Condensed matter physics 2013
Problem series 11

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*Problem 41 – 2P

a) Read chapter 5.3 onwards of the manuscript.

b) Order the binding types in solids in respect to their typical binding energies and give a brief explanation about the mechanisms behind them. (0.5/2)

c) Calculate the binding energy in a metal with the following model: Assume a free electron gas of density n which has a constant charge density ρ. The gas is combined with a lattice of ions, each having the charge $+e$. Neglecting electron-electron interactions, you may focus on a sphere with radius R around one single ion. (1/2)

  i) Plot qualitatively the total energy $E = E_{\text{kin}} + E_{\text{pot}}$ of the electrons.
  ii) Determine the equilibrium distance r_{eq} and binding energy E_B per unit cell.
  iii) How do r_{eq} and E_B compare to the real world?

d) Calculate the Madelung constant of a two-dimensional NaCl crystal using Evjen's method (cf. pp. 5.36 in the manuscript). How many steps are necessary to obtain this precision? What is the physical meaning of this constant? (0.5/2)

Problem 42

Draw the four lowest energy bands in the dispersion relation $E(\boldsymbol{k})$ in an fcc-crystal in the direction Γ-X [corresponds to the (100) direction], assuming a parabolic dependence like in a free electron gas.

* Problem 43 – 2P

Calculate the bandstructure for quasi-free 1D electrons in a weak potential $V(x)$ of period a.

a) Sketch the electronic bands in the periodic zone scheme. Find the points in k space where two electronic wave functions have the same energy.

b) Of what form are the unperturbed wave functions? Write down formally the Fourier components V_{k_1,k_2} of the perturbing potential in Dirac notation or integral form (do not calculate them just yet).

c) Using non-degenerate perturbation theory, calculate the correction (i. e., the energy shift) for $k \neq n\frac{\pi}{a}$ $(n \in \mathbb{Z})$. Assume a very large system and use $\lim_{L\to\infty} \frac{1}{L} \int\limits_{-L/2}^{L/2} e^{ikx} dx = \delta(k)$, i.e. the integral becomes the Fourier transform of a constant, which is the Direc-Delta function.

d) For $k = n\frac{\pi}{a}$, use degenerate perturbation theory to calculate the eigenenergies. Plot these schematically in the diagram in **a)**. Explain why a gap opens in the $E(\boldsymbol{k})$ relation.

e) What are the eigenfunctions at this point in k space?

* Problem 44 – 2P

Introduction – We assume that an electron bound to a single atomic core is described by the atomic Hamiltonian $H_{\mathrm{at}} = -\frac{\hbar^2}{2m}\vec{\nabla}^2 + V_{\mathrm{at}}(\boldsymbol{r})$ with the atomic core potential $V_{\mathrm{at}}(\boldsymbol{r})$, which leads to the Eigen functions $\psi_n(\boldsymbol{r})$ (we will leave the index from now on, but these are the labels that give the names of the electronic bands later). The latter we assume to be known. We now focus at the potential near a given atom (at position 0) in a crystal with N such atoms at positions $\boldsymbol{R}_j$, the potential has to be corrected by $\delta V(\boldsymbol{r})$, since the correct potential is given by $\sum_j V_{\mathrm{at}}(\boldsymbol{r} - \boldsymbol{R}_j)$. This is nothing but a new notation so that we can write the Hamiltonian of the complete crystal as $H_{\mathrm{cryst}} = H_{\mathrm{at}} + \delta V$ (periodic). We now look at the order zero approximation of the wave function, which corresponds to $\delta V \cdot \psi_n = 0$ for all n (δV disappears where $\psi_n \neq 0$). In this case the ψ_n are also solutions to the crystal Hamiltonian with the same Eigen energy as for the atomic orbital (in this approximation these are the same!). But this applies to each atom position, which leads to N degenerate Eigen states, which we can combine linearly to functions $\Psi(\boldsymbol{r}) = \sum_j c_{\boldsymbol{R}_j}\psi(\boldsymbol{r} - \boldsymbol{R}_j)$ (this is the reason why this method is sometimes also called *linear combination of atomic orbitals*). Choosing $c_j = e^{i\boldsymbol{k}\boldsymbol{R}_j}$ for a given $\boldsymbol{k}$ leads to the zero-order crystal wave function

$$\Psi(\boldsymbol{r}) = \sum_j e^{i\boldsymbol{k}\boldsymbol{R}_j}\psi(\boldsymbol{r} - \boldsymbol{R}_j).$$

a) Show that this function obeys the Bloch condition $\Psi(\boldsymbol{r} + \boldsymbol{R}) = \Psi(\boldsymbol{r})e^{i\boldsymbol{k}\boldsymbol{R}}$.

b) Assume ψ is an s-state wave function. Draw schematically the real part of the one-dimensional wave function $\Psi(r)$ for $k = 0$ and $k = \pi/(3a)$ with a the lattice constant.