**Übung Quantenmechanik 2 WS 2024/25**

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## 1. Emergent Dirac physics

Based on the graphene exercise of the previous exercise sheet:

(a) Obtain the graphene dispersion around the K and K' points by linearizing the eigenvalues $\varepsilon_{\pm}(\mathbf{k})$.
**Hint:** Define $\mathbf{k} = \mathrm{K} + \mathbf{q}$, with $|\mathbf{q}| << |\mathrm{K}|$, and perform a linear expansion in $\mathbf{q}$.

(b) Linearize in the same way the Bloch Hamiltonian $h(\mathbf{k})$ around K and K'. Show that we can write $h(K' + \mathbf{q}) = \hbar v_F \mathbf{q} \cdot \boldsymbol{\sigma}$ and $h(K + \mathbf{q}) = \hbar v_F (\mathbf{q} \cdot \boldsymbol{\sigma})^*$, where $v_F = 3ta/2\hbar$ is the Fermi velocity, and $\boldsymbol{\sigma}$ is the vector of Pauli matrices in the A/B sublattice basis.
**Hint:** Perform a $\pi/3$ phase rotation of the basis vector $\psi(\mathbf{k})$, *i.e.*

$$h(K' + \mathbf{q}) \to \begin{bmatrix} e^{i\pi/3} & 0 \\ 0 & e^{-i\pi/3} \end{bmatrix} h(K' + \mathbf{q})$$

after the linearization in $\mathbf{q}$.

(c) Make the analogy between the above calculated linearized graphene Hamiltonian and the 2D massless Dirac Hamiltonian. A little literature search (a la wikipedia, don't overdo it) is helpful. We will discuss this later in the lecture.

## 2. Peierls substitution

A Bloch state of a one-band Hamiltonian with a periodic potential $U(\boldsymbol{r} + \boldsymbol{R}) = U(\boldsymbol{r})$ (where $\boldsymbol{R}$ is a linear combination of the lattice basis vectors with integer coefficients) is given by

$$\psi_{\boldsymbol{k}\sigma}(\boldsymbol{r}) = u_{\boldsymbol{k}\sigma}(\boldsymbol{r}) e^{i\boldsymbol{k}\boldsymbol{r}} \chi_{\sigma}, \tag{1}$$

where $u_{\boldsymbol{k}\sigma}(\boldsymbol{r})$ has the same periodicity as the crystal. For the following calculation we will neglect the spin index $\sigma$ and its respective wave function $\chi_{\sigma}$. Then the *Wannier* functions are defined by

$$\phi_{\boldsymbol{R}}(\boldsymbol{r}) = \frac{1}{\sqrt{N}} \sum_{\boldsymbol{k}} \psi_{\boldsymbol{k}}(\boldsymbol{r}) e^{i\boldsymbol{k}\boldsymbol{R}}, \tag{2}$$

where $N$ is the number of unit cells.

(a) Show that two Wannier states are orthonormal. You may use $\langle \psi_{\boldsymbol{k}}(\boldsymbol{r}) | \psi_{\boldsymbol{k}'}(\boldsymbol{r}) \rangle = \delta_{\boldsymbol{k},\boldsymbol{k}'}$.

We now introduce a magnetic field with vector potential $\boldsymbol{A}(\boldsymbol{r})$, leading to the modified Hamiltonian $H = \frac{1}{2m}\left(\boldsymbol{p} - \frac{e}{c}\boldsymbol{A}(\boldsymbol{r})\right)^2 + U(\boldsymbol{r})$. Ultimately, we are interested in the hopping amplitude between the lattice sites

$$t_{lm} = \int d\boldsymbol{r} \phi_{\boldsymbol{R}_l}(\boldsymbol{r})^* H(\boldsymbol{r}) \phi_{\boldsymbol{R}_m}(\boldsymbol{r}). \tag{3}$$

(b) Show that the vector potential $\boldsymbol{A}(\boldsymbol{r})$ does only lead to a phase factor $\exp\left(i\frac{e}{\hbar c}\int_{\boldsymbol{R}}^{\boldsymbol{r}} d\boldsymbol{r}'\boldsymbol{A}(\boldsymbol{r}')\right)$ in the Wannier states, where the integral is understood to be a line integral from $\boldsymbol{R}$ to $\boldsymbol{r}$. Why do we choose the lower boundary to be $\boldsymbol{R}$?
<u>Hint</u>: Consider

$$\phi_{\boldsymbol{R}}(\boldsymbol{r}) = \exp\left(i\frac{e}{\hbar c}\int\limits_{\boldsymbol{R}}^{\boldsymbol{r}} d\boldsymbol{r}'\boldsymbol{A}(\boldsymbol{r}')\right)\tilde{\phi}_{\boldsymbol{R}}(\boldsymbol{r}) \tag{4}$$

and show that $\exp\left(i\frac{e}{\hbar c}\int_{\boldsymbol{R}}^{\boldsymbol{r}} d\boldsymbol{r}'\boldsymbol{A}(\boldsymbol{r}')\right) H(\boldsymbol{A}\to 0)\tilde{\phi}_{\boldsymbol{R}}(\boldsymbol{r}) = H(\boldsymbol{A}\neq 0)\phi_{\boldsymbol{R}}(\boldsymbol{r})$.

(c) Calculate now the hopping element $t_{lm}$ in presence of a vector potential $\boldsymbol{A}(\boldsymbol{r})$ to show that

$$t_{lm}(\boldsymbol{A}\neq 0) = \exp\left(i\frac{e}{\hbar c}\int\limits_{\boldsymbol{R}_m}^{\boldsymbol{R}_l} d\boldsymbol{r}'\boldsymbol{A}(\boldsymbol{r}')\right) t_{lm}(\boldsymbol{A}\to 0). \tag{5}$$

Assume that the integral $\int_{\boldsymbol{R}\to\boldsymbol{r}\to\boldsymbol{R}'\to\boldsymbol{R}} d\boldsymbol{s}\boldsymbol{A}$ is approximately zero.

## 3. Application II: Flux band structure on a square lattice

Consider a tight binding model of spin-less electrons on a 2D square lattice with lattice constant $a$ in a uniform magnetic field $\boldsymbol{B}$ perpendicular to the lattice which is generated by the vector potential

$$\boldsymbol{A}(\boldsymbol{x}) = \frac{1}{2}\frac{\hbar c}{e}\frac{\pi}{a^2} y\hat{\boldsymbol{x}}, \tag{6}$$

where $\hat{\boldsymbol{x}}$ is the unit vector in $x$ direction. The Hamiltonian of such a system is given by

$$H = \sum_{\langle lm\rangle} t_{lm} c_l^\dagger c_m \quad \text{with} \quad t_{lm} = t_0 \exp\left(\frac{ie}{\hbar c}\int\limits_m^l d\boldsymbol{s}\boldsymbol{A}(\boldsymbol{x})\right), \tag{7}$$

where the sum extends over all pairs of neighbouring sites $l$ and $m$ (each pair is therefore counted twice). In (7), the bare hopping parameter $t_0$ is constant, $c_l^\dagger$ creates an electron on the site $l$, and $c_m$ annihilates an electron on site $m$.

(a) Which axiom of quantum mechanics would be violated, if we were to count the pairs only once?

(b) Calculate the magnetic flux per plaquette (= cell of area $a \times a$) in units of $\phi_0/2\pi$, where $\Phi_0 = \frac{hc}{e}$ is the Dirac flux quantum.

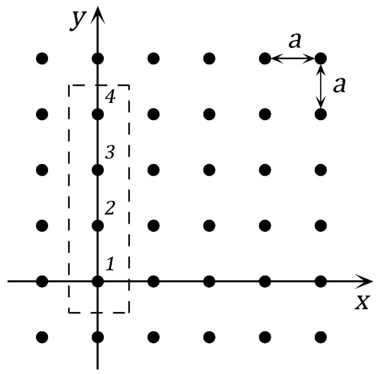


Figure 1: Sketch of lattice

(c) Sketch the lattice including the phases of the hopping parameters $t_{lm}$ between neighbouring sites.

(d) How many lattice sites must the unit cell of the lattice contain to calculate the band structure? (The unit cell has to be chosen such that the model, including the hopping phases, is invariant under translation by full unit cells.)

Now choose a unit cell with four sites $1, 2, 3$ and $4$ above each other as sketched in Fig. 1.

(e) Sketch the corresponding Brillouin zone (BZ). How many solutions will we obtain for each point in the BZ? (Or, in other words, how many bands will we obtain?)
How many possible values for the lattice momenta $\hbar\boldsymbol{q}$ are there for a lattice with $N$ sites and periodic boundary conditions (PBCs)?

(f) Consider the momentum space creation operators

$$c^\dagger_{\boldsymbol{q},\alpha} = \sqrt{\frac{4}{N}} \sum_j c^\dagger_{j,\alpha} e^{-i\boldsymbol{R}_{j,\alpha}\boldsymbol{q}}, \tag{8}$$

where $\alpha = 1, 2, 3, 4$ labels the basis of the unit cell, the index $j$ the unit cells and $\boldsymbol{R}_{j,\alpha} = \boldsymbol{R}_j + \boldsymbol{r}_\alpha$ the position of these sites within the real space unit cell. Show that the Hamiltonian can be written in the following form

$$H = t \sum_{\boldsymbol{q}} \begin{pmatrix} c_{\boldsymbol{q},1} \\ c_{\boldsymbol{q},2} \\ c_{\boldsymbol{q},3} \\ c_{\boldsymbol{q},4} \end{pmatrix}^\dagger \begin{pmatrix} 2\cos(q_x a) & e^{-iq_y a} & 0 & e^{iq_y a} \\ e^{iq_y a} & -2\sin(q_x a) & e^{-iq_y a} & 0 \\ 0 & e^{iq_y a} & -2\cos(q_x a) & e^{-iq_y a} \\ e^{-iq_y a} & 0 & e^{iq_y a} & 2\sin(q_x a) \end{pmatrix} \begin{pmatrix} c_{\boldsymbol{q},1} \\ c_{\boldsymbol{q},2} \\ c_{\boldsymbol{q},3} \\ c_{\boldsymbol{q},4} \end{pmatrix}. \tag{9}$$

For the following exercises use Mathematica or a similar mathematical symbolic computation program.

(g) Calculate the energy bands for the model.

(h) Show that around the $\Gamma = (0, 0)$ point the part of the spectrum can be expanded to an equation defining an ellipse $E(\Gamma + \delta\boldsymbol{k}) = \pm\sqrt{a(\delta k_x)^2 + b(\delta k_y)^2}$.

(i) Sketch the bands on a path from the $\Gamma$ point to the $X = (\pi, 0)$ point. In which sense is the spectrum relativistic?

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