Institut für Theoretische Festkörperphysik
Karlsruher Institut für Technologie

Prof. Dr. M. Garst
Dr. J. Masell
Dr. S. Sorn

Condensed Matter Theory 1 — Exercise 8

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https://ilias.studium.kit.edu/goto.php?target=crs_2219528
To be discussed on: *Thursday 2023/12/21*

1. Tight-binding band structure of graphene

Graphene is a single sheet of carbon atoms which form a hexagonal lattice. The goal of this exercise is to determine the band structure of graphene in the tight-binding approximation.

A hexagonal lattice is not a Bravais lattice. The primitive unit cell consists of two atoms, leading to the red and blue sublattice in Fig. 1. The Bravais lattice vectors $\boldsymbol{a}$ and the vectors $\boldsymbol{u}$ which connect atoms on adjacent lattice sites are given by

$$\boldsymbol{a}_1 = \frac{a}{2}\begin{pmatrix}\sqrt{3}\\1\end{pmatrix},\ \boldsymbol{a}_2 = \frac{a}{2}\begin{pmatrix}\sqrt{3}\\-1\end{pmatrix} \tag{1}$$

and

$$\boldsymbol{u}_1 = \frac{a}{2}\begin{pmatrix}\frac{1}{\sqrt{3}}\\1\end{pmatrix},\ \boldsymbol{u}_2 = a\begin{pmatrix}-\frac{1}{\sqrt{3}}\\0\end{pmatrix},\ \boldsymbol{u}_3 = \frac{a}{2}\begin{pmatrix}\frac{1}{\sqrt{3}}\\-1\end{pmatrix}\ , \tag{2}$$

where a is the lattice constant. We restrict the discussion to only one orbital per atom, the so-called π-orbital, with the wave function $\phi(\boldsymbol{r}-\boldsymbol{r}_0)$ for an atom at position $\boldsymbol{r}_0$. The tight-binding ansatz for the total wave function is then given as

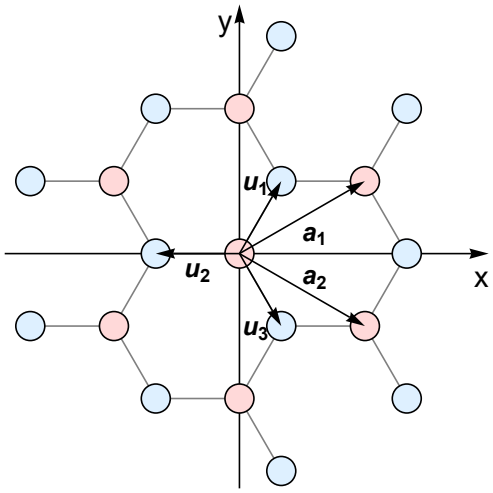

Figure 1: The hexagonal atomic lattice of graphene consists of the blue and red sublattice.

$$\Psi_{\boldsymbol{k}} = a_{\boldsymbol{k}}\Psi^{(A)}_{\boldsymbol{k}} + b_{\boldsymbol{k}}\Psi^{(B)}_{\boldsymbol{k}} \tag{3}$$

where

$$\Psi^{(\alpha)}_{\boldsymbol{k}} = \sum_{\boldsymbol{R}\in\text{Bravais lattice}} e^{i\boldsymbol{k}\boldsymbol{R}}\phi\left(\boldsymbol{r}-(\boldsymbol{R}-\boldsymbol{\delta}_\alpha)\right) \quad \text{with} \quad \alpha = A, B\ . \tag{4}$$

The respective basis vectors $\boldsymbol{\delta}_\alpha$ in Eq. (4) are $\boldsymbol{\delta}_A = \boldsymbol{0}$ and $\boldsymbol{\delta}_B = \boldsymbol{u}_1$. The coefficients are given by the eigenvalue problem $\mathcal{H}_{\boldsymbol{k}}\begin{pmatrix}a_{\boldsymbol{k}}\\b_{\boldsymbol{k}}\end{pmatrix} = \varepsilon(\boldsymbol{k})\begin{pmatrix}a_{\boldsymbol{k}}\\b_{\boldsymbol{k}}\end{pmatrix}$ which determines the dispersion $\varepsilon(\boldsymbol{k})$ in the tight-binding approximation. When considering only hopping between nearest neighbors, the tight-binding Hamiltonian in the most simple case is given by

$$\mathcal{H}_{\boldsymbol{k}} = \begin{pmatrix}\varepsilon_A & \gamma(\boldsymbol{k})\\ \gamma^*(\boldsymbol{k}) & \varepsilon_B\end{pmatrix} = \begin{pmatrix}\varepsilon_A & -t\sum_{n=1}^{3} e^{i\boldsymbol{u}_n\cdot\boldsymbol{k}}\\ -t\sum_{n=1}^{3} e^{-i\boldsymbol{u}_n\cdot\boldsymbol{k}} & \varepsilon_B\end{pmatrix}\ . \tag{5}$$

Here, t is the hopping amplitude. ε_A and ε_B are the orbital eigenenergies on sites A and B, respectively. In this exercise, we set $\hbar = 1$.

a) Assume that the two sublattices are equivalent, $\varepsilon_A = \varepsilon_B = \varepsilon/2$. In the following, consider an energy shift such that $\varepsilon = 0$. Calculate the dispersion $\varepsilon_\pm(\boldsymbol{k})$ of the two bands and plot them, for example using Mathematica. Show that the two bands touch at the so-called *Dirac points*

$$\boldsymbol{K} = \begin{pmatrix} 0 \\ \frac{4\pi}{3a} \end{pmatrix} \quad \text{and } \boldsymbol{K'} = \begin{pmatrix} 0 \\ -\frac{4\pi}{3a} \end{pmatrix} \tag{6}$$

in the 1. BZ where $\varepsilon_\pm(\boldsymbol{K}) = \varepsilon_\pm(\boldsymbol{K'}) = 0$.

b) Show that the dispersion around the Dirac points takes the form

$$\varepsilon_\pm(\boldsymbol{K} + \boldsymbol{k}) \approx \pm v_F |\boldsymbol{k}| \tag{7}$$

and similarly for $\boldsymbol{K'}$. This linear dispersion is the reason for the special electric properties of graphene. Determine the Fermi velocity v_F of graphene and express it by a and t.

c) Consider now the case $\varepsilon_A \neq \varepsilon_B$. This inequivalence may be caused, for example, by the substrate underneath the two-dimensional graphene. Expand the tight-binding Hamilton operator around the Dirac points and show that it can be written in the form

$$\mathcal{H}_{\boldsymbol{K}+\boldsymbol{k}} \approx v_F(k_y\sigma^x - k_x\sigma^y) + \Delta\sigma^z + \varepsilon\mathbb{1} \tag{8}$$

where the σ^i are the Pauli matrices. Here, $\Delta = (\varepsilon_A - \varepsilon_B)/2$ and $\varepsilon = (\varepsilon_A + \varepsilon_B)/2$.

d) Diagonalize the Hamiltonian matrix of Eq. (8). Show that the degeneracy of the bands is lifted if $\Delta \neq 0$, i.e., they do not touch anymore.

2. Berry curvature

Consider the tight-binding Hamilton matrix $\mathcal{H}_\mathbf{k} = -\vec{d}_\mathbf{k} \cdot \vec{\sigma}$ which is defined via the three-dimensional vector $\vec{d}_\mathbf{k}$. The wave vector is $\mathbf{k} = (k_x, k_y, k_z)$. Let $|u_\mathbf{k}\rangle$ denote a state with $\langle u_\mathbf{k}|u_\mathbf{k}\rangle = 1$ which fulfills

$$\hat{d}_\mathbf{k} \cdot \vec{\sigma}|u_\mathbf{k}\rangle = |u_\mathbf{k}\rangle \ , \tag{9}$$

where $\hat{d}_\mathbf{k} = \vec{d}_\mathbf{k}/|\vec{d}_\mathbf{k}|$ is normalized. For this to be well-defined, we assume in the following that the length of $\vec{d}_\mathbf{k}$ is finite everywhere in the 1. BZ, $|\vec{d}_\mathbf{k}| > 0$. The Berry curvature, which gives rise to transport properties, is in momentum space defined as $\vec{\Omega} = \vec{\nabla}_\mathbf{k} \times \vec{A}_\mathbf{k}$ with the vector potential $\vec{A}_\mathbf{k} = -i\langle u_\mathbf{k}|\vec{\nabla}_\mathbf{k}|u_\mathbf{k}\rangle$. The goal of this exercise is to express the Berry curvature by properties of the unit vector $\hat{d}_\mathbf{k}$.

a) Using Eq. (9), show that

$$(\partial_{k_j}\hat{d}^i_\mathbf{k})\sigma^i|u_\mathbf{k}\rangle = 2P\partial_{k_j}|u_\mathbf{k}\rangle \tag{10}$$

with $j = x, y, z$ and Einstein's summation convention for the index i. Moreover, we defined the projector $P = \frac{1}{2}(\mathbb{1} - \hat{d}_\mathbf{k}\vec{\sigma}) = \mathbb{1} - |u_\mathbf{k}\rangle\langle u_\mathbf{k}|$ with $P = P^2$. Based on this result, show that

$$4(\partial_n\langle u_\mathbf{k}|)P(\partial_m|u_\mathbf{k}\rangle) = (\partial_n\hat{d}^i_\mathbf{k})(\partial_m\hat{d}^j_\mathbf{k})(\delta_{ij} + i\varepsilon_{ij\ell}d^\ell_\mathbf{k}) \ , \tag{11}$$

which is written in shortened notation where $\partial_{k_j} \equiv \partial_j$.
Reminder: $\sigma^i\sigma^j = \delta_{ij} + i\varepsilon_{ij\ell}\sigma^\ell$.

b) Calculate the curvature $\Omega_i = \varepsilon_{ij\ell}\partial_j A_\ell$ and show that it is given by

$$\Omega_n = \frac{1}{4}\varepsilon_{nm\ell}\hat{d}_{\mathbf{k}} \cdot \left((\partial_m \hat{d}_{\mathbf{k}}) \times (\partial_\ell \hat{d}_{\mathbf{k}})\right) \ . \tag{12}$$

The expression in Eq. (12) has a geometric interpretation where $\vec{\Omega}$ is the solid angle spanned by the derivatives $\hat{d}_{\mathbf{k}}$ on the unit sphere. The sources of Berry curvature $\vec{\nabla} \cdot \vec{\Omega}$ are monopoles in momentum space.

c) As an example for the geometric interpretation, consider $\vec{d}_{\mathbf{k}} = v_F \hbar \vec{k}$ whose amplitude $|\vec{d}_{\mathbf{k}}|$ vanishes at $\mathbf{k} = 0$. Calculate $\vec{\Omega}$ and the monopole charge. For the latter, use Gauss' law $\int_V d^3k \vec{\nabla} \cdot \vec{\Omega} = \int_{\partial V} d\hat{\sigma} \cdot \vec{\Omega}$ where the volume is a ball around $\mathbf{k} = 0$ with radius k_r. Sketch $\hat{d}_{\mathbf{k}}$ (you may either draw or use a computer program).

d) As a second example, consider now the tight-binding Hamilton matrix $\mathcal{H} = v_F\hbar(k_x\sigma^x + k_y\sigma^y) + \Delta\sigma^z$ with $v_F > 0$, c.f. Eq. (8). Determine its unit vector $\hat{d}_{\mathbf{k}}$ and calculate the Berry curvature with the help of Eq. (12). As the vector $\hat{d}_{\mathbf{k}}$ varies only in the k_x-k_y-plane, $\vec{\Omega}$ has only one non-vanishing component

$$\Omega_z = \frac{1}{2}\hat{d}_{\mathbf{k}} \left((\partial_{k_x} \hat{d}_{\mathbf{k}}) \times (\partial_{k_y} \hat{d}_{\mathbf{k}})\right). \tag{13}$$

Show that the integral over the two-dimensional plane yields the universal result $\int dk_x dk_y \Omega_z = \pi \mathrm{sign}(\Delta)$ which only depends on the sign of Δ. Sketch $\hat{d}_{\mathbf{k}}$ (you may either draw or use a computer program).