{M}}^{-1}(n\,\vec{k}) \cdot \vec{e}_{\vec{q}} .$$

Here, m is the electron mass and $\overline{\overline{M}}^{-1}(n\,\vec{k})$ is the tensor of the inverse effective mass (see lecture).

Problem 12: Hole operator **(3 points)**

In the discussion of excited states in a semiconductor, it is useful to introduce special creation and annihilation operators $\hat{d}_v^\dagger$, $\hat{d}_v$ for valence band electrons. These operators describe so-called *holes*. Starting from electron creation and annihilation operators $\hat{c}_v^\dagger$, $\hat{c}_v$, they are defined by

$$\hat{d}_v^\dagger = \hat{c}_v \quad \text{and} \quad \hat{d}_v = \hat{c}_v^\dagger \quad \text{for} \quad v = n,\vec{k} \quad \text{with} \quad n \in \text{valence band} .$$

a) Calculate the following anticommutator relations

i) $[\hat{d}_v,\, \hat{d}_{v'}]_+$,

ii) $[\hat{d}_v,\, \hat{d}_{v'}^\dagger]_+$,

iii) $[\hat{c}_l,\, \hat{d}_v]_+$,

iv) $[\hat{c}_l,\, \hat{d}_v^\dagger]_+$.

b) Consider a system in the ground state which is given in the Hartree-Fock approximation by

$$|\phi_0\rangle = \prod_j \hat{c}_j^\dagger\, |0\rangle \qquad \text{for all} \qquad j \in \text{valence bands} .$$

Calculate the expectation value for the number operator of a hole $\hat{N}^{\text{hole}} = \sum_v \hat{d}_v^\dagger\, \hat{d}_v$ for a state

$$|\phi_1\rangle = \hat{d}_{v'}^\dagger\, \hat{c}_l^\dagger\, \hat{d}_{v''}^\dagger\, |\phi_0\rangle .$$

c) Consider excited states of the form $|\phi_1\rangle = \hat{c}_l^\dagger\, \hat{d}_v^\dagger\, |\phi_0\rangle$. Here, one electron from conduction band l and one hole from valence band v have been created. Determine the following matrix elements

i) $\langle\phi_0|\hat{d}_{v'}\, \hat{c}_{l'} \quad \hat{c}_{l_1}^\dagger\, \hat{c}_{l_2} \quad \hat{c}_l^\dagger\, \hat{d}_v^\dagger|\phi_0\rangle$,

ii) $\langle\phi_0|\hat{d}_{v'}\, \hat{c}_{l'} \quad \hat{d}_{v_1}^\dagger\, \hat{d}_{v_2} \quad \hat{c}_l^\dagger\, \hat{d}_v^\dagger|\phi_0\rangle$,

iii) $\langle\phi_0|\hat{d}_{v'}\, \hat{c}_{l'} \quad \hat{c}_{l_1}^\dagger\, \hat{c}_{l_2}\, \hat{d}_{v_1}^\dagger\, \hat{d}_{v_2} \quad \hat{c}_l^\dagger\, \hat{d}_v^\dagger|\phi_0\rangle$.

Problem 13: Bogoliubov transformation (3 points)

The Hamilton operator of two interacting electrons has the form

$$\hat{H} = A\,(\hat{c}_1^\dagger\, \hat{c}_1 + \hat{c}_2^\dagger\, \hat{c}_2) - B\,(\hat{c}_1^\dagger\, \hat{c}_2^\dagger + \hat{c}_2\, \hat{c}_1)$$

with the constants $A,\, B > 0$. Using the new operators $\hat{\alpha}$, $\hat{\beta}$, $\hat{\alpha}^\dagger$ and $\hat{\beta}^\dagger$ with

$$\hat{c}_1 = u\,\hat{\alpha} + v\,\hat{\beta}^\dagger , \qquad \hat{c}_1^\dagger = u\,\hat{\alpha}^\dagger + v\,\hat{\beta} , \qquad \hat{c}_2 = u\,\hat{\beta} - v\,\hat{\alpha}^\dagger , \qquad \hat{c}_2^\dagger = u\,\hat{\beta}^\dagger - v\,\hat{\alpha} ,$$

$\hat{H}$ can be transformed into diagonal form. Here, u and v are real constants.

a) Calculate the anticommutators

$$[\hat{\alpha},\, \hat{\alpha}^\dagger]_+ , \qquad [\hat{\alpha},\, \hat{\beta}^\dagger]_+ \qquad \text{and} \qquad [\hat{\beta},\, \hat{\beta}^\dagger]_+$$

for the case $u^2 + v^2 = 1$.

b) Use the transformation given above to show that $\hat{H}$ can be put into the form

$$\hat{H} = F\,(\hat{\alpha}^\dagger\, \hat{\alpha} + \hat{\beta}^\dagger\, \hat{\beta}) + G$$

if u and v are chosen in an appropriate way (under the requirement $u^2 + v^2 = 1$). Here, F and G are constants.

c) Determine the ground state energy of the system.