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Fachbereich Physik

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Einführung in die Theoretische Festkörperphysik

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Exercise 3

(Due date: 11.11.2019)

Problem 1 (**Chemical Binding Energy**) (4 points)

The interaction energy between two ions i and j of an ionic solid is give by

$$U_{ij} = \frac{Z_i Z_j e^2}{4\pi\varepsilon_0 r_{ij}} + \lambda e^{-r_{ij}/\rho}, \quad \lambda > 0, \tag{1}$$

where Z_i is the charge of the i-th ion and r_{ij} is the distance between the i-th ion and the j-th ion.

a) The first term is the Coulomb interaction between the ions. What does the second term qualitatively represent?

b) Calculate the binding energy in the case of a one-dimensional ionic solid with alternating charges +e and -e.
Hinweis: The second term in equation (1) is so strongly decaying that you only have to consider it for your nearest neighbor.

c) Calculate the equilibrium distance between the ions. Suppose $\rho = 0.35$ Å and $\lambda = 0.5 \cdot 10^{-8}$ erg.
Hinweis: Calculate the solution numerically, e.g. using the bisection method or by entering the relevant terms in a common coordinate system. For a numeric method to converge, you may need to select appropriate units. SI units are not helpful here because the numbers are too small.

Problem 2 (**Coupling Constant**) (3 points)

Consider a 1D atomic chain where the atoms are located at positions $R_n = na$, $n \in \mathbb{N}$. Let a be the lattice parameter. The force between two atoms can be modeled by Hooke's law with stiffness $K_{ij} = K(R_i - R_j)$, i.e. the atoms are coupled not only to the nearest neighbors. Assume a linear dispersion ($\omega(k) = \eta|k|$), where η is a constant. Determine K_{ij}.
Hint: Write down $K_{ij}(k)$ explicitly and calculate the inverse Fourier transform.

Problem 3 (**Photoelectric Effect**) (3 points)

Let a hydrogen atom be in its ground state with well-known wave function:

$$\langle \vec{r}|0\rangle = \frac{e^{-r/a_0}}{\sqrt{\pi a_0^3}}, \tag{2}$$

where a_0 is the Bohr radius. This atom is being radiated by a radiation field with polarisation vector $\vec{\epsilon} = \hat{z}$ and the electron is emitted. The final state is given by

$$\langle \vec{r}|f\rangle = \frac{e^{i\vec{p}_f\cdot\vec{r}/\hbar}}{(2\pi\hbar)^{3/2}}. \tag{3}$$

In the electric dipole approximation we get – in this special case – a "transition probability"

$$\omega_{0\to f} \propto \left|\left\langle 0 \middle| \hat{A} \middle| f \right\rangle\right|^2 \delta(E_f - E_0 - \hbar\omega), \tag{4}$$

where $\left\langle \vec{r} \middle| \hat{A} \middle| \vec{r}' \right\rangle = \delta(\vec{r} - \vec{r}')\frac{\partial}{\partial z}$, E is the state energy and $\hbar\omega$ is the photon energy. Calculate the transition probability explicitly. How does it depend on the emission direction of the photo-electron?