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Summer 2020

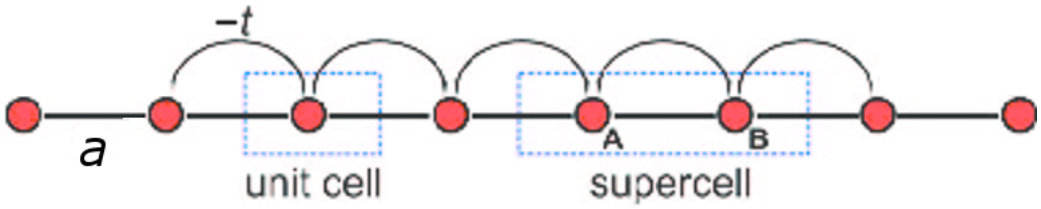
6.4.2020

http://ctcm.kfkl.cz/srfp2020

Seminar on problem solving in physics NFPL087, Wed 10:40, F052

Problem Sheet 5

1 Linear chain: repetition using Bloch functions



We consider a linear chain of atoms represented by single orbitals, as shown in the figure. The distance between atoms is a, the tunneling amplitude between nearest neighbors is $-t$ and we disregard the overlap between neighboring orbitals. It is well known that the electronic states form a cosine band (*Ashcroft & Mermin, Chap. 10*). In this problem you will rederive this simple result. It is recommended that you review the calculation of the band from the Sheet 3, Problem 2.

The Hamiltonian reads

$$\hat{H} = -t \sum_{n=1}^{N} \Big[|n\rangle\langle n+1| \; + \; |n+1\rangle\langle n| \Big]. \tag{1}$$

In this problem, we will calculate the band using the Bloch theorem. The smallest unit cell has a single orbital (atom). We will adopt periodic boundary conditions, namely, that the chain has total N sites; the site $N+1$ is identical to the site 1, *i.e.* the chain is a ring. Rederive the familiar cosine band in the following steps.

(a) Introduce the Bloch states $|k\rangle$ via the relation

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

The periodic boundary condition $|1\rangle = |N+1\rangle$ imposes a constraint on the allowed values of k inside the interval $\langle -\frac{\pi}{a}, \frac{\pi}{a} \rangle$. You can obtain the constraint in the following way: Use Eq. (2) on the left and right hand sides of the condition $|1\rangle = |N+1\rangle$. Because $|k\rangle$ are linearly independent, it holds that $e^{-\mathrm{i}kNa} = 1$. Write the allowed values of k! *Optionally,* you can convince yourself that the number of Bloch states is the same as the number of sites N in the ring.[1]

[1] In fact, Eq. (2) is just a discrete Fourier transform.

(b) Insert the above expansion, Eq. (2), in the Hamiltonian and simplify the result using the formula $\frac{1}{N}\sum_n e^{-\mathrm{i}na(k-k')} = \delta_{kk'}$, where on the right side there is the Kronecker delta.

(c) Convince yourself, that the Hamiltonian is diagonal in $|k\rangle$, namely, $\hat{H} = \sum_k \varepsilon(k)|k\rangle\langle k|$. Verify, that the dispersion relation $\varepsilon(k)$ is the same as in Problem **2** of Sheet 3.

2 A doubled unit cell and a reduced Brillouin zone

In the previous problem, 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 dispersion, 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

$$\hat{H} = -t\sum_{n=1}^{N}\Big[|\mathrm{A},n\rangle\langle\mathrm{B},n| + |\mathrm{B},n\rangle\langle\mathrm{A},n| + |\mathrm{B},n\rangle\langle\mathrm{A},n+1| + |\mathrm{A},n+1\rangle\langle\mathrm{B},n|\Big]. \tag{3}$$

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

$$|\mathrm{A},n\rangle = \frac{1}{\sqrt{N}}\sum_k e^{-\mathrm{i}kn\cdot 2a}|\mathrm{A},k\rangle, \quad |\mathrm{B},n\rangle = \frac{1}{\sqrt{N}}\sum_k e^{-\mathrm{i}kn\cdot 2a}|\mathrm{B},k\rangle, \quad \text{where } k \in \left\langle -\frac{\pi}{2a}, \frac{\pi}{2a}\right\rangle. \tag{4}$$

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

(a) Introduce the expansion from Eq. (4) into the Hamiltonian. Convince yourself, that

$$\hat{H} = -t\sum_k\Big[|\mathrm{A},k\rangle\langle\mathrm{B},k|\left(1+e^{\mathrm{i}2ak}\right) + |\mathrm{B},k\rangle\langle\mathrm{A},k|\left(1+e^{-\mathrm{i}2ak}\right)\Big]. \tag{5}$$

(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,

$$\hat{H}(k) = \begin{pmatrix} 0 & 1+e^{\mathrm{i}2ak} \\ 1+e^{-\mathrm{i}2ak} & 0 \end{pmatrix}. \tag{6}$$

It is easy to find the eigenvalues of $\hat{H}$: for every k, find the two eigenvalues $\varepsilon_\pm(k)$ of the matrix (6). 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) Instead of a single band (Problem **1**) there are now two bands. Convince yourself, that the spectrum is the same, independent on the choice of the unit cell. Note: 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!

(e) 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.

3 **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

$$\hat{H} = -t \sum_{n_x,n_y=1}^{N} \Big[|n_x, n_y\rangle\langle n_x+1, n_y| \; + \; |n_x+1, n_y\rangle\langle n_x, n_y| + |n_x, n_y\rangle\langle n_x, n_y+1| \; + \; |n_x, n_y+1\rangle\langle n_x, n_y| \Big] \tag{7}$$

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

$$|n_x, n_y\rangle = \frac{1}{\sqrt{N^2}} \sum_{k_x,k_y} e^{-\mathrm{i}(k_x n_x + k_y n_y)a} |k_x, k_y\rangle, \quad \text{where } k_x, k_y \in \left\langle -\frac{\pi}{a}, \frac{\pi}{a} \right\rangle . \tag{8}$$

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.

Note: Having mastered these three problems, you will find it straightforward to calculate the interesting and important band structure of graphene from Problem Sheet 3.