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Problem Set 2
Energy bands in solids

1 Monatomic tight-binding chain

Let us consider a very simple model of a one-dimensional crystal consisting of N sites, each separated by a distance a. On such a lattice, a single electron can sit only on the locations of the ions (and is thus tightly bound to each lattice site, hence the name *tight-binding approximation*). However, the electron has some small probability to hop to a neighboring site due to quantum tunneling.

When the electron sits on the n^{th} site of the chain ($n = 1, \ldots, N$), we denote its quantum eigenstate by $|n\rangle$, with corresponding onsite energy ε. We assume that these states are orthogonal to one another, *i.e.*, $\langle n|m\rangle = \delta_{nm}$.

The tight-binding Hamiltonian corresponding to the present model reads

$$H = \varepsilon \sum_{n=1}^{N} |n\rangle\langle n| - t \sum_{n=1}^{N} \big(|n\rangle\langle n+1| + |n+1\rangle\langle n|\big), \tag{1}$$

where t (assumed for simplicity to be real and positive, *i.e.*, $t \in \mathbb{R}^+$) denotes the hopping parameter that characterizes the probability amplitude for the electron to hop to a nearest-neighbor lattice site. We further consider periodic boundary conditions (by putting the lattice on a circle) and set $|N+1\rangle = |1\rangle$.

1.1 Solving the tight-binding model

We first aim at finding the eigenenergies E corresponding to the (exactly-solvable) Hamiltonian (1). To this end, we expand an eigenstate $|\psi\rangle$ of the tight-binding Hamiltonian H on the basis of the eigenstates $|n\rangle$ of H when the hopping amplitude $t = 0$ as $|\psi\rangle = \sum_{n=1}^{N} c_n |n\rangle$, with $c_n \in \mathbb{C}$.

(a) With the help of the stationnary Schrödinger equation $H|\psi\rangle = E|\psi\rangle$, show that the coefficients c_n obey the following equation:

$$(E - \varepsilon)c_n + t(c_{n+1} + c_{n-1}) = 0. \tag{2}$$

(b) Let us now make the ansatz

$$c_n = \frac{1}{\sqrt{N}}\, \mathrm{e}^{\mathrm{i}kna}, \tag{3}$$

with k some wavenumber.

(i) Convince yourself that the set of solutions to the Schrödinger equation remains the same if we shift $k \to k + 2\pi/a$, so that the wavenumber takes values $k \in \,]-\pi/a, +\pi/a]$ in the so-called (first) Brillouin zone.

(ii) Show that the wavenumber k is quantized in units of $2\pi/Na$, so that there are exactly N states of the form (3).

(iii) Finally, demonstrate that the eigenenergies of the Hamiltonian (1) are given by

$$E_k = \varepsilon - 2t\cos(ka). \tag{4}$$

(c) Plot the energy band (4) as a function of k.

(d) Compute the electron group velocity corresponding to the dispersion (4). In which direction travels an electron with $k > 0$ ($k < 0$)?

(e) Show that for small wavenumber (long wavelength $\lambda = 2\pi/k$), the dispersion relation is quadratic and takes the form

$$E_k \simeq (\varepsilon - 2t) + \frac{\hbar^2 k^2}{2m_*},$$

with the *effective* mass $m_* = \hbar^2/2ta^2$.

1.2 Metals *vs.* insulators

We now fill the energy band with many electrons.

(a) Remembering that electrons are spin 1/2 elementary particles and obey the Pauli exclusion principle, how many electrons at most can you put on the energy band (4)?

(b) Imagine putting N electrons on the energy band. What is then the Fermi wavenumber k_{F} and the corresponding Fermi energy E_{F}. Argue that the system is in a metallic phase.

(c) Consider now having $2N$ electrons on the lattice. Argue that the system is then in an insulating phase.

2 Two orbitals per atom

We now consider that each atom of the chain has two orbitals, which we call A and B, having eigenergies ε_A and ε_B, respectively. We denote by $|n, A\rangle$ ($|n, B\rangle$) the eigenstate of the electron if it sits on site n and resides on the A (B) orbital. We assume there is a hopping amplitude t_{AA} (t_{BB}) which allows an electron on orbital A (B) to hop to orbital A (B) of a nearest-neighbor atom. We suppose in addition that there is a hopping amplitude $t_{AB} = t_{BA}$ that allows an electron on orbital A to hop to the orbital B of the neighboring atom, and *vice versa*. For simplicity, we consider t_{AA}, t_{BB}, and $t_{AB} = t_{BA}$ to be real and positive.

2.1 Tight-binding Hamiltonian

Inspired by Eq. (1), construct a tight-binding Hamiltonian for the two-orbital model at hand.

2.2 $t_{AB} = 0$

(a) Consider first the case $t_{AB} = 0$. Using your results of Part 1, give the dispersion relation of the resulting two enery bands.

(b) Sketch these two energy bands.

(c) If each atom is divalent (*i.e.*, the atomic chain has $2N$ valence electrons), derive a condition on the quantities $\varepsilon_A - \varepsilon_B$, as well as t_{AA} and t_{BB}, that determines whether the system is a metal or an insulator.

2.3 $t_{AB} \neq 0$

We now consider the case in which t_{AB} is nonzero. Using what you have learned from Part 1 of this Problem Set, derive and discuss the bandstructure of the corresponding Hamiltonian.