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Low energy properties of Graphene : tight-binding model

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, and in the next session we will analyse the effect of an impurity on the local density of states. We mainly follow the content of [1] and [2].

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.

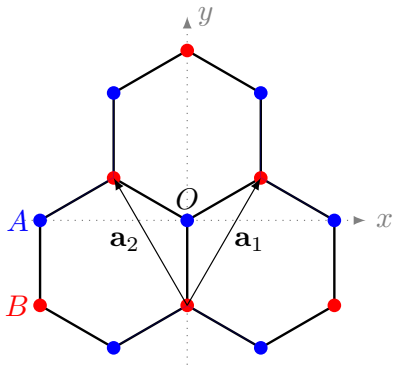

Figure 1: A and B labels the two sublattices of graphene. $\mathbf{a}_1$ and $\mathbf{a}_2$ are direct space basis vectors.

Every atom A (respectively B) has three nearest neighbors 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 ($a = 0.142$nm) is set to unity. The reciprocal lattice is spanned by the vectors $\mathbf{b}_1$ and $\mathbf{b}_2$ 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:

$$H = t\sum_{\langle i,j\rangle} \left(|\phi_i\rangle\langle\phi_j| + h.c.\right), \qquad \langle\phi_i|\phi_j\rangle = \delta_{i,j} \tag{4}$$

The state $|\phi_i\rangle$ describes the bound state in which the electron is localized around the carbon atom i, whose position is $\mathbf{r}_i$[1]. 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

1 Momentum space

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 $\mathbf{a}_\alpha$ (for $\alpha = 1, 2$). What is T_α in second quantization (** and in first quantization ? why is not simply $e^{\pm \mathbf{a}_\alpha \cdot \nabla}$?). Check that $[H, T_\alpha] = 0$. 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[2] for the Fourier transform

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

   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 $\mathcal{A}_{\rm BZ}$?

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 the 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

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

   Show that states of the form $c^\dagger_A(q_1)\cdots c^\dagger_A(q_m)c^\dagger_B(q_{m+1})\cdots c^\dagger_B(q_n)|0\rangle$ are eigenstates of both T_α and $\mathcal{T}_\alpha$.

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

$$\boxed{H = \int_{BZ} \frac{d^2q}{|\mathbf{b}_1 \wedge \mathbf{b}_2|} \mathbf{c}^\dagger(\mathbf{q}) \underbrace{\begin{pmatrix} 0 & f(\mathbf{q}) \\ f(\mathbf{q})^* & 0 \end{pmatrix}}_{h(\mathbf{q})} \mathbf{c}(\mathbf{q}), \qquad c(\mathbf{q}) = \begin{pmatrix} c_A(\mathbf{q}) \\ c_B(\mathbf{q}) \end{pmatrix}.}$$

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

7. What is the one-body spectrum of H ? What are the eigenstates ? Write the Hamiltonian in diagonal form

$$H = \int_{BZ} \frac{d^2q}{|\mathbf{b}_1 \wedge \mathbf{b}_2|} \Big(\epsilon_+(\mathbf{q}) d^\dagger_+(\mathbf{q}) d_+(\mathbf{q}) + \epsilon_-(\mathbf{q}) d^\dagger_-(\mathbf{q}) d_-(\mathbf{q})\Big)$$

[1] Each carbon atom hosts many bound states, but only the lowest energy one contributes to the low energy properties of graphene. Technically the tight-binding approximation amounts to a projection of the Hilbert space to the low energy subspace spanned by the $|\phi_i\rangle$.

[2] The unusual term $e^{-i\mathbf{q}\cdot\mathbf{d}_3}$ in the Fourier transform on the B sublattice is conventional, and is there to ensure the periodicity of all quantities w.r.t. to shifts $\mathbf{q} \to \mathbf{q} + \mathbf{b}_i$. This amounts to forget the relative position of the B sublattice w.r.t. the A sublattice.

2 Dirac points

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

9. What is the Fermi surface (FS) ?

10. We define the corners of the Brillouin zone by

$$\mathbf{K}_\xi = \xi \frac{\mathbf{b}_1 - \mathbf{b}_2}{3} \tag{6}$$

where $\xi = \pm 1$ is called the chirality. Check that to first order in $\mathbf{q}$ we have: $f(\mathbf{K}_\xi + \mathbf{q}) \simeq -\xi v_F |\mathbf{q}| e^{i\xi\theta_\mathbf{q}}$, with $v_F = \frac{3t}{2}$ and $\theta_\mathbf{q}$ is the polar angle of the wave vector $\mathbf{q}$ with respect to the direction $\mathbf{a}_1 - \mathbf{a}_2$. $\xi\theta_\mathbf{q}$ is called in the literature the *pseudospin*.

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

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

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

$$H = \sum_\xi v_F \int \frac{d^2q}{\mathcal{A}_{BZ}} \, c_\xi^\dagger(\mathbf{q}) \left(-\xi q_x \sigma_x + q_y \sigma_y\right) c_\xi(\mathbf{q})$$

Each term $\xi = \pm$ is now a two-dimensional Dirac Hamiltonian. At low energy graphene has effectively two independent Dirac fermions.

3 Retarded Green's function

14. Argue that the retarded Green function $G^0(\omega)$ is of the form :

$$G^0(\omega) = \int_{BZ} \frac{d^2\mathbf{q}}{|\mathbf{b}_1 \wedge \mathbf{b}_2|} \mathbf{c}^\dagger(\mathbf{q}) G^0(\mathbf{q}, \omega) \mathbf{c}(\mathbf{q})$$

Show that the 2 by 2 retarded Green function $G^0(\mathbf{q}, \omega)$ is

$$G^0(\mathbf{q}, \omega) = \frac{1}{(\omega + i\eta)^2 - |f(\mathbf{q})|^2} \begin{pmatrix} \omega + i\eta & f(\mathbf{q}) \\ f(\mathbf{q})^* & \omega + i\eta \end{pmatrix} \tag{7}$$

15. Show that the 2×2 matrix retarded Green function of the operators $c(A, \mathbf{K}_\xi + \mathbf{q})$ and $c(B, \mathbf{K}_\xi + \mathbf{q})$ in the neighborhood of $\mathbf{K}_\xi$ is:

$$G^\xi(\mathbf{q}, \omega) = \frac{1}{(\omega + i0^+)^2 - v^2|\mathbf{q}|^2} \begin{pmatrix} \omega & -\xi v_F q e^{i\xi\theta} \\ -\xi v_F q e^{-i\xi\theta} & \omega \end{pmatrix} \tag{8}$$

4 Symmetries of graphene

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

16. Chirality symmetry is a unitary operator Γ such that

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

Check that Γ anti-commute with H. Since Γ does not commute with H, it is not associated with any conserved quantity. However $\{\Gamma, H\} = 0$ implies that the energy spectrum of H is symmetric about zero (show that). What is $\Gamma c^\dagger(A, \mathbf{q})\Gamma^\dagger$? $\Gamma c^\dagger(B, \mathbf{q})\Gamma^\dagger$? Check that $\Gamma d_\pm(\mathbf{q})\Gamma^\dagger = d_\mp(\mathbf{q})$.

17. Time-reversal symmetry is an anti-linear, anti-unitary[3] operator $\mathcal{T}$ defined by

$$\mathcal{T} c_i \mathcal{T}^\dagger = c_i, \quad \mathcal{T} c_i^\dagger \mathcal{T}^\dagger = c_i^\dagger$$

Show that graphene is invariant under time-reversal symmetry (*i.e.* $[\mathcal{T}, H] = 0$). What are $\mathcal{T} c^\dagger(A, \mathbf{q})\mathcal{T}^\dagger$ and $\mathcal{T} c^\dagger(B, \mathbf{q})\mathcal{T}^\dagger$?

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

19. 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.

References

[1] Cristina Bena. Effect of a single localized impurity on the local density of states in monolayer and bilayer graphene. *Phys. Rev. Lett.*, 100:076601, Feb 2008.

[2] C. Dutreix and M. I. Katsnelson. Friedel oscillations at the surfaces of rhombohedral n-layer graphene. *Phys. Rev. B*, 93:035413, Jan 2016.

[3] An operator A is said to be anti-linear if $A(\lambda u + v) = \bar{\lambda} A(u) + A(v)$. An anti-unitary operator is an anti-linear operator A such that $\langle Au, Av\rangle = \overline{\langle u, v\rangle}$. The hermitian conjugate of anti-linear operator A is the operator $A^\dagger$ obeying $\langle Au, v\rangle = \overline{\langle u, A^\dagger v\rangle}$ for all u, v. Therefore anti-unitary operators are anti-linear operators such that $AA^\dagger = 1$.