Excitons

Exercise 4.1 One-dimensional model of a semiconductor

Let us consider electrons moving on a one-dimensional chain. We use the so-called tight-binding approximation. Thus, we assume that each atom has a localized electron state and that the electrons are able to hop between neighboring atoms. This hopping process describes the kinetic energy term.
It is most convenient to use a second-quantized language. For simplicity, we assume spinless electrons. Let c_i and $c_i^\dagger$ be the creation and annihilation operators for an electron at site i, respectively. The overlap integral between neighboring electron states is denoted by $-t$. Then, the kinetic energy operator is written as

$$H_0 = -t \sum_i \left(c_i^\dagger c_{i+1} + c_{i+1}^\dagger c_i \right). \tag{1}$$

We assume that the chain contains N atoms and in the following we set the lattice constant $a = 1$. Furthermore, we assume that two consecutive atoms are nonequivalent which is modeled by an alternating potential of the form

$$V = v \sum_i (-1)^i \; c_i^\dagger c_i. \tag{2}$$

[a] Consider first the case $v = 0$. Show that the states created by

$$c_k^\dagger = \frac{1}{\sqrt{N}} \sum_j e^{-ikj} c_j^\dagger \tag{3}$$

are eigenstates of H_0 with energy $\epsilon_k = -2t \cos k$. Here, k belongs to the first Brillouin zone $[-\pi, \pi)$.

[b] For $v \neq 0$ the eigenstates are created by

$$a_k^\dagger = u_k c_k^\dagger + v_k c_{k+\pi}^\dagger, \qquad b_k^\dagger = v_k c_k^\dagger - u_k c_{k+\pi}^\dagger \tag{4}$$

where $u_k^2 + v_k^2 = 1$ for all k in the reduced Brillouin zone $[-\pi/2, \pi/2)$. Diagonalize the Hamilton operator and show that it can be written in the form

$$H_0 + V = \sum_{k \in [-\frac{\pi}{2}, \frac{\pi}{2})} \left(-E_k a_k^\dagger a_k + E_k b_k^\dagger b_k \right), \qquad E_k = \sqrt{\epsilon_k^2 + v^2}. \tag{5}$$

[c] Consider now the ground state of the half-filled chain ($N/2$ electrons). What is the difference between the cases [a] and [b]?

Exercise 4.2 Coulomb interaction - excitons

Electrons are charged particles and therefore they repel. We use a simplified version of the Coulomb potential, namely, we assume that the energy of the system is increased by u whenever two electrons are on neighboring atoms (note that due to the Pauli principle two spinless electrons can not be on the same site.) In second quantized form the interaction term is written as follows:

$$U = u \sum_i n_i n_{i+1} = u \sum_i c_i^\dagger c_{i+1}^\dagger c_{i+1} c_i. \tag{6}$$

We assume that $u \ll v, t$. In this case, only the states with momentum in the vicinity of $\pm\pi/2$ are considerably affected by the Coulomb interaction.

[a] Show that the repulsive interaction between the electrons leads to an attractive interaction between electrons in the conduction band and holes in the valence band:

$$U \approx -\frac{4u}{N} \sum_{k,k',q} \cos(k-k')\; a_{k+q} b_k^\dagger b_{k'} a_{k'+q}^\dagger. \tag{7}$$

In deriving the above expression we have replaced all the v_k's and u_k's by $v_{-\pi/2}$ $(= v_{\pi/2})$ and $u_{-\pi/2}$ $(= u_{\pi/2})$.

[b] Let us now calculate the energy of an exciton. We make the following ansatz for the wave function of an exciton with momentum q:

$$|\psi_q\rangle = \sum_k A_k^q a_{k+q} b_k^\dagger |\Omega\rangle \tag{8}$$

where $|\Omega\rangle$ is the ground state of the system without interaction. Since we consider a small u we expect that the electron-hole pair is only weakly bound and that the wave function extends over a large region in real space. On the other hand, in reciprocal space, we expect that the exciton state is strongly localized. Therefore, we replace $\cos(k-k')$ in Eq. (7) by 1. Show that the energies ω_q of the exciton excitations $|\psi_q\rangle$ are given by the solution of

$$\frac{1}{4u} = \frac{1}{N} \sum_k \frac{1}{E_k + E_{k+q} - \omega_q}. \tag{9}$$

Discuss the solution graphically. How is the excitation spectrum modified by the interaction?

[c] Show that for small q the energy of the exciton is

$$\omega_q = 2v - \frac{u^2 v}{t^2} + \frac{q^2}{2(2m^*)} \tag{10}$$

where $m^* = v/(4t^2)$ is the effective mass at the band minimum.

Exercise 4.3 Excitons in real semiconductors

We consider a semiconductor with parabolic valence and conduction band characterized by the effective masses m_v and m_c. Compute the binding energy E_0 of the hydrogen-like bound state between an electron and a hole. The dielectric constant is denoted by ϵ. Compare the binding energy E_0 with the band gap Δ in GaAs with $\epsilon \approx 15$. ($\Delta = 1.5$ eV, $m_\mathrm{c} = 0.07 m_\mathrm{e}$ and $m_\mathrm{v} = 0.7 m_\mathrm{e}$.)