Solid State Theory II: Ex 3 **(SS 2015)** **Prof. Krüger**

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Problem 8: Limit $\vec{q} \to 0$ of the dielectric function (4 points)

The dielectric function $\varepsilon(\vec{q}, \omega)$ contains matrix elements of the form

$$I(\vec{q}) = \int \psi^*_{n', \vec{k}+\vec{q}}(\vec{r})\, e^{i\,\vec{q}\,r}\, \psi_{n,\vec{k}}(\vec{r})\, d^3 r \ .$$

They describe transitions between the bands n and n'. Consider the case of small wave vectors $\vec{q}$.

The Bloch functions have the form

$$\psi_{n,\vec{k}}(\vec{r}) = e^{i\,\vec{k}\,\vec{r}}\, u_{n,k}(\vec{r}) \qquad \text{and} \qquad \psi_{n',\vec{k}+\vec{q}}(\vec{r}) = e^{i\,(\vec{k}+\vec{q})\,r}\, u_{n',k+q}(\vec{r}) \ .$$

a) Use the lattice periodic functions $u_{n,\vec{k}}$ and $u_{n',\vec{k}+\vec{q}}$ to represent $I(\vec{q})$.

b) The lattice periodic functions fulfill the following Schrödinger equations

$$\hat{H}(\vec{k})\, u_{n,\vec{k}}(\vec{r}) = E_{n,\vec{k}}\, u_{n,\vec{k}}(\vec{r}) \ , \qquad \hat{H}(\vec{k}+\vec{q})\, u_{n',k+\vec{q}}(r) = E_{n',\vec{k}+\vec{q}} u_{n',\vec{k}+q}(\vec{r}) \ .$$

Determine $\hat{H}(\vec{k})$ and $\hat{H}(\vec{k}+\vec{q})$.

c) $\hat{U} := \hat{H}(\vec{k}+\vec{q}) - \hat{H}(\vec{k})$ is a small perturbation for small wave vectors $\vec{q}$. Use first order perturbation theory to represent $u_{n',\vec{k}+\vec{q}}(\vec{r})$ by $u_{n,\vec{k}}(\vec{r})$. Employ this result to calculate $I(\vec{q})$. (*Hint*: the functions are orthonormal.) Use the matrix elements of the momentum operator

$$\vec{p}_{n',n}(\vec{k}) = \int u^*_{n',\vec{k}}(\vec{r})\, \hat{\vec{p}}\, u_{n,\vec{k}}(\vec{r})\, d^3 r$$

to represent your final result.

Problem 9: Sum rule for dielectric function (4 points)

A general property (which is called “sum rule“) of the dielectric function is discussed in this problem.

a) Consider a Hamilton operator $\hat{H}$ with a complete orthonormal set of eigenfunctions $|\psi_\alpha\rangle$ and an additional operator $\hat{A}$.

   i) Calculate the double commutator $[[\hat{H}, \hat{A}]_-, \hat{A}]_-$ and show that

$$\langle\psi_\alpha|[[\hat{H}, \hat{A}]_-, \hat{A}]_-|\psi_{\alpha'}\rangle = \sum_\beta (E_\alpha + E_{\alpha'} - 2\,E_{\beta)}\, \langle\psi_\alpha|\hat{A}|\psi_\beta\rangle\, \langle\psi_\beta|\hat{A}|\psi_{\alpha'}\rangle \ .$$

   ii) Use the general result of i) together with $\hat{A} = e^{-i\,\vec{q}\,\vec{r}}$ to calculate

$$S = \sum_\beta (E_\alpha - E_\beta)\, \left|\langle\psi_\alpha|e^{-i\,\vec{q}\,\vec{r}}|\psi_\beta\rangle\right|^2 \ .$$

b) The imaginary part of a dielectric function is given by

$$\varepsilon_2(\vec{q},\,\omega) \;=\; \frac{\pi}{\Omega}\,\frac{e^2}{\varepsilon_0\,q^2} \sum_{\substack{\delta,\,\vec{k},\,\vec{k}\,'\\ n,\,n'}} f\left(E_{n,\,\vec{k}}\right)\,\left|\langle\psi_{n\,\vec{k}}|e^{-i\,\vec{q}\,\vec{r}}|\psi_{n'\,\vec{k}\,'}\rangle\right|^2$$

$$\cdot\left(\delta\left(E_{n\,\vec{k}} - E_{n'\,\vec{k}\,'} + \hbar\,\omega\right) - \delta\left(E_{n\,\vec{k}} - E_{n'\,\vec{k}\,'} - \hbar\,\omega\right)\right).$$

A sum rule for $\varepsilon_2(\vec{q},\,\omega)$ has the form

$$\int_0^\infty \omega\,\varepsilon_2(\vec{q},\,\omega)\,d\omega \;=\; \alpha\,\omega_p^2\;.$$

Here, ω_p ist the plasma frequency. Use the result of a) to prove this sum rule and to calculate α.

c) The dielectric function in the Drude model has the form

$$\varepsilon(\omega) \;=\; \left(1 - \frac{\omega_p^2}{\omega^2 + i\,\gamma\,\omega}\right) \qquad \text{with} \qquad \gamma > 0 \qquad \text{and} \qquad \gamma \to 0\;.$$

ω_p is the plasma frequency.

Calculate

$$\text{a)} \qquad \int_0^\infty \omega\,Im\left(\varepsilon(\omega)\right)d\omega\;, \qquad \text{b)} \qquad \int_0^\infty Im\left(\frac{1}{\varepsilon(\omega)}\right)d\omega$$

by explicit evaluation of the integrals in the limit $\gamma \to 0$.

Problem 10: Current density operator (2 points)

The current density operator for a system of N particles with charge Q under the influence of a vector potential $\vec{A}$ is defined in terms of the momentum and position operators $\hat{\vec{p}}_l = \frac{\hbar}{i}\vec{\nabla}_{\vec{r}_l}$ and $\hat{\vec{r}}_l$ of the l-th particle as follows

$$\vec{J}(\vec{r},\,t) \;=\; \hat{\vec{j}}(\vec{r}) + \hat{\vec{j}}_{\rm dia}(\vec{r},\,t)$$

with a *paramagnetic*

$$\hat{\vec{j}}(\vec{r}) \;=\; \frac{1}{2}\,\frac{Q}{m}\sum_{l=1}^{N}\left(\hat{\vec{p}}_l\,\delta\left(\vec{r} - \hat{\vec{r}}_l\right) + \delta\left(\vec{r} - \hat{\vec{r}}_l\right)\hat{\vec{p}}_l\right)$$

and a *diamagnetic* part

$$\hat{\vec{j}}_{\rm dia}(\vec{r},\,t) \;=\; -\frac{Q^2}{m}\sum_{l=1}^{N}\delta\left(\vec{r} - \hat{\vec{r}}_l\right)\vec{A}\left(\hat{\vec{r}}_l,\,t\right)\;.$$

i) Calculate $\hat{\vec{J}}(\vec{r},\,t)$ in the occupation number representation for a basis of plane waves

$$\psi_{\vec{k},\,\sigma}(\vec{r}) \;=\; \frac{1}{\sqrt{\Omega}}\,e^{i\,\vec{k}\cdot\vec{r}}\,\chi_\sigma\;.$$

ii) Determine the Fourier transform of the operator resulting in i).