Problem 3: Screened point charge (5 points)

As discussed in the lecture, electrostatic response can be expressed in terms of three potentials $\delta\varphi_{\rm ext}(\vec{r})$, $\delta\varphi_{\rm ind}(\vec{r})$, and $\delta\varphi(\vec{r})$. $\delta\varphi_{\rm ext}$ is provided "from outside", $\delta\varphi_{\rm ind}$ constitutes the system's response, and $\delta\varphi = \delta\varphi_{\rm ext} + \delta\varphi_{\rm ind}$ is the resulting, "total" potential. The charge-density response $\delta\rho_{\rm ind}(\vec{r})$ can be expressed as $\delta\rho_{\rm ind} = \chi_0 \circ \delta\varphi$ (with charge susceptibility χ_0), resulting in $\delta\varphi_{\rm ind} = V \circ \delta\rho_{\rm ind}$ (with Coulomb interaction $V(\vec{r}-\vec{r}\,') = \frac{1}{|\vec{r}-\vec{r}\,'|}$).

For a homogeneous system, Fourier transform

$$f(\vec{r}) = \frac{1}{(2\pi)^3}\int f(\vec{q})\, e^{i\vec{q}\vec{r}}\, d^3q\,, \qquad f(\vec{q}) = \int f(\vec{r})\, e^{-i\vec{q}\vec{r}}\, d^3r$$

turns the convolutions into multiplications, i.e.

$$\delta\varphi_{\rm ind}(\vec{q}) = V(\vec{q}) \cdot \chi_0(\vec{q}) \cdot \delta\varphi(\vec{q})\,.$$

By defining $\varepsilon(\vec{r}, \vec{r}\,')$ such that $\varepsilon \circ \delta\varphi = \delta\varphi_{\rm ext}$ one arrives at $\varepsilon = \delta(\vec{r}-\vec{r}\,') - V \circ \chi_0$ (or, for a homogeneous system, $\varepsilon(\vec{q}) = 1 - V(\vec{q}) \cdot \chi_0(\vec{q})$).

Alternatively, the charge-density response can be expressed as $\delta\rho_{\rm ind} = \chi \circ \delta\varphi_{\rm ext}$ (with $\chi \neq \chi_0$!), finally resulting (for a homogeneous system) in $\frac{1}{\varepsilon(\vec{q})} = 1 + V(\vec{q})\,\chi(\vec{q})$.

The static dielectric function of a homogeneous, infinitely large semiconductor may be given by

$$\varepsilon(q) = 1 + \frac{1}{(\varepsilon_0 - 1)^{-1} + q^2/\bar{q}^2}$$

with $\varepsilon_0 = \varepsilon(q = 0)$ the static dielectric constant and $\bar{q}$ being some characteristic wave number (e.g., $q_{\rm TF}$ in a metal). Consider an external point charge Q at $\vec{r} = 0$ (e.g. due to a defect atom), resulting in $\delta\varphi_{\rm ext}(\vec{r}) = \frac{Q}{r}$.

a) Calculate and plot the induced charge density $\delta\rho_{\rm ind}(\vec{r})$. Show that the entire induced charge amounts to $(\varepsilon_0^{-1} - 1)\,Q$.

b) Calculate and plot $\delta\varphi_{\rm ind}(\vec{r})$ and $\delta\varphi(\vec{r})$. Show that for $r \to \infty$,

$$\delta\varphi(\vec{r}) \quad\longrightarrow\quad \frac{Q}{\varepsilon_0\, r}\,.$$

c) What do you get for a simple metal?

Problem 4: Commutator relations for fermions (3 points)

a) The anticommutator of the operators $\hat{A}$ and $\hat{B}$ is given by

$$[\hat{A}, \hat{B}]_+ = \hat{A}\,\hat{B} + \hat{B}\,\hat{A}\,.$$

Show that the following relation holds for an additional operator $\hat{D}$

$$[\hat{A}, \hat{B}\,\hat{D}]_- = [\hat{A}, \hat{B}]_+\,\hat{D} - \hat{B}\,[\hat{A}, \hat{D}]_+\,.$$

b) The creation and annihilation operators $\hat{c}_j^+$ and c_j have been introduced in the lecture. Use the anticommutator relations of these operators to calculate the following commutator $[\hat{A},\, \hat{B}]_- \,=\, \hat{A}\,\hat{B} \,-\, \hat{B}\,\hat{A}$

i)

$$[\hat{n}_j,\, \hat{c}_k]_- \qquad \text{and} \qquad [\hat{n}_j,\, \hat{c}_k^+]_- \qquad \text{with} \qquad \hat{n}_j \,=\, \hat{c}_j^+\,\hat{c}_j \;.$$

ii)

$$[\hat{c}_i^+\,\hat{c}_j,\, \hat{c}_l^+\,\hat{c}_m]_- \,=\, \alpha\,\cdot\,\hat{c}_i^+\,\hat{c}_m \,+\, \beta\,\hat{c}_l^+\,\hat{c}_j \;.$$

Calculate α and β.

iii)

$$\begin{aligned}[\hat{c}_i^+\,\hat{c}_j\,\hat{c}_l^+\,\hat{c}_m,\, \hat{c}_n^+\,\hat{c}_p]_- \;&=\; (\alpha\,\cdot\,\hat{c}_i^+\,\hat{c}_p \,+\, \beta\,\cdot\,\hat{c}_n^+\,\hat{c}_j)\,\hat{c}_l^+\,\hat{c}_m \\ &+\; \hat{c}_i^+\,\hat{c}_j\,(\gamma\,\cdot\,\hat{c}_l^+\,\hat{c}_p \,+\, \zeta\,\cdot\,\hat{c}_n^+\,\hat{c}_m)\;.\end{aligned}$$

Calculate α, β, γ and ζ.

Useful relation:

$$[\hat{A}\,\hat{B},\, \hat{D}]_- \,=\, [\hat{A},\, \hat{D}]_-\,\hat{B} \,+\, \hat{A}\,[\hat{B},\, \hat{D}]_- \;.$$

Problem 5: Expectation values for fermions (2 points)

The eigenstates of the Hamilton operator

$$\hat{H} \,=\, \sum_{j=1}^{\infty} \varepsilon_j\,\hat{c}_j^+\,\hat{c}_j \qquad \text{have the form} \qquad |\phi\rangle \,=\, \prod_{j=1}^{\infty} (\hat{c}_j^+)^{n_j}\,|0\rangle \;.$$

a) Calculate $\hat{n}_l\,|\phi\rangle$ with $\hat{n}_l \,=\, \hat{c}_l^+\,\hat{c}_l$.

b) Determine the expectation values

$$\text{a)} \qquad \langle\phi|\hat{c}_l^+\,\hat{c}_m|\phi\rangle \;,$$

$$\text{b)} \qquad \langle\phi|\hat{c}_i^+\,\hat{c}_l^+\,\hat{c}_k\,\hat{c}_m|\phi\rangle \;.$$

Use the occupation numbers n_k and n_m to represent your result.

Problem 6: Two-level system (3 points)

The Hamilton operator of a system with two spin degenerate energy levels ε_a and ε_b has the form

$$\hat{H} \,=\, \varepsilon_a\,\left(\hat{c}_{a\uparrow}^+\,\hat{c}_{a\uparrow} \,+\, \hat{c}_{a\downarrow}^+\,\hat{c}_{a\downarrow}\right) \,+\, \varepsilon_b\,\left(\hat{c}_{b\uparrow}^+\,\hat{c}_{b\uparrow} \,+\, \hat{c}_{b\downarrow}^+\,\hat{c}_{b\downarrow}\right) \;.$$

a) Show that the state $|\phi_1\rangle \,=\, \hat{c}_{a\uparrow}^+\,\hat{c}_{b\uparrow}^+\,|0\rangle$ is an eigenstate of the system. Which energy has the system in this state?

b) Show that the state $|\phi_2\rangle \,=\, \frac{1}{\sqrt{2}}\left(\hat{c}_{a\uparrow}^+ \,+\, \hat{c}_{a\downarrow}^+\right)\,\hat{c}_{b\uparrow}^+\,|0\rangle$ is normalized. Is $|\phi_2\rangle$ an eigenstate of the system?

c) Calculate for $|\phi_1\rangle$ and $|\phi_2\rangle$, respectively, the expectation values for the spin operators

$$\hat{S}_z \,=\, \frac{\hbar}{2}\sum_j \left(\hat{c}_{j\uparrow}^+\,c_{j\uparrow} \,-\, \hat{c}_{j\downarrow}^+\,\hat{c}_{j\downarrow}\right) \quad \text{and} \quad \hat{S}_x \,=\, \frac{\hbar}{2}\sum_j \left(\hat{c}_{j\uparrow}^+\,\hat{c}_{j\downarrow} \,+\, \hat{c}_{j\downarrow}^+\,c_{j\uparrow}\right) \quad \text{with} \quad j = a,\, b\,.$$