# Concepts in Condensed Matter Physics: Exercise 1

## Spring 2020

Due date: 28/05/2020

1. **The robustness of Dirac fermions in Graphene**

   We know that the lattice structure of Graphene has unique symmetries (e.g. 3-fold rotational symmetry of the honeycomb lattice). The question is: What protects the Dirac spectrum? Namely, what inherent symmetry in Graphene do we need to violate in order to destroy the massless Dirac spectrum of the electrons at low energies (i.e. open a band gap)? In this question, consider only nearest neighbor terms.

   (a) Stretching the Graphene lattice - one way to reduce the symmetry of Graphene is to stretch its lattice in one direction. **Which symmetry is broken in this case?** In non-stretched Graphene the hopping of an electron from a carbon atom to its three nearest-neighbors has equal amplitudes ($t_1 = t_2 = t_3 = t$). Stretching a carbon-carbon bond reduces the hopping element along this bond. A simple way to take into account the stretching is to keep the hexagonal geometry of Graphene fixed but write a tight-binding Hamiltonian with non-equal hopping matrix elements:

   $$H = -\sum_{\vec{R},\sigma} \sum_{a} \left[ t_a A^{\dagger}_{\vec{R},\sigma} B_{\vec{R}+\vec{\delta}_a,\sigma} + \text{h.c.} \right], \tag{1}$$

   where the vectors $\vec{\delta}$, connecting the $A$ atoms to their nearest neighbors, are given by

   $$\vec{\delta}_1 = \tfrac{a}{2}\left(1,\sqrt{3}\right) \quad \vec{\delta}_2 = \tfrac{a}{2}\left(1,-\sqrt{3}\right) \quad \vec{\delta}_3 = a\left(-1,0\right). \tag{2}$$

   i. Write the Bloch Hamiltonian for the generic case ($t_1 \neq t_2 \neq t_3$) and find the corresponding energy bands and wave functions. Use the form $h(\vec{k}) = \vec{d}(\vec{k}) \cdot \vec{\sigma}$, where the $\vec{\sigma}$ are the Pauli matrices acting on the A-B space, and find $\vec{d}(\vec{k})$. In what follows you can plot the energy bands numerically.

ii. What happens to the Dirac cones in homogeneous stretching (change the values of the $t$'s but keep them equal)?

iii. How are the two Dirac points and cones affected in the following two different cases: (i) $t_1 = t_3 > t_2$, and (ii) $t_1 = t_3 < t_2$? For what values of $r \equiv \frac{t_2}{t_1}$ do the Dirac cones gap out? Plot the band structure of the Bloch Hamiltonian for several representative values of $r$ leading up to $r^*$ where the cones gap out. Plot the phase of the pseudo-spin wave-function as a function of $\vec{k}$ for these values of $r$ in the vicinity of the Dirac points. (Similar to what you saw in class for non-stretched case.) Try explaining what happens to the Dirac cones in terms of vortices in k-space as $r$ is modified.

iv. For the non-stretched case, we found the Hamiltonian

$$\tilde{H} = \hbar v_F \left( k_x \sigma_x + \tau_z k_y \sigma_y \right), \tag{3}$$

with $\tau_z = \pm 1$ labeling the valley degree of freedom. How does Eq. (3) change when the graphene is stretched? (You may assume $r \ll r^*$.) Compare this to the coupling of the Dirac fermions to the electromagnetic gauge field $p_\mu \to p_\mu - qA_\mu$.

(b) What happens when one introduces a term proportional to $\sigma_z$ (for example $d_z = $ const.) to $h(\vec{k})$? What is the physical meaning of such a term, and how does it manifest in the microscopic tight-binding Hamiltonian? What symmetry of Graphene does it break?

2. **Bilayer Graphene**

In this problem we will discuss the electronic properties of two sheets of Graphene stacked one on top of the other. We will consider a particular stacking (which is energetically favored when stacking Graphene), the so-called "Bernal stacking" (or "AB stacking"). In this configuration, an A-atom of layer 2 ($A_2$) is positioned directly above a B atom of layer 1 ($B_1$), while $A_1$ and $B_2$ are exactly aligned with the hexagon center of their opposing layer, see Fig. 1.

(a) Let us consider the tight-binding Hamiltonian of bilayer Graphene. There are three hopping processes we want to account for: (i) the intra-layer hopping (you are already familiar with), with amplitude $t$; (ii) the "strong" inter-layer hopping, which couples overlapping $A_2$ and $B_1$ atoms, with amplitude $\gamma_1$; and finally (iii) the much smaller coupling between neighboring $A_1$ and $B_2$ atoms, with amplitude $\gamma_3$.

Write down the tight-binding Hamiltonian in terms of creation/annihilation operators on the sites $A_1, B_1, A_2, B_2$. Transform it to k-space to find the Bloch Hamiltonian, and write it in the
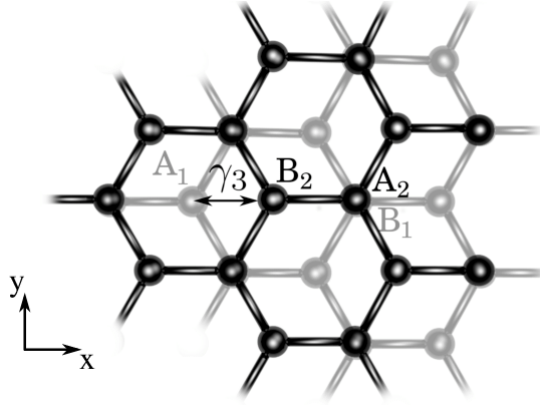
Figure 1: Stacking of two layers of Graphene. Atoms of the bottom layer "1" appear in gray, while in the to player "2" appear in black. In the stacking depicted, $A_2$ and $B_1$ atoms overlap and have a hopping amplitude of $\gamma_1$, whereas $A_1$ atoms are located in the center of layer-2 hexagons, and $B_2$ atoms are centered with respect to layer-1 hexagons. Nearby $A_1$ and $B_2$ atoms are connected by a hopping amplitude $\gamma_3$.

form

$$H = \sum_{\vec{k}} \Psi^\dagger\left(\vec{k}\right) h\left(\vec{k}\right) \Psi\left(\vec{k}\right), \tag{4}$$

with $\Psi\left(\vec{k}\right) = \left(\psi_{A_1,\vec{k}}, \psi_{B_1,\vec{k}}, \psi_{A_2,\vec{k}}, \psi_{B_2,\vec{k}}\right)$ a spinor of annihilation operators.

(b) From this point on, we will use the fact that $\gamma_3 \ll \gamma_1$ and set $\gamma_3 = 0$. Diagonalize the Hamiltonian and plot its spectrum as a function of $\vec{k}$ for $\gamma_1 \ll t$, and $\gamma_1 \lesssim t$. Compare your results with the spectrum we obtained for single-layer Graphene. Is the spectrum gapped?

(c) Expand the Bloch Hamiltonian around the $K/K'$ points and find its low-momentum description. How does the spectrum behave at low energies and small momenta?

Using second-order perturbation theory in $\frac{v_F|\vec{k}|}{\gamma}$, derive the effective low-energy $2\times2$ Hamiltonian acting on the spinor $\tilde{\Psi}\left(\vec{k}\right) = \left(\psi_{A_1,\vec{k}}, \psi_{B_2,\vec{k}}\right)$ (You may want to consult the book of Sakurai, Chapter 5.2.). Can you define (and find) the mass of the electrons from the spectrum?

(d) Add to the $2 \times 2$ Bloch Hamiltonian you found a term accounting for a chemical potential bias between the layers. In other words, an energy "cost" for electrons to be located on layer-1 atoms, and an identical energy "gain" for being located on layer-2. Such a setup can be experimentally achieved by, e.g., placing the bilayer inside a two-plate capacitor. What is the effect of such a term on the spectrum?

3. **"Magic angle" Twisted Bilayer Graphene** (Bonus question)

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In this exercise, we will explore a system on the cutting edge of contemporary condensed matter physics, the theoretical prediction (similar to what you will do in this exercise) and discovery of which has recently been awarded the prestigious Wolf prize. The system is comprised of two sheets of graphene, with a very small in-plane rotation of one sheet relative to the other, of the order of $\sim 1°$. As you will see, the spectrum of such systems is exceptionally "flat" (and has for example a tiny Dirac velocity) as compared to plain monolayer Graphene. This in turn seems to strongly enhance correlations between the electrons and may lead to rather exciting phenomena.

For those of you interested, you can check out the following talk on YouTube: `https://www.youtube.com/watch?v=O2HVCjhuJlE`, where roughly the first half of the talk is relevant to this exercise (although all of it is quite interesting).
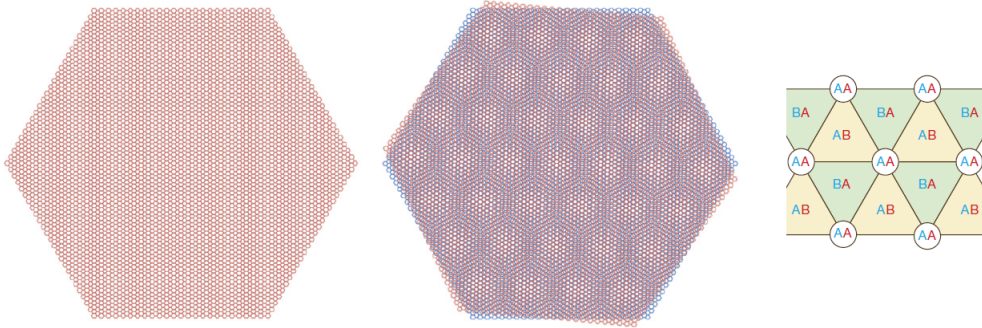


Figure 2: Twisted bilayer Graphene. Left: lattice structure of a single layer of Graphene. Middle: two Graphene layers with a small relative twist. The periodic Moiré pattern is formed in real-space, and one finds alternating areas of $AA$, $AB$, and $BA$ stacking, pointed out explicitly to the right. The inter-layer hopping captured in Eq. (6) is modulated by this Moiré potential.

The twisted-bilayer Graphene structure gives rise to a Moiré periodic pattern, see Fig. 2, with an enlarged unit cell of $\mathcal{O}\left(10^3\right)$ carbon atoms. The Moiré pattern effectively modulates the inter-layer hopping matrix elements, with a triangular lattice pattern spanned by

$$\vec{q}_1 = k_\theta\left(0, -1\right), \quad \vec{q}_2 = \frac{k_\theta}{2}\left(\sqrt{3}, 1\right), \quad \vec{q}_3 = \frac{k_\theta}{2}\left(-\sqrt{3}, 1\right),$$

with $k_\theta = 2k_D \sin\left(\theta/2\right)$, $k_D = 4\pi/(3a)$ being the (monolayer) Dirac momentum, $a$ is the Graphene lattice constant, and $\theta$ the relative twist-angle.

(a) Begin with the low-energy Dirac Hamiltonian of a single layer *near a single valley* for simplicity, and transform it to real-space. This produces a $2\times 2$ matrix with derivatives in real-space $h_0\left(\vec{r}\right)$. Find $h_{0,\Theta}\left(\vec{r}\right)$, which is defined as rotating $h_0\left(\vec{r}\right)$ around the $z$-axis by an angle $\Theta$. (Hint: the

generator of in-plane rotations is the $\sigma_z$ Pauli matrix.)

(b) The continuum Hamiltonian can now be expressed by

$$\mathcal{H} = \int d^2\vec{r}\Psi^\dagger \left(\vec{r}\right) h_{\text{eff.}} \left(\vec{r}\right) \Psi \left(\vec{r}\right),$$

with $\Psi = (\psi_{A,1}\psi_{B,1}, \psi_{A,2}\psi_{B,2})$ and (notice that $h_{\text{eff.}}$ is a $4 \times 4$ matrix just like that of bilayer Graphene, and that each element in the matrix below is a $2 \times 2$ matrix)

$$h_{\text{eff.}} \left(\vec{r}\right) = \begin{pmatrix} h_{0,\theta/2} \left(\vec{r}\right) & T \left(\vec{r}\right) \\ T^\dagger \left(\vec{r}\right) & h_{0,-\theta/2} \left(\vec{r}\right) \end{pmatrix}. \tag{5}$$

The matrix $T$ embodies the Moiré-modulated inter-layer hopping, and is given by

$$T \left(\vec{r}\right) = \sum_{j=1}^{3} \begin{pmatrix} w_0 & w_1 e^{-i(j-1)\phi} \\ w_1 e^{i(j-1)\phi} & w_0 \end{pmatrix} e^{-i\vec{q}_j \cdot \vec{r}} \equiv \begin{pmatrix} w_0 F_0 \left(\vec{r}\right) & w_1 F_{1+} \left(\vec{r}\right) \\ w_1 F_{1-} \left(\vec{r}\right) & w_0 F_0 \left(\vec{r}\right) \end{pmatrix}, \tag{6}$$

with $\phi = 2\pi/3$. The functions $F_\lambda$ represent the Moiré modulation in space. To understand their form, plot $|F_0 \left(\vec{r}\right)|, |F_{1\pm} \left(\vec{r}\right)|$ as a function of position.

Perform a Fourier transform on the continuum Hamiltonian to find its form in k-space. Notice the Hamiltonian is no longer diagonal in $\vec{k}$ as all the cases we have considered so far (monolayer and bilayer Graphene) due to the periodic modulation. Specifically, you should find the Hamiltonian takes the form

$$\left[\psi_1^\dagger \left(\vec{k}\right), \psi_2^\dagger \left(\vec{k} + \vec{q}_1\right), \psi_2^\dagger \left(\vec{k} + \vec{q}_2\right), \psi_2^\dagger \left(\vec{k} + \vec{q}_3\right)\right] \mathcal{H}_{\vec{k}} \left[\psi_1 \left(\vec{k}\right), \psi_2 \left(\vec{k} + \vec{q}_1\right), \psi_2 \left(\vec{k} + \vec{q}_2\right), \psi_2 \left(\vec{k} + \vec{q}_3\right)\right]$$

(plus an Hermitian conjugate) with $\psi_\ell \left(\vec{k}\right) = \left(\psi_{A,\ell} \left(\vec{k}\right), \psi_{B,\ell} \left(\vec{k}\right)\right)$. Find the explicit form of $\mathcal{H}_{\vec{k}}$.

(c) Next, we want to take a closer look at the spectrum around one of the Dirac points, so we will find the effective Hamiltonian connecting $\psi_1^\dagger \left(\vec{k}\right)$ and $\psi_1 \left(\vec{k}\right)$.

Recall that for an Hamiltonian of the form

$$H = \begin{pmatrix} H_A & T_{AB} \\ T_{BA} & H_B \end{pmatrix},$$

one can formulate an effective $A$-Hamiltonian which produces the same Schrodinger equation

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solution with energy $E$ (you should check this explicitly),

$$H_A^{\text{eff}}(E) = H_A - T_{AB}(H_B - E)^{-1}T_{BA}. \tag{7}$$

After approximating $h_{0,\theta/2} \approx h_{0,0}$, The $\mathcal{H}_{\vec{k}}$ you found in the previous part should be of the form

$$\mathcal{H}_{\vec{k}} = \begin{pmatrix} h\left(\vec{k}\right) & T_{01} & T_{02} & T_{03} \\ T_{10} & h\left(\vec{k}+\vec{q}_1\right) & & \\ T_{20} & & h\left(\vec{k}+\vec{q}_2\right) & \\ T_{30} & & & h\left(\vec{k}+\vec{q}_3\right) \end{pmatrix}, \tag{8}$$

with $h\left(\vec{k}\right) = v_F \vec{k} \cdot \sigma$. Using a generalized form of Eq. (7) at the vicinity of $E = 0$, find the effective Hamiltonian $\psi_1^\dagger\left(\vec{k}\right) h_{\text{eff}}\left(\vec{k}\right) \psi_1\left(\vec{k}\right)$. Expand it to first order in $\vec{k}$ to extract the modified Dirac velocity $v^\star$. How does it depend on $v_F, w_{0,1}, k_\theta$? Take $v_F k_D = 9.9$ eV, $w_1 = 110$ meV, $w_0 = 82$ meV. Plot $v^\star$ as a function of the twist angle. What is the "magic angle" at which the band becomes flat? Compare this to the case $w_0 \to 0$.

You might find references [1, 2, 3] useful for this exercise.

# References

[1] Rafi Bistritzer and Allan H. MacDonald. Moiré bands in twisted double-layer graphene. *Proceedings of the National Academy of Sciences*, 108(30):12233–12237, 2011.

[2] J. M. B. Lopes dos Santos, N. M. R. Peres, and A. H. Castro Neto. Graphene bilayer with a twist: Electronic structure. *Phys. Rev. Lett.*, 99:256802, Dec 2007.

[3] Grigory Tarnopolsky, Alex Jura Kruchkov, and Ashvin Vishwanath. Origin of magic angles in twisted bilayer graphene. *Phys. Rev. Lett.*, 122:106405, Mar 2019.