Solid State Theory
Exercise 5

SS 08
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Linear Response Theory

In this exercise we want to use linear response theory to first, reproduce the result for the dielectric susceptibility for free electrons obtained in the script and then, calculate the dielectric susceptibility for a semiconductor.

Exercise 5.1 Formalism

We want to consider a (external) scalar Field $V(\vec{r},t)$ that couples to the local density operator[1]

$$\hat{n}(\vec{r},t) = \hat{\psi}^\dagger(\vec{r},t)\hat{\psi}(\vec{r},t), \tag{1}$$

thus leading to a perturbation of the system of the form

$$\mathcal{H}' = \int d^3\vec{r}\, V(\vec{r},t)\hat{n}(\vec{r},t). \tag{2}$$

The linear response of the system is then given by

$$\langle \delta\hat{n}(\vec{r},t)\rangle = \int dt' \int d^3\vec{r}\,'\chi(\vec{r}-\vec{r}\,',t-t')V(\vec{r},t) \tag{3}$$

where $\chi(\vec{r},t)$ is the density-density correlation function

$$\chi(\vec{r}-\vec{r}\,',t-t') = \frac{i}{\hbar}\Theta(t-t')\langle[\hat{n}^\dagger(\vec{r},t),\hat{n}(\vec{r}\,',t')]\rangle_{\mathcal{H}} \tag{4}$$

and $\langle\ldots\rangle_{\mathcal{H}}$ denotes the thermal mean value with respect to the (unperturbed) Hamiltonian $\mathcal{H}$.
In momentum and frequency space, eq. (3) simplifies to

$$\langle \delta\hat{n}(\vec{q},\omega)\rangle = \chi(\vec{q},\omega)V(\vec{q},\omega). \tag{5}$$

Show that the dielectric susceptibility is given by

$$\chi(\vec{q},\omega) = \sum_{n,n'} \frac{e^{-\beta\epsilon_n}}{Z}|\langle n|\hat{n}_{\vec{q}}|n'\rangle|^2 \left\{\frac{1}{\hbar\omega-\epsilon_{n'}+\epsilon_n+i\hbar\eta} - \frac{1}{\hbar\omega-\epsilon_n+\epsilon_{n'}+i\hbar\eta}\right\} \tag{6}$$

with Z the partition function,

$$\hat{n}_{\vec{q}} = \int d^3r\hat{n}(\vec{r})e^{-i\vec{q}\cdot\vec{r}}, \tag{7}$$

the Fourier transform of the local density operator and the sum over n,n' runs over all possible many-particle states.

[1]Since we are doing time-dependent perturbation theory, we have to use the Heisenberg representation of the operators.

Exercise 5.2 Dielectric susceptibility of free electrons

For free electrons the field operators are given as

$$\hat{\psi}(\vec{r}) = \frac{1}{\sqrt{\Omega}} \sum_{\vec{k},s} e^{i\vec{k}\cdot\vec{r}} \hat{c}_{\vec{k}s}, \qquad \hat{\psi}^\dagger(\vec{r}) = \frac{1}{\sqrt{\Omega}} \sum_{\vec{k},s} e^{-i\vec{k}\cdot\vec{r}} \hat{c}^\dagger_{\vec{k}s} \tag{8}$$

with $\hat{c}_{\vec{k}s}$ ($\hat{c}^\dagger_{\vec{k}s}$) annihilating (creating) an electron with momentum $\vec{k}$ and spin s.
Derive eq. (3.32) of the script using linear response theory.

Exercise 5.3 Dielectric susceptibility in a semiconductor

We now want to recapitulate the calculations from above, this time however for a semiconductor. Therefore, we need two changes:

- Instead of one single band we have two bands, a valence band (V) and a conduction band (C), respectively.
- In addition, the eigenstates of the Hamiltonian are now given as Bloch-states and thus, the field operators read

  $$\hat{\psi}^\dagger(\vec{r}) = \frac{1}{\sqrt{\Omega}} \sum_{\alpha=\mathrm{V,C}} \sum_{\vec{k}s} u^*_{\alpha\vec{k}}(\vec{r}) e^{-i\vec{k}\cdot\vec{r}} c^\dagger_{\alpha\vec{k}s} \tag{9}$$

  with $u_{\alpha\vec{k}}(\vec{r}+\vec{R}) = u_{\alpha\vec{k}}(\vec{r})$ for all lattice vectors $\vec{R}$.

a) Calculate the Fourier transform $\hat{n}_{\vec{q}}$ of the local density operator $\hat{n}(r)$.

b) Use eq. (6) to show that the dielectric susceptibility for $T = 0$ is given by

$$\chi(\vec{q},\omega) = \sum_{\vec{k}} \frac{n_F(\epsilon^{\mathrm{V}}_{\vec{k}}) - n_F(\epsilon^{\mathrm{C}}_{\vec{k}+\vec{q}})}{\omega - \epsilon^{\mathrm{V}}_{\vec{k}} + \epsilon^{\mathrm{C}}_{\vec{k}+\vec{q}}} |M(\vec{k},\vec{q})|^2 \tag{10}$$

where $\epsilon^{\mathrm{V/C}}_{\vec{k}}$ is the energy of a quasi-particle in the valence and conduction band, respectively and

$$M(\vec{k},\vec{q}) = \frac{1}{\Omega_{\mathrm{UC}}} \int_{\mathrm{UC}} d^3\vec{r}\; u^*_{C\vec{k}+\vec{q}}(\vec{r}) u_{V\vec{k}}(\vec{r}). \tag{11}$$

Hint: use the periodicity of $u_{\alpha\vec{k}}(\vec{r})$ to reduce integrals over the whole space to an integral over one unit cell.

c) We now want to consider the static case ($\omega = 0$) for $\vec{q} \to 0$. Show that $M(\vec{k},\vec{q}) \propto \vec{q}\cdot\vec{r}_{CV}$ and thus, the dielectric constant

$$\varepsilon(\vec{q},0) = 1 + \frac{4\pi e^2}{q^2}\chi(\vec{q},0) \approx \text{const.} \tag{12}$$

How does a semiconductor screen a point charge for $|\vec{r}| \to \infty$?
Hint: use the orthogonality of the Bloch states in different bands.