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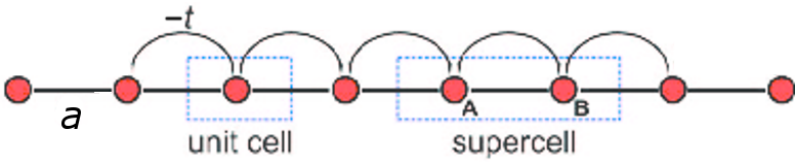
http://ctcm.kfkl.cz/srfp2020

Seminar on problem solving in physics NFPL087, Tue 15:00

Problem Sheet 5

1 Linear tight-binding chain: a doubled unit cell and a reduced Brillouin zone



In the Problem **3** on Sheet 4, the chain was solved using the smallest unit cell. In this problem, we use a unit cell with two atoms (a *supercell*, see the figure above). Naturally, we obtain the same energy spectrum, but the calculation offers interesting new aspects, both methodological and physical.

We shall label the two atoms inside the supercell as A and B and denote all states by $|\mathrm{A}, n\rangle$ and $|\mathrm{B}, n\rangle$, where n indexes the supercells. The Hamiltonian reads[1]

$$\hat{H} = -t \sum_{n=-\infty}^{\infty} \Big[|\mathrm{A}, n\rangle\langle \mathrm{B}, n| + |\mathrm{B}, n\rangle\langle \mathrm{A}, n| + |\mathrm{B}, n\rangle\langle \mathrm{A}, n+1| + |\mathrm{A}, n+1\rangle\langle \mathrm{B}, n| \Big]. \tag{1}$$

The above equation states that the electron can only tunnel from A to B, either within a single supercell or to the neighboring supercells.

We introduce two kinds of Bloch states, $|\mathrm{A}, n\rangle$ and $|\mathrm{B}, n\rangle$, by the expressions

$$|\mathrm{A}, n\rangle = \frac{1}{\sqrt{N}} \sum_k e^{-\mathrm{i}kn\cdot 2a} |\mathrm{A}, k\rangle, \quad |\mathrm{B}, n\rangle = \frac{1}{\sqrt{N}} \sum_k e^{-\mathrm{i}kn\cdot 2a} |\mathrm{B}, k\rangle, \quad \text{where } k \in \left\langle -\frac{\pi}{2a}, \frac{\pi}{2a} \right\rangle. \tag{2}$$

Notice that the length of the supercell is $2a$.

(a) Introduce the expansion from Eq. (2) into the Hamiltonian. Convince yourself, that

$$\hat{H} = -t \sum_k \Big[|\mathrm{A}, k\rangle\langle \mathrm{B}, k| \left(1 + e^{\mathrm{i}2ak}\right) + |\mathrm{B}, k\rangle\langle \mathrm{A}, k| \left(1 + e^{-\mathrm{i}2ak}\right) \Big]. \tag{3}$$

[1] In this problem, and in others, we do not write the on-site energies in the Hamiltonian. The onsite energies have the form

$$\varepsilon \sum_n \Big[|\mathrm{A}, n\rangle\langle \mathrm{A}, n| + |\mathrm{B}, n\rangle\langle \mathrm{B}, n| \Big]$$

. You can convince yourself, that these terms merely shift the resulting bands.

(b) Notice, that $\hat{H}$ is now block-diagonal in k, *i.e* it has the form $\hat{H} = \sum_k \hat{H}(k)$, where $\hat{H}(k)$ acts on states $|\mathrm{A}, k\rangle$ and $|\mathrm{B}, k\rangle$ only. In fact, $\hat{H}(k)$ can be simply represented by a 2×2 matrix in these states,

$$\hat{H}(k) = \begin{pmatrix} 0 & 1 + e^{\mathrm{i}2ak} \\ 1 + e^{-\mathrm{i}2ak} & 0 \end{pmatrix}. \tag{4}$$

It is easy to find the eigenvalues of $\hat{H}$: for every k, find the two eigenvalues, $\varepsilon_\pm(k)$, of the matrix (4). Verify, that $\varepsilon_\pm(k) = \pm 2t\,|\cos(ak)|$.

(c) Plot the dispersion relation in the Brillouin zone $\langle -\frac{\pi}{2a}, \frac{\pi}{2a} \rangle$!

(d) Compare with the result of Problem **3**, Sheet 4. Convince yourself, that the energy spectrum is the same, independent on the choice of the unit cell.

(e) The two bands that you obtained in this problem can be obtained easily in a simpler way by the construction of a *reduced* Brillouin zone (*Ashcroft & Mermin, ch. 9*). In practice, you can take the band with a single-atom unit cell, and fold it to the reduced zone $\langle -\frac{\pi}{2a}, \frac{\pi}{2a} \rangle$, obtaining the two bands of the doubled unit cell. Try it!

(f) Discussion: The two bands obtained in the supercell touch at a degeneracy point. Discuss the implications. What types of transitions can occur in the system? Hint: Peierls instability.

2 Band structure of a square lattice

Calculate the band structure of a square lattice of atoms represented by single orbitals, with the same assumptions as in the previous problems: consider only nearest neighbor coupling and neglect the overlaps. The Hamiltonian reads

$$\hat{H} = -t \sum_{n_x, n_y = 1}^{N} \Big[|n_x, n_y\rangle\langle n_x + 1, n_y| \,+\, |n_x + 1, n_y\rangle\langle n_x, n_y| + |n_x, n_y\rangle\langle n_x, n_y + 1| \,+\, |n_x, n_y + 1\rangle\langle n_x, n_y| \Big] \tag{5}$$

where the basis functions $\{|n_x, n_y\rangle\}$ now reflect the two-dimensional nature, carrying two integer indices n_x, n_y. The respective Bloch states $|k_x, k_y\rangle$ are labelled by a two-dimensional wavenumber (k_x, k_y) and we introduce them by the (inverse) relations

$$|n_x, n_y\rangle = \frac{1}{\sqrt{N^2}} \sum_{k_x, k_y} e^{-\mathrm{i}(k_x n_x + k_y n_y)a} |k_x, k_y\rangle, \quad \text{where } k_x, k_y \in \left\langle -\frac{\pi}{a}, \frac{\pi}{a} \right\rangle. \tag{6}$$

Analogously with Problem **1**, obtain the two-dimensional bands $\varepsilon(k_x, k_y)$! Plot the band structure along at least three directions in the Brillouin zone. You can choose the so called high-symmetry points.

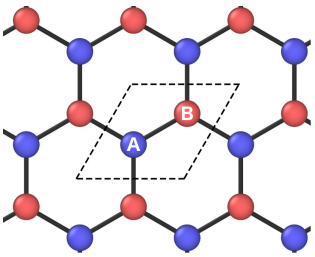
3 Electronic and crystalline structure of graphene

Graphene, a carbon allotrope, is a two-dimensional material in which the carbon atoms are arranged in a honeycomb pattern.

(a) Familiarize yourself with the crystalline structure of graphene. Discuss the symmetry properties of graphene: inversion symmetry, reflection planes, *etc.*

(b) Suggest a unit cell of graphene. What is the minimum number of atoms in a unit cell? Write the direct and reciprocal lattice vectors!

(c) Familiarize yourself with the concept of sp^2 hybridization and π bonds.



The picture on the left shows part of a hexagonal lattice, divided into two sublattices, A (blue) and B (red). Notice that every atom has three nearest neighbors from the other sublattice (one in the same unit cell and two in the neighboring cells). Lattices in which every atom binds only to the atoms of the other sublattice are called bipartite. The dashed line in the picture encloses a unit cell.

(d) Motivated by the intuitive picture of the sp^2 hybridization, we introduce a simple model of the electronic structure of graphene, which contains a single orbital (the p_z orbital) per site and does not involve electron-electron interactions *explicitly*. Thus, the basis functions can be labelled as $|\mathbf{R}, l\rangle$, where $\mathbf{R}$ labels the unit cell (vector from a direct lattice) and $l = A, B$ is the sublattice index; see figure below. Furthermore, we assume a simple tight-binding picture, in which the electron can tunnel to the nearest neighboring site only, and we disregard overlaps of the basis functions, *i.e* $\langle \mathbf{R}, l|\mathbf{R}', l'\rangle = \delta_{\mathbf{R}\mathbf{R}'}\delta_{ll'}$. The Hamiltonian reads

$$\hat{H} = -t \sum_{\langle \mathbf{R},l;\mathbf{R}',l'\rangle} \left[|\mathbf{R}, l\rangle\langle \mathbf{R}', l'| + |\mathbf{R}', l'\rangle\langle \mathbf{R}, l| \right], \tag{7}$$

where the sum runs over pairs of nearest neighbors. Use Bloch's theorem to find the energy eigenvalues, $\varepsilon_b(\mathbf{k})$, where b is a band index and $\mathbf{k}$ runs in the first Brillouin zone!

(e) Analyze the properties of $\varepsilon_b(\mathbf{k})$! Describe the properties of the spectrum (symmetry in the reciprocal space, particle-hole symmetry, Fermi surface). Find a linear approximation to the spectrum near the Fermi energy and comment in its form! What other (quasi-)particles have the same dispersion relation?

Literature: band-structure: A. H. Castro Neto, *et al.* The electronic properties of graphene, Rev. Mod. Phys. 81(1), 109 (2009),
original work: P. R. Wallace, The band theory of graphite, Phys. Rev. 71 (1947), 622–34