ICFP M1 - QUANTUM MATTER - TD n°2 - Exercises
Graphene in the Tight-Binding Approximation

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Graphene is a honeycomb lattice of carbon atoms with one valence electron. The remaining three electrons per carbon atom are involved in the formation of strong covalent σ bonds, and can be considered as frozen as far as the low energy electronic properties of graphene are concerned. Here we study the low energy properties of graphene.

The graphene lattice is made of two triangular Bravais sublattices spanned by

$$\mathbf{a}_1 = \left(\frac{\sqrt{3}}{2}, \frac{3}{2}\right), \qquad \mathbf{a}_2 = \left(-\frac{\sqrt{3}}{2}, \frac{3}{2}\right). \tag{1}$$

They are denoted A and B according to Fig. 1.

Every atom of A (respectively B) has three nearest neighbors in B (respectively A), whose relative positions are given by the three unit vectors

$$\mathbf{d}_1 = \left(\frac{\sqrt{3}}{2}, \frac{1}{2}\right), \qquad \mathbf{d}_2 = \left(-\frac{\sqrt{3}}{2}, \frac{1}{2}\right), \qquad \mathbf{d}_3 = (0, -1). \tag{2}$$

The distance a between two carbon atoms ($a = 1.42$ **r**A) is set to unity. The reciprocal lattice is spanned by the vectors b_1 and b_2 defined by

$$\mathbf{a}_i \cdot \mathbf{b}_j = 2\pi\delta_{ij}. \tag{3}$$

The low energy properties of graphene are captured by a tight-binding approximation, in which we consider a spinless nearest-neighbor model on an infinite honeycomb lattice:

$$\mathcal{H} = t \sum_{<i,j>} \left(|\phi_i\rangle\langle\phi_j| + \text{h.c.}\right) \quad \text{where} \quad \langle\phi_i|\phi_j\rangle = \delta_{i,j}. \tag{4}$$

The state $|\phi_i\rangle$ describes the bound state in which the electron is localized around the carbon atom i, whose position is $\mathbf{r}_i$. The corresponding wavefunctions are of the form $\langle\mathbf{r}|\phi_i\rangle = \phi(\mathbf{r} - \mathbf{r}_i)$.

1. Rewrite the tight-binding Hamiltonian in second quantization.

2. The honeycomb lattice is invariant under discrete translations of $\mathbf{a}_1$ and $\mathbf{a}_2$. We denote by T_α the unitary operator that translates a single electron by $\mathbf{a}_\alpha$. What is T_α in first and second quantization? Check that $[\mathcal{H}, T_\alpha] = 0$. What is the standard method to exploit this symmetry ?

3. Since the honeycomb lattice is made of two Bravais sublattices A and B, one has to define two Fourier modes (one for each sublattice). In this tutorial we work with the following convention for the Fourier transform

$$|\psi^A_{\mathbf{q}}\rangle = \sum_{\mathbf{r}\in A} e^{i\mathbf{q}\cdot\mathbf{r}}|\phi_{\mathbf{r}}\rangle \qquad |\psi^B_{\mathbf{q}}\rangle = \sum_{\mathbf{r}\in B} e^{i\mathbf{q}\cdot(\mathbf{r}-\mathbf{d}_3)}|\phi_{\mathbf{r}}\rangle = \sum_{\mathbf{r}\in A} e^{i\mathbf{q}\cdot\mathbf{r}}|\phi_{\mathbf{r}+\mathbf{d}_3}\rangle. \tag{5}$$

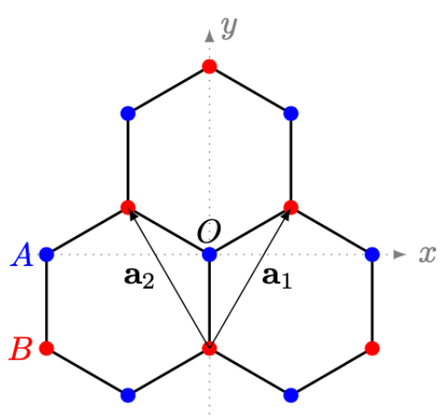

Figure 1: Crystallographic structure of Graphene.

Check that these states are indeed eigenstates of T_α. Check that $|\psi^A_{\mathbf{q}}\rangle = |\psi^A_{\mathbf{q}+\mathbf{b}_i}\rangle$ and $|\psi^B_{\mathbf{q}}\rangle = |\psi^B_{\mathbf{q}+\mathbf{b}_i}\rangle$. What is the Brillouin zone ? What is its area $\mathcal{A}_{\text{BZ}}$?

4. What are the creation operators $c^\dagger_A(\mathbf{q})$ and $c^\dagger_B(\mathbf{q})$ corresponding to $|\psi^A_{\mathbf{q}}\rangle$ and $|\psi^B_{\mathbf{q}}\rangle$? What is their inverse Fourier transform ? Compute their anti-commutation relations $\{c_\alpha(\mathbf{q}), c^\dagger_{\alpha'}(\mathbf{q}')\}$.

5. For a system that can contain many electrons, we can also consider the operators $\mathcal{T}_\alpha$ that translates all electrons. They are defined by

$$\mathcal{T}_\alpha c_{\mathbf{r}} \mathcal{T}^\dagger_\alpha = c_{\mathbf{r}+\mathbf{a}_\alpha} \qquad \mathcal{T}_\alpha|0\rangle = |0\rangle \tag{6}$$

Show that states of the form $c^\dagger_A(\mathbf{q}_1)\dots c^\dagger_A(\mathbf{q}_m)c^\dagger_B(\mathbf{q}_{m+1})\dots c^\dagger_B(\mathbf{q}_n)|0\rangle$ are eigenstates of both T_α and $\mathcal{T}_\alpha$.

6. Show that the tight-binding Hamiltonian in momentum space is

$$\mathcal{H} = \int_{\text{BZ}} \frac{\mathrm{d}\mathbf{q}}{\mathcal{A}_{\text{BZ}}} \mathbf{c}^\dagger(\mathbf{q}) h(\mathbf{q}) \mathbf{c}(\mathbf{q}) \quad \text{where } \mathbf{c}(\mathbf{q}) = \begin{pmatrix} c_A(\mathbf{q}) \\ c_B(\mathbf{q}) \end{pmatrix}, \quad h(\mathbf{q}) = \begin{pmatrix} 0 & f(\mathbf{q}) \\ f(\mathbf{q})^* & 0 \end{pmatrix} \tag{7}$$

with $f(q) = t(1 + e^{i\mathbf{q}\cdot\mathbf{a}_1} + e^{i\mathbf{q}\cdot\mathbf{a}_2})$.

7. What is the one-body spectrum of $\mathcal{H}$? What are the eigenstates ? Write the Hamiltonian in diagonal form

$$\mathcal{H} = \int_{\text{BZ}} \frac{\mathrm{d}\mathbf{q}}{\mathcal{A}_{\text{BZ}}} (\mathbf{d}^\dagger_+(\mathbf{q})\epsilon_+(\mathbf{q})\mathbf{d}_+(\mathbf{q}) + \mathbf{d}^\dagger_-(\mathbf{q})\epsilon_-(\mathbf{q})\mathbf{d}_-(\mathbf{q})). \tag{8}$$

where $d_\pm$ and $\epsilon_\pm$ are to specify.

8. We want to describe undopped graphene. What is the corresponding filling of the spinless tight-binding model ?

9. What is the Fermi surface?

10. We define the corners of the Brillouin zone by

$$\mathcal{K}_\zeta = \zeta \frac{\mathbf{b}_1 - \mathbf{b}_2}{3}. \tag{9}$$

where $\zeta = \pm 1$ is called the chirality. Check that to first order in $\mathbf{q}$ we have: $f(\mathcal{K}_\zeta + \mathbf{q}) \approx -\zeta v_{\text{F}} |\mathbf{q}| e^{i\zeta\theta_{\mathbf{q}}}$ with $v_{\text{F}} = 3t/2$ and $\theta_{\mathbf{q}}$ is the polar angle of the wave vector $\mathbf{q}$ with respect to the direction $\mathbf{a}_1 - \mathbf{a}_2$. The quantity $\zeta\theta_{\mathbf{q}}$ is called in the literature the pseudospin.

11. What are the excitation energies in the neighborhood of $\mathcal{K}_\zeta$ (to first order in $\mathbf{q}$) ?

12. Show that the mode $\mathbf{q}$ eigenvectors near $\mathcal{K}_\pm$ are $\frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ \mp\zeta e^{-i\zeta\theta_\theta} \end{pmatrix}$.

13. Argue that the low-energy effective Hamiltonian of graphene at half-filling is given by:

$$\mathcal{H} = \sum_\zeta v_{\text{F}} \int_{\text{BZ}} \frac{\mathrm{d}\mathbf{q}}{\mathcal{A}_{\text{BZ}}} c^\dagger_\zeta(\mathbf{q})(-\zeta q_x \sigma_x + q_y \sigma_y) c_\zeta(\mathbf{q}) \tag{10}$$

which is the sum of two Dirac Hamiltonians. At low energy graphene has effectively two independent Dirac fermions.

Besides translation invariance, the tight-binding model of graphene has many symmetries.

14. Chirality symmetry is a unitary operator Γ such that

$$\Gamma c_i \Gamma^\dagger = \begin{cases} c_i \text{ if } i \in A \\ -c_i \text{ if } i \in B \end{cases} \tag{11}$$

Check that Γ anti-commute with $\mathcal{H}$. It implies that the energy spectrum of H is symmetric about zero (show it). What is $\Gamma c^\dagger_A(\mathbf{q})\Gamma^\dagger$? $\Gamma c^\dagger_B(\mathbf{q})\Gamma^\dagger$? Check that $\Gamma d^\dagger_\pm(\mathbf{q})\Gamma^\dagger = d^\dagger_\mp(\mathbf{q})$.

15. Time-reversal symmetry is an anti-linear, anti-unitary operator θ defined by

$$\theta c_i \theta^\dagger = c_i, \quad \theta c^\dagger_i \theta^\dagger = c^\dagger_i. \tag{12}$$

Show that graphene is invariant under time-reversal symmetry (i.e. $[\theta, \mathcal{H}] = 0$). What is $\theta c^\dagger_A(\mathbf{q})\theta\dagger$? $\theta c^\dagger_B(\mathbf{q})\theta^\dagger$?

16. Inversion symmetry is a a unitary operator I such that $I c_{\mathbf{r}} I^\dagger = c_{\mathbf{d}_3 - \mathbf{r}}$. Check that graphene is invariant under inversion. What is $I c^\dagger_A(\mathbf{q}) I^\dagger$? $I c^\dagger_B(\mathbf{q}) I^\dagger$?

17. Show that under time-reversal we have $h(\mathbf{q}) \to h(-\mathbf{q})^*$ while under inversion we have $h(\mathbf{q}) \to \sigma_x h(-\mathbf{q})\sigma_x$. Check this way that graphene is indeed time-reversal and inversion symmetric.

Reminder of Pauli matrices:

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \qquad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \qquad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$