Twisted Bilayer Graphene

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Twisted Bilayer Graphene
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- Tight-Binding Model

- The Hofstadter Butterfly describes spectral properties of non-interacting electron in a magnetic field. It arises in many situations
- It was discovered in 1976 by Douglas Hofstadter
- The diagram shows fractal structure
- It starts out with Landau levels and with increasing field, these levels split due to the periodic potential
- The band gaps in the butterfly are described by the equation

$$\frac{n}{n_0} = t\frac{\Phi}{\Phi_0} + s$$

  where t, s are integers. This comes from the filling up of Landau levels

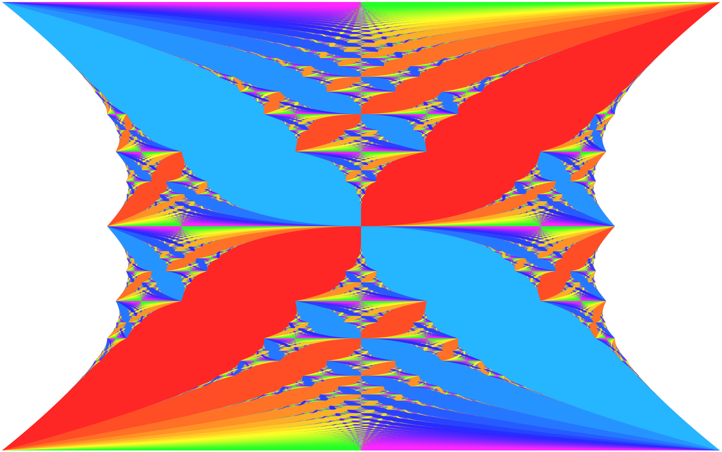
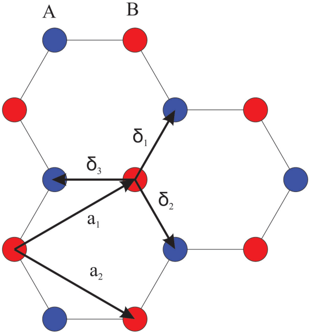


Figure: Hofstader 1976

Single-Layer Graphene

Graphene Structure (Real and Momentum space)



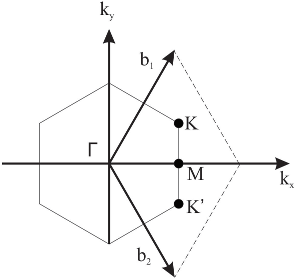


Figure: Honeycomb lattice and its Brillouin zone. Lattice structure of graphene, made out of two interpenetrating triangular lattices A and B, a_1 and a_2 are the lattice unit vectors, and δ_i, i= 1, 2, 3 are the nearest-neighbor vectors, the right diagram represents the corresponding Brillouin zone.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

In this kind of model, we assume that each electron is bound to a lattice site and can only jump between lattice sites.

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

$$\{a_{\sigma,i}, a^{\dagger}_{\sigma',i'}\} = \{b_{\sigma,i}, b^{\dagger}_{\sigma',i'}\} = \delta_{ii'} \delta_{\sigma\sigma'}$$

$$\{a_{i,\sigma}, b_{i',\sigma'}\} = 0$$

The creation and annihilation operators anticommute as the electrons are fermions

Rewriting the above Hamiltonian in Fourier modes, we obtain the following dispersion relation:

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

$$g(\vec{k}) = \sum_{\delta} e^{i\vec{k}\cdots\delta} = -t\left[e^{-ik_x a} + 2e^{ik_x a/2}\cos\frac{k_y a\sqrt{3}}{2}\right]$$

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

Taylor expanding around the Dirac points,

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

Energy Spectrum

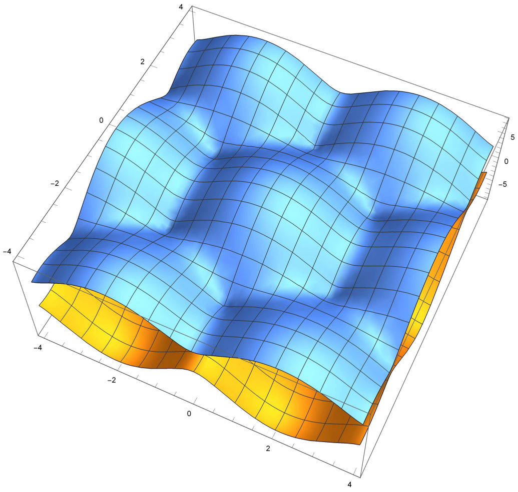


Figure: Electron dispersion in honeycomb lattice

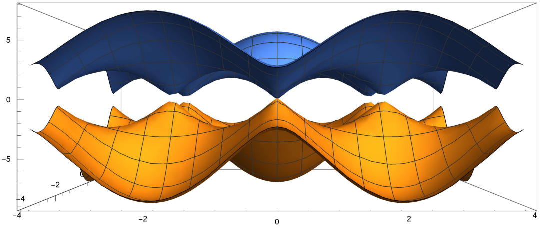


Figure: Energy spectrum in units of t for finite values of t and t', with $t = 2.7eV$ and $t' = 0.2t$. Image highlights the energy bands close to one of the Dirac points.

Expanding around this dirac point and putting $t' = 0$ we get

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

. Putting this into the Hamiltonian, we get

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

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

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

Twisted Bilayer Graphene

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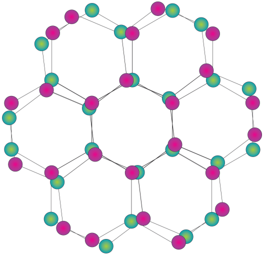
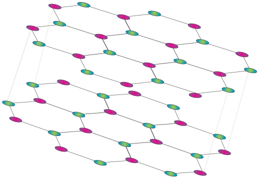


Figure: AB bilayer graphene stacks, twisted by a small angle



We can write a tight-binding model for twisted bilayer graphene by including all the relavant hopping terms between all possible sublattices in both layers and including only nearest neighbour interactions

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

By doing a similar calculation as done in graphene, we can derive the continuum model for tBLG. The intralayer part is exactly the same as in graphene, just rotated.

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

where and

$$h(\theta) = i v_F \vec{\sigma}\left(\theta\right) \cdot \vec{\nabla}$$

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

Twisted Bilayer Graphene in a megnetic Field

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

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

- In the presence of a constant perpendicular magnetic field, we can take $\mathbf{A} = (-By, 0, 0)$.

Landau Level Description

$WhenwecouplethecontinuummodeloftBLGtoamagneticfield, thestat$

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

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

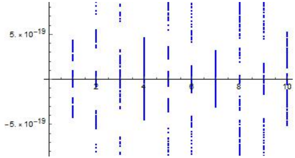


Figure: 10 landau levels for 10 rational values

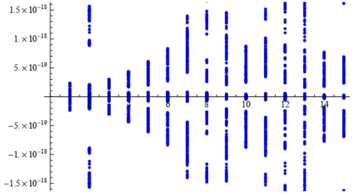


Figure: 15 landau levels for 15 rational vaues each