

A simple semiconductor and the formation of excitons

Band Structure

We can model a semiconductor by considering electrons in a one-dimensional chain lattice subject to an alternating (chemical) potential. The corresponding Hamilton operator reads in second quantized form:

$$H = -t \sum_{j=1}^N \left(c_j^\dagger c_{j+1} + c_{j+1}^\dagger c_j \right) + v \sum_{j=1}^N (-1)^j n_j . \quad (1)$$

Here $c_j^\dagger$ (c_j) creates (annihilates) a spinless electron at site i . $n_j = c_j^\dagger c_j$ is the number operator on site j . You can treat Eq. (1) by transforming the Hamiltonian into k -space and rewriting it as a matrix equation.

(a) Bring Eq. (1) into the form

$$H = \sum_{\#k} \bar{c}_k^\dagger H(k) \bar{c}_k , \quad (2)$$

where $\bar{c}_k^\dagger = (c_k^\dagger, c_{k+\pi}^\dagger)$. The hash # indicates, that the sum is to be taken over the reduced Brillouin zone, i.e. here $k \in (-\pi/2, \pi/2]$.

(b) Find the unitary transformation $U = \begin{pmatrix} -u_k & v_k \\ v_k^* & u_k^* \end{pmatrix}$, which diagonalizes $H(k)$ and determine the eigenenergies E_k of $H(k)$. Furthermore, determine the band gap Δ .

(c) Introduce the operators $\bar{\alpha}_k^\dagger = (a_k^\dagger, b_k^\dagger) = \bar{c}_k^\dagger U^\dagger$, to show that the Hamiltonian can be expressed as

$$H = \sum_{\#k} \left[-E_k a_k^\dagger a_k + E_k b_k^\dagger b_k \right] . \quad (3)$$

(d) Find the ground state $|\Omega\rangle$ of H at electron density $n_k = c_k^\dagger c_k = 1/2$ (half-filling) and think of an interpretation for the new particles created by $a_k^\dagger$ and $b_k^\dagger$.

Wigner crystallization

In this example we consider the Jellium model of metals where the ionic lattice is replaced by a homogeneously charged background and the electrons can move around freely (see lecture). For typical densities the electrons form an electron gas and are described by a filled Fermi sea. Due to the fermionic character of electrons, however, at low densities the electrons will form a lattice structure instead of an electron gas. This process is called *Wigner crystallization* and should be considered in a simple version in this exercise.

Let us consider that the electrons are localized on a lattice and are exposed to a uniform positive background charge. For a single electron let us now consider a sphere of radius $d = r_s a_B$ where a_B is the Bohr radius. Each electron will be at the center of such a sphere and the total background charge inside a single sphere is equal to the electron charge $+e$ such that there is no total electric field outside

of a sphere. The spheres are regularly placed in a lattice such that they do not overlap. Therefore, we can neglect all interactions between different spheres.

We will now compute the potential energy for a single sphere which is built from only two terms, the potential energy between the positive background charge inside a sphere with itself, U_{pp} , and the potential energy between the electron at the center and the positive background charge within a sphere, U_{ep} .

- (a) Compute the charge density ρ of the positive background charge within a sphere. Use Gauss' law $4\pi Q = \oint \mathbf{E} \cdot d\mathbf{A}$ to compute the electric field $E_p(r)$ of the positive background inside the sphere $r \leq r_s a_B$. Q is the total charge within the surface of the integral. What is the field $E_p(r)$ outside the sphere?

- (b) From $E_p(r)$ compute the potential $V_p(r)$ and make it continuous at the $r = r_s a_B$. Show that

$$V_p(r) = \begin{cases} \frac{e}{2r_s a_B} \left(3 - \frac{r^2}{(r_s a_B)^2} \right), & r \leq r_s a_B \\ \frac{e}{r}, & r > r_s a_B. \end{cases} \quad (4)$$

- (c) Use the previous result to compute the self-energy of the uniformly charged background in a sphere, U_{pp} , and show that

$$U_{pp} = \frac{3}{5} \frac{e^2}{r_s a_B}. \quad (5)$$

- (d) Compute the potential energy between the background and the electron at the center of the sphere to show that

$$U_{ep} = -\frac{3}{2} \frac{e^2}{r_s a_B}. \quad (6)$$

- (e) We now have to add the kinetic energy for a single electron. We make a very simple assumption and consider that the electron in the sphere is described by a free wave with wavelength $\lambda \approx r_s a_B$. Compute the kinetic energy of the electron and the total energy for an electron in the Wigner crystal E_{Wigner} .

- (f) Let us now compare the energy of the Wigner crystal with the energy per electron in the Fermi sea, E_F . According to Sommerfeld-Pauli theory of metals, the energy density $n(E) = \frac{3}{2\epsilon_F^{3/2}} E^{1/2}$. Use this to show that $E_F = 3/5 \epsilon_F$ for $T = 0$, where E_F is the average energy per electron in the Fermi sea. Then use the relations

$$a_B = \frac{\hbar^2}{m e^2} \quad \text{and} \quad k_F = \left(\frac{9\pi}{4} \right)^{1/3} \frac{1}{r_s a_B},$$

to determine for which values of r_s the Wigner crystal has lower energy than the Fermi-sea!