Exercise 7 for Theoretical Solid State Physics in Summer 2023

Prof. Dr. Andreas Klümper
Dr. Vladislav Popkov

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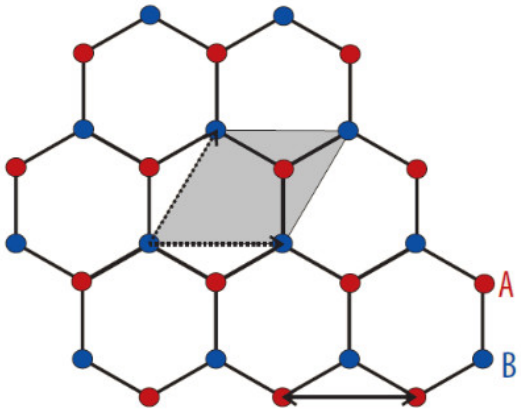
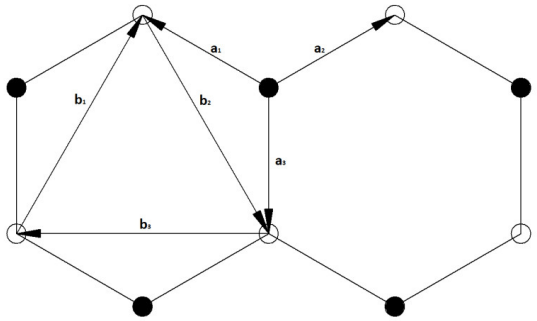
Discussion: 24.05.2023, 14:15

1. **Band structure of a bcc lattice in tight binding approximation (4 points)**
   Consider a bcc lattice with a one-atomic basis. Calculate the band structure in tight binding approximation, considering only the s orbitals and the matrix elements of the nearest neighbors.

2. **Band structure of electrons on graphene (14 points)**
   We study electrons on the graphene lattice, see figures. The red (blue) points on the left correspond to the full (open) circles on the right. We consider the red points forming sublattice A and the blue points forming sublattice B. The unit cells contain exactly one A and one B point. The edges of the hexagons have length a.





   (a) By definition the vectors connecting nearest neighbours are $\vec{a}_1$, $\vec{a}_2$, $\vec{a}_3$. (Attention: these vectors are not to be confused with primitive vectors.) In standard Cartesian coordinates $\vec{a}_3$ is

$$\vec{a}_3 = a \begin{pmatrix} 0 \\ -1 \end{pmatrix}$$

   Write down the expressions for $\vec{a}_1$, $\vec{a}_2$.

(b) The vectors connecting next-nearest neighbours are $\vec{b}_1$, $\vec{b}_2$, $\vec{b}_3$ (not to be confused with primitive vectors of the reciprocal lattice). Can (any) two of these vectors be used as primitive vectors of the Bravais lattice?

(c) We want to apply the tight binding (LCAO) method. Per unit cell we take into account only two orbitals, one s-orbital for each of the two atoms at sites A and B. The matrix elements of the Hamiltonian between electronic states on nearest neighbour points be t. (In the terminology of the lecture this corresponds to $\tilde{h}_{A,B}(\vec{R}) = t$ and $\tilde{h}_{B,A}(\vec{R}) = t$ for certain Bravais vectors $\vec{R}$.) We consider this matrix element as a *hopping rate* between nearest neighbour sites. Hence we use 2-component Bloch functions for the electrons in the crystal.

$$\Psi(\vec{r}) = \begin{pmatrix} \psi_A \\ \psi_B \end{pmatrix} \mathrm{e}^{\mathrm{i}\vec{k}\vec{r}}$$

where $\vec{r}$ takes values of the Bravais lattice, i.e. the position vectors of the unit cells, and the upper (lower) component refers to the A (B) site within the cell.

One may think of the electrons to sit on the discrete points and to hop under the action of the Hamiltonian between nearest neighbours.

We want to find energy eigenstates

$$E\Psi = H\Psi\,.$$

Explain that the first component of the equation reads

$$E \cdot \psi_A \, \mathrm{e}^{\mathrm{i}\vec{k}\vec{r}} = t\,\psi_B \left(\mathrm{e}^{\mathrm{i}\vec{k}(\vec{r}+\vec{a}_1)} + \mathrm{e}^{\mathrm{i}\vec{k}(\vec{r}+\vec{a}_2)} + \mathrm{e}^{\mathrm{i}\vec{k}(\vec{r}+\vec{a}_3)} \right).$$

Write down the second component.

(d) Show that

$$E\Psi = t \begin{pmatrix} 0 & \sum_{j=1}^{3} \mathrm{e}^{\mathrm{i}\vec{k}\vec{a}_j} \\ \sum_{j=1}^{3} \mathrm{e}^{-\mathrm{i}\vec{k}\vec{a}_j} & 0 \end{pmatrix} \Psi$$

(e) Derive/write

$$H = t \left(\sum_{j=1}^{3} \cos(\vec{k}\vec{a}_j) \right) \sigma_1 - t \left(\sum_{j=1}^{3} \sin(\vec{k}\vec{a}_j) \right) \sigma_2$$

where $\sigma_{1,2}$ are the standard Pauli matrices.

(f) What are the energy eigenvalues $E_\pm$ (as function of $\vec{k}$)?

(g) Can you produce 3d plots with Mathematica or Maple?

(h) At which $\vec{k}$-points do you find energy 0? Or: where does the gap between $E_+(\vec{k})$ and $E_-(\vec{k})$ close?

Hint: One set of these points is

$$\vec{K} = \begin{pmatrix} \frac{2}{\sqrt{3}a}\left(2\pi m \pm \frac{2\pi}{3}\right) \\ \frac{2n\pi}{3a} \end{pmatrix}$$

for arbitrary integer m and even integer n. What is the second set of points with vanishing gap? Draw a figure of these points.

(i) What is the expansion of $E_\pm(\vec{k})$ at these points?