TWISTED BILAYER GRAPHENE

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Abstract. — This project is an attempt to study the energy spectrum of the twisted bilayer graphene. We wished to reproduce the Hoffstatder butterfly pattern in the eigenvalue support of the tBLG. We start with a tight binding model for single layer graphene, see it's extension to the bilayer graphene and further study the system in the presence of a magnetic field. The Hamiltonian is represented as Landau levels. In tBLG case, we stick to the low energy hamiltonian which is an extension of the continuum limit of single layer graphene instead of going for the more general tight binding to keep our model semi analytical, we stick to small twist angles.

Contents

1. Single Layer- Graphene

Graphene is a material made of a single atomic layer. This two dimensional system is made of Carbon atoms, arranged in a honeycomb lattice with nearest site distance $a = 1.42\,\text{Å}$. This can be thought of as two intercepting triangular lattices A and B (Figure 1). We want to calculate the spectrum

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of non-interacting electron. Graphene has one accessible electron per atom. We restrict ourselves here to the case of nearest-neighbor tunneling terms only. Working directly in second quantization, and define the annihilation and creation operators of an electron at the lowest orbital centered around sites A and B.

For single layer graphene, the Hamiltonian is given by

$$H = -t \sum_{\langle i,j\rangle,\sigma} a^\dagger_{\sigma,i} b_{\sigma,j} - t' \sum_{\langle\langle i,j\rangle\rangle,\sigma} \left(a^\dagger_{\sigma,i} a_{\sigma,j} + b^\dagger_{\sigma,i} b_{\sigma,j} \right) + \text{H.c.}$$
$$\{a_{\sigma,i}, a^\dagger_{\sigma',i'}\} = \{b_{\sigma,i}, b^\dagger_{\sigma',i'}\} = \delta_{ii'}\delta_{\sigma\sigma'}$$
$$\{a_{i,\sigma}, b_{i',\sigma'}\} = 0$$

where $a_{i,\sigma}$ ($b_{i,\sigma}$) annihilates an electron with spin σ at the site $\vec{R}_i$ on sublattice A (B), $t = \approx 2.8$eV is the nearest-neighbour hopping energy (between different sublattices) and t' is the next nearest-neibour hopping energy (on the same sublattice). t' satisfies $0.02t \leq t' \leq 0.2t$. The third next-nearest hopping term can also be included but it has hopping energy of about 0.07eV, so we neglect it. The energy-momentum dispersion relation we get from this tight-banding Hamiltonian is

$$E_\pm \left(\vec{k}\right) = \pm t \sqrt{3 + f\left(\vec{k}\right)} - t' f\left(\vec{k}\right)$$

where

$$f\left(\vec{k}\right) = 2\cos\left(\sqrt{3}k_y a\right) + 4\cos\left(\frac{\sqrt{3}}{2}k_y a\right)\sin\left(\frac{3}{2}k_x a\right)$$

The points $K, K' = \left(\frac{2\pi}{3a}, \pm\frac{2\pi}{3\sqrt{3}a}\right)$ are called Dirac points. They are the corners of the graphene Brilouin zone. Expanding the dispersion relation around the Dirac point as $k = K + q$ gives

$$E_\pm \approx 3t' \pm v_F|\vec{q}| - \left(\frac{9t'a^2}{4} \pm \frac{3t^2 a}{8}\sin\left(3\tan^{-1}\left(\frac{q_y}{q_x}\right)\right)\right)|\vec{q}|^2$$

Notice that the two bands touch at some points in the first Brillouin zone. Since Graphene has one accessible electron per atom, we get by taking spin into account that the lower band is exactly filled. This means that if we would like to discuss small excitations above the ground state, the excitations that will contribute are those near the crossing points. These points (Dirac Points) can be found by setting $f(\vec{k}) = 0$. Expanding around this dirac point and putting $t' = 0$ we get

$$f(\vec{K} + \vec{q}) \approx -\frac{3ta}{2}e^{-i\phi}(q_y + iq_x) + \text{h.c.}$$

. Putting this into the Hamiltonian, we get

$$H(\vec{K}+\vec{q}) = -\frac{3ta}{2}\begin{pmatrix} 0 & e^{i\phi}(q_y+iq_x) \\ e^{-i\phi}(q_y-iq_x) & 0 \end{pmatrix}$$

On defining new fields $\Psi_i = (a_i, b_i)$ and expanding the tight-binding hamiltonian to order δ, it takes some algebra to see that the tight-binding hamiltonian has the following continuum model as a low-energy (large distance) limit

$$H = -iv_F \int \mathrm{d}x\mathrm{d}y \left[\hat{\Psi}_1^\dagger(\vec{r})\,\vec{\sigma}\cdot\vec{\nabla}\Psi_1(\vec{r}) + \hat{\Psi}_2^\dagger(\vec{r})\,\vec{\sigma}^*\cdot\vec{\nabla}\Psi_2(\vec{r})\right]$$

where $\vec{\sigma} = (\sigma_x, \sigma_y)$ and $\vec{\sigma}^* = (\sigma_x, -\sigma_y)$ are the Pauli matrices and $v_F = \frac{3ta}{2}$

2. Twisted Bilayer

The tight-binding Hamiltonian for bilayer graphene is given by

$$\begin{aligned} H = &- \sum_{\langle i,j\rangle,m,\sigma} \gamma_0\, a^\dagger_{m,i,\sigma} b_{m,j,\sigma} \\ &- \sum_{j,\sigma}\left(\gamma_1\, a^\dagger_{1,j,\sigma} a_{2,j,\sigma} + \gamma_4\,(a^\dagger_{1,j,\sigma} b_{2,j,\sigma} + a^\dagger_{2,j,\sigma} b_{1,j,\sigma}) + \gamma_3\, b^\dagger_{1,j,\sigma} b_{2,j,\sigma}\right) \\ &+\text{H.c.} \end{aligned}$$

where $a_{m,i,\sigma}(b_{m,i,\sigma})$ annihilates an electron with spin σ, on a sublattice A(B), in a layer $m = 1, 2$ at the site $\mathbf{R}_i$.

Low energy theories operate mainly on the electronic states near the Dirac cones, which the tBLG inherits from its two constituent layers. In tBLG, the Dirac cones having their origins at K *and* K_θ are located close to each other in momentum space (for $\theta < 30°$). This allows constructing an effective low-energy Hamiltonian for the Dirac electrons moving in each graphene layer with additional inter-layer hopping terms.
To make the expression more symmetric, we rotate both layers by $\frac{\theta}{2}$ opposite to each other instead of rotating one layer by θ
Expanding around the dirac points, we get a low energy continuum description given by hamiltonian density

$$\mathcal{H} = \begin{pmatrix} h(-\theta/2) & T(\vec{r}) \\ T^\dagger(\vec{r}) & h(\theta/2) \end{pmatrix}$$

where $h(\theta) = iv_F\vec{\sigma}(\theta)\cdot\vec{\nabla}$ as we derived for single layer graphene and

$$T(\vec{r}) = w\sum_j e^{-i\vec{q}_j\cdot\vec{r}}\, T_j$$

where $\vec{q_1} = k_\theta(0,-1)$, $\vec{q_2} = k_\theta(\sqrt{3},1)/2$, $\vec{q_3} = k_\theta(-\sqrt{3},1)/2$ where $k_\theta = 2k_D \sin\left(\frac{\theta}{2}\right)$ these are the hopping direction and k_D is the dirac momentum (which is the magnitude of the difference between $\vec{K}$ and $\vec{K_\theta}$. Next,

$$T_1 = \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix} \quad T_2 = \begin{pmatrix} e^{-i\phi} & 1 \\ e^{i\phi} & e^{-i\phi} \end{pmatrix} \quad T_3 = \begin{pmatrix} e^{i\phi} & 1 \\ e^{-i\phi} & e^{i\phi} \end{pmatrix}$$

where $\phi = \frac{2\pi}{3}$ $T_{i\alpha\beta}$ describes the hopping from the α sublattice of layer 1 to β sub latttice of layer 2 in the $\vec{q_i}$ hopping direction.

3. Twisted Bilayer in a magnetic field

When an electron moves in the presence of a magnetic field, the wavefunction picks up a phase of $e^{-iq\int_\gamma \vec{A}\cdot \mathrm{d}\vec{r}}$ where $\vec{A}$ is the vector potential. To simulate this effect (cf. Aharonov-Bohm) in the presence of a magnetic field, we replace the hopping energies by doing a Peierls substitution, that is, replace γ_i by

$$\gamma_i e^{-\frac{ie}{\hbar}\int_{\mathbf{R}}^{\mathbf{R}'} \mathbf{A}\cdot d\mathbf{r}}$$

In the presence of a constant perpendicular magnetic field, we can take $\mathbf{A} = (-By, 0, 0)$.
Doing a similar calculation as done for single-layer graphene, we obtain a continuum model with Hamiltonian in the basis $|Ln\alpha y\rangle$ (L layer, n Landau level, α sublattice and y guiding centre). This basis can be thought of as $|L\alpha\rangle \otimes |ny\rangle$ where the first component defines a 4-component dirac spinor is the continuum model.

$$\mathcal{H} = h\left(\frac{\theta}{2}\right) + T + \text{h.c.}$$

where

$$h(\theta) = -\omega_c \sum_{Lny} e^{-i\theta}\sqrt{n+1}|Ln+1Ay\rangle\langle LnBy|$$

$$T = w \sum_{nmy\alpha\beta} T^{(0)}_{\alpha\beta mn}|2n\alpha y\rangle\langle 1m\beta y| + T^{(R)}_{\alpha\beta mn}|2n\alpha y+\Delta\rangle\langle 1m\beta y| + T^{(L)}_{\alpha\beta mn}|2n\alpha y-\Delta\rangle\langle 1m\beta y|$$

where $w \approx 110$meV is the interlayer hopping amplitude, $\Delta = \frac{\sqrt{3}}{2} k_\theta l^2$, $l = \sqrt{\frac{\Phi_0}{2\pi B}}$.

$$T^{(0)}_{mn\alpha\beta} = T_{1\alpha\beta} F_{mn}\left(\frac{\vec{q}_1 l}{\sqrt{2}}\right) e^{-ik_\theta y}$$
$$T^{(R)}_{mn\alpha\beta} = T_{2\alpha\beta} F_{mn}\left(\frac{\vec{q}_2 l}{\sqrt{2}}\right) e^{-\frac{i}{4}k_\theta(2y-\Delta)}$$
$$T^{(L)}_{mn\alpha\beta} = T_{3\alpha\beta} F_{mn}\left(\frac{\vec{q}_3 l}{\sqrt{2}}\right) e^{-\frac{i}{4}k_\theta(2y+\Delta)}$$

where the T_i and q_i are defined above and

$$F_{nm}(z_x, z_y) = \sqrt{\frac{m!}{n!}} (-z_x + i z_y)^{n-m} e^{-\frac{z_x^2+z_y^2}{2}} \mathcal{L}_m^{n-m}\left(z_x^2 + z_y^2\right)$$

from $n \geq m$. For $n < m$ define $F_{nm}(z) = F_{mn}(-z)^*$. Here $\mathcal{L}$ are the associated Laguerre polynomials.

4. Hoffstatder Butterfly

Moiré Patterns occur when there are two overlapping periodic layers with a relative shift between them (translational or rotational). When the two layers are superimposed, at specific values of the shift, a pattern with longer period emerges. The magneto-electronic spectra of the twisted-bilayer graphene also demonstrates such a Moiré pattern.
For small twist angles this spectrum has a fractal butterfly-like structure. The fractal Hoffstatder spectrum occurs when there is incommensurate length scales (a and l) involved in the graphene. Generally magneto-Bloch (periodic) hamiltonians are give eigenvalues only when the flux Φ through a unit cell is a rational multiple of the magnetic flux quantum Φ_0.

$$\alpha = \frac{\Phi_0}{\Phi} = \frac{p}{q} \propto \frac{\theta^2}{B}$$

We took the Langau-level hamiltonian and numerically diagonalised it at $\alpha = p/q$ (q=75) where p is integer and with $n_0 = 30$ landau levels. The dimension of the Hamiltonian becomes $4n_0 q$ as there are two layers and two sublattices.

Literature and sources

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5. Figures

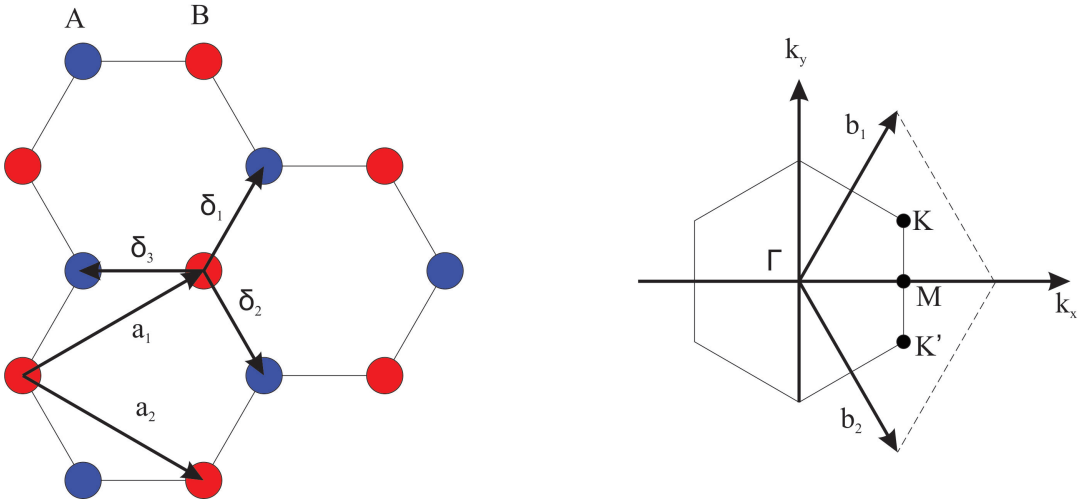

Figure 1. Honeycomb lattice and its Brillouin zone. Lattice structure of graphene, made out of two interpenetrating triangular lattices A and B, a_1 and a_2 are the lattice unit vectors, and δ_i, i= 1, 2, 3 are the nearest-neighbor vectors, the right diagram represents the corresponding Brillouin zone. The Dirac cones are located at the K and K' points.

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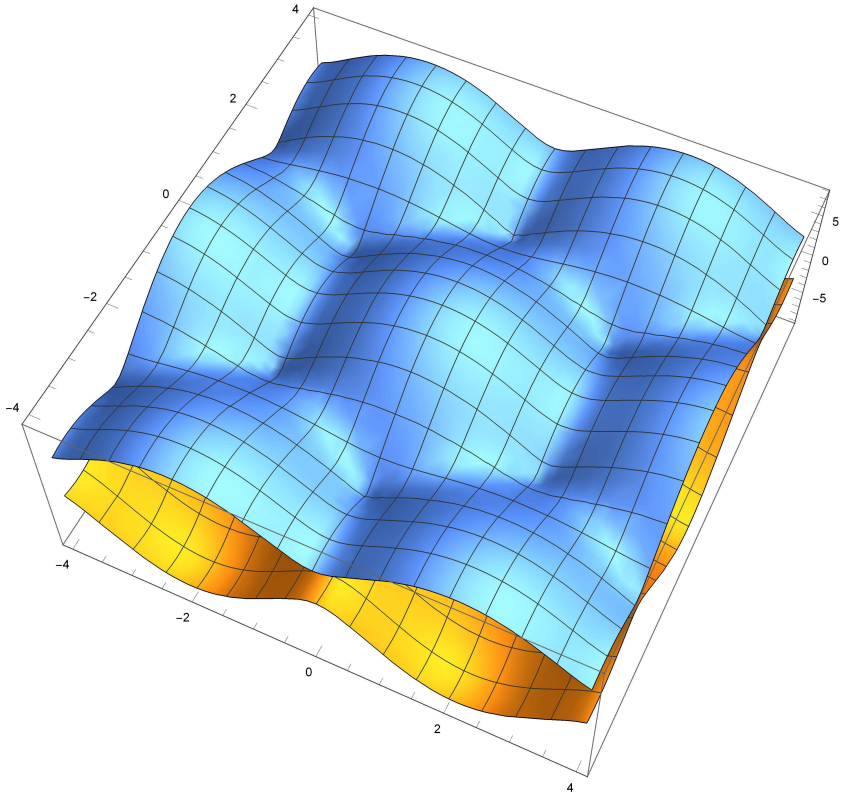

FIGURE 2. Electron dispersion in honeycomb lattice

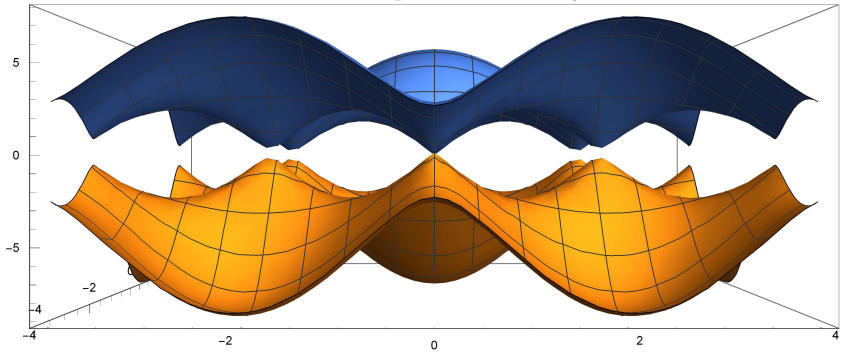

FIGURE 3. energy spectrum in units of t for finite values of t and t', with $t = 2.7eV$ and $t' = 0.2t$. Image highlights the energy bands close to one of the Dirac points.

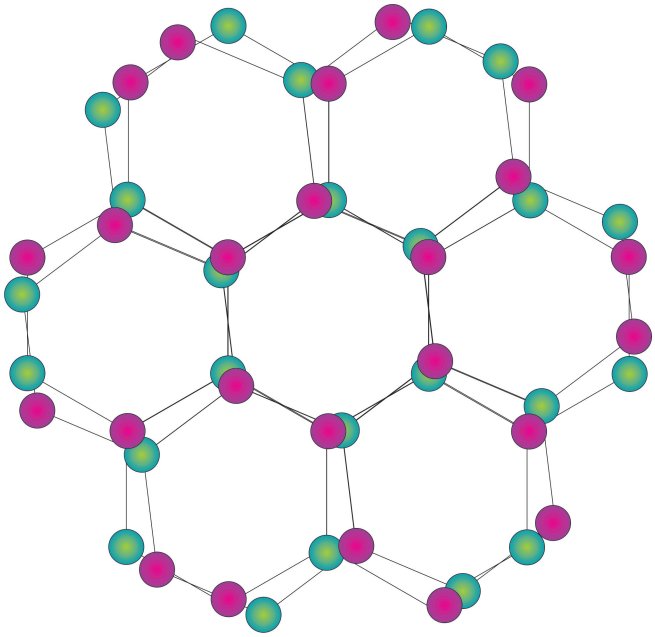

FIGURE 4. AB bilayer graphene stacks, twisted by a small angle

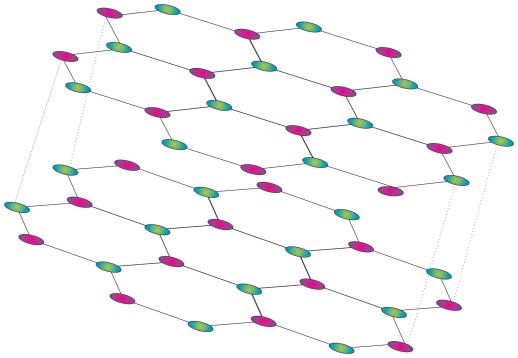

FIGURE 5. Crstal structure of AB stacked bilayer graphene, twisted by a small angle

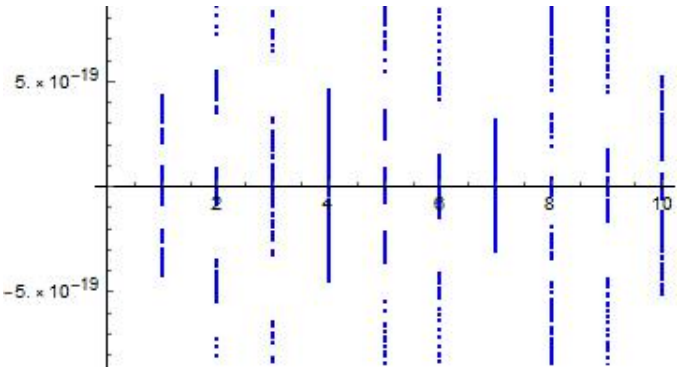

FIGURE 6. 10 landau levels for 10 rational values

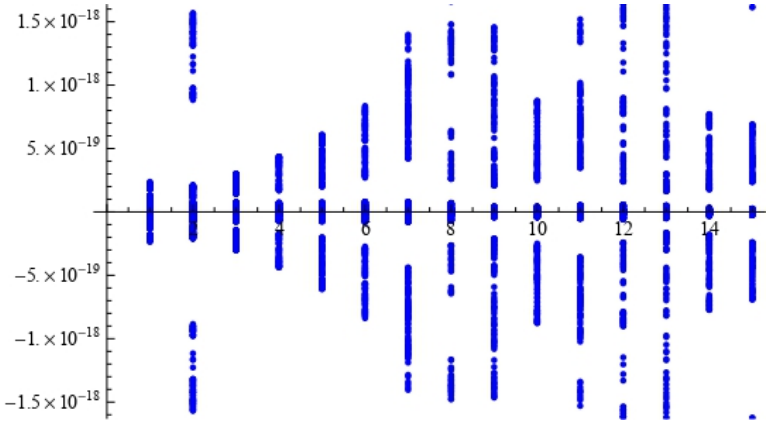

FIGURE 7. 15 landau levels for 15 rational vaues each