24/09/19

Lectures on 2D materials

IV Twisted bilayer graphene

Outline

A] Introduction

B] k.p approach

C] Flat bands

D] Interactions

A] Introduction

(see slides)

Overlaying two honeycomb lattices - two graphene monolayers - with a relative twist results in a new pattern (called Moiré) with a long-wavelength periodicity on top of the original hexagonal lattice.

B] k.p approach

In the absence of tunneling between layers, we have two Dirac cones (one for each layer) in the valley K that are slightly shifted by the small twist angle θ.

Dirac cones

K_1 bottom layer

$K_2 = R_\theta K_1$ top layer

R_θ is the rotation around the z-axis (θ is small)

<u>No interlayer hopping</u>:

$$H = \begin{pmatrix} \hbar v_F \vec{k}\cdot\vec{\sigma} & 0 \\ 0 & \hbar v_F \vec{k}\cdot\vec{\sigma} \end{pmatrix}$$

bottom layer quasimomentum is $\vec{K}_1 + \vec{k}$

top layer quasimomentum is $R_\theta \vec{K}_1 + \vec{k}$

and the Bloch wavefunctions are

$$\underset{\substack{\downarrow \\ \eta = A, B}}{\psi_\eta^{\overset{\text{top, bottom}}{a}}}(k, r) = \sum_m e^{i(\vec{K}_a + \vec{k})\cdot(\vec{R}_m^a + \vec{t}_\eta^a)} \underbrace{\varphi_\pi}_{\pi\text{- orbital of graphene } (p_z)} \left[\vec{r} - (\vec{R}_m^a + \vec{t}_\eta^a)\right]$$

$\vec{R}_m^a + \vec{t}_\eta^a$ describes the different positions of the hexagonal lattice a.

Notation: $\varphi_\pi\left[r-(R_n^a+t_\eta^a)\right]=\langle r|R_n^a+t_\eta^a\rangle$

We now include interlayer hoppings with the matrix elements

$$\langle r|H_T|r'\rangle = t(r-r') = \sum_{\vec{p}} t_p \, e^{i\vec{p}\cdot(\vec{r}-\vec{r}')}$$

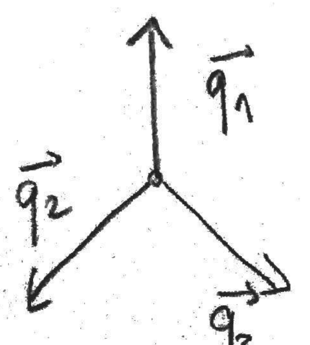
A tedious computation leads to

$$\langle \psi_\eta^d(k)|H_T|\psi_{\eta'}^t(k')\rangle = t_K \sum_{j=1}^{3} (T_j)_{\eta\eta'} \, \delta_{k,k'+q_j}$$

$$T_1 = \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix} \quad T_2 = \begin{pmatrix} 1 & \omega^* \\ \omega & 1 \end{pmatrix} \quad T_3 = T_2^*$$

where $\omega = e^{2i\pi/3}$

$$\vec{q_1} = \vec{K_2} - \vec{K_1} = R_\theta \vec{K_1} - \vec{K_1}, \quad \vec{q_2} = C_3 \vec{q_1}, \quad \vec{q_3} = C_3 \vec{q_2}$$



$$|\vec{q_1}| = 2\sin\frac{\theta}{2}|K| \simeq \theta |K| = \frac{4\pi}{3\sqrt{3}a}\theta$$

Physically, the quasimomentum $\vec{k}$ is (almost) conserved when changing layers. But the origin goes from $\vec{K}_1$ to $\vec{K}_2$, therefore $\vec{k}$ is shifted by $\vec{K}_2 - \vec{K}_1$ when the electron is transferred from top to bottom, and also $C_3(\vec{K}_2 - \vec{K}_1)$, $C_3^2(\vec{K}_2 - \vec{K}_1)$.

With the rescaling $q_1 \to |K|\theta q_1$ (such that $|q_1| = 1$), the Hamiltonian is

$$\boxed{\frac{H}{\hbar v_F |K|} = \vec{k}.\vec{\sigma}\, \delta_{k,k'} + \alpha \sum_j T_j\, \delta_{k,k'+q_j}} \quad (1)$$

$$\alpha = \frac{t_K}{\hbar v_F |K| \theta} \sim \frac{1}{\theta}$$

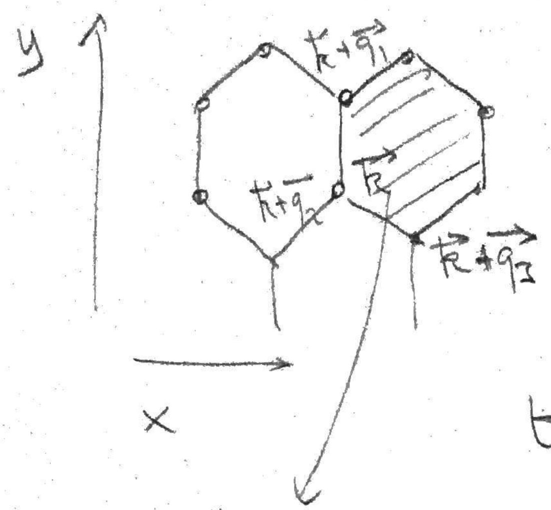
α is the dimensionless layer coupling

$\alpha \to \infty$ for $\theta \to 0$

strong coupling

Moiré Brillouin zone:

$\vec{k}$ is coupled to $\vec{k} + \vec{q}_{1,2,3}$



← these different quasimomenta are equivalent – or, equivalently, they form a single eigenstate

Moiré Brillouin zone (MBZ) generated by $\vec{q}_1, \vec{q}_2, \vec{q}_3 \sim \theta$

- MBZ gets smaller with θ as the superlattice increases in size.
- Solution of Eq. (1) gives two bands at the Fermi energy almost flat when $\theta \simeq 1.05°$ (see slides)

C] Flat bands

Why flat bands?

Real space formulation of Eq. (1)

$$H = \begin{pmatrix} \hbar v_F \,\vec{k}\cdot\vec{\sigma} & t_K \sum_j T_j e^{-i\vec{q}_j\cdot\vec{r}} \\ t_K \sum_j T_j e^{i\vec{q}_j\cdot\vec{r}} & \hbar v_F \,\vec{k}\cdot\vec{\sigma} \end{pmatrix}$$

where $\vec{k} = \frac{1}{i}\begin{pmatrix}\partial_x \\ \partial_y\end{pmatrix}$

$$H\,\psi(x,y) = \varepsilon\,\psi(x,y)$$

→ has the periodicity of the large superlattice.

Symmetry $C_{2z}T$ $\quad \vec{q}\to\vec{q} \quad \vec{r}\to-\vec{r}$

note that $\sigma_x T_j^* \sigma_x$ so $\sigma_x H_{-r}^* \sigma_x = H_r$

Expansion in position $\vec{r}$

$$e^{i\vec{q_j}\cdot\vec{r}} \simeq 1 + i\vec{q_j}\cdot\vec{r} + \dots$$

$$t_K \sum_j T_j e^{i\vec{q_j}\cdot\vec{r}} \simeq 3t_K + \frac{3}{2} t_K |q_1| (y\sigma_x - x\sigma_y)$$

$$H = \hbar v_F \left(\vec{k} - \frac{e}{\hbar}\vec{A}\,\tau_y\right)\cdot\vec{\sigma} + 3t_K\tau_x$$

τ_x, τ_y act in the top/down space

$$\vec{A} = \frac{3}{2} t_K |K| \theta \frac{1}{e v_F} \begin{pmatrix} y \\ -x \end{pmatrix} = \frac{2\pi t_K}{e v_F L_s} \begin{pmatrix} y \\ -x \end{pmatrix}$$

size of superlattice

rotation $\tau_y \to \tau_z$

$$H = \hbar v_F \begin{pmatrix} (\vec{k} - \frac{e}{\hbar}\vec{A})\cdot\vec{\sigma} & 0 \\ 0 & (\vec{k} + \frac{e}{\hbar}\vec{A})\,\vec{\sigma} \end{pmatrix} + 3t_K\tau_x$$

LL in a magnetic field

$$\vec{B} = \mp \frac{4\pi t_K}{e v_F L_s} \vec{u_z}$$

$\simeq 120T$ at $\theta \simeq 1°$

$$\hbar v_F \left(\vec{k} - \frac{e}{\hbar} \vec{A} \right) \cdot \vec{\sigma}$$

$$\hookrightarrow E_\pm = \pm \hbar \omega_c \sqrt{N} \quad N \in \mathbb{N}$$

$$\hbar \omega_c = \sqrt{\frac{8\pi \hbar v_F t_K}{L_S}} \qquad l_B = \sqrt{\frac{L_S \hbar v_F}{4\pi t_K}}$$

- zero-energy modes $N=0$ $\quad \underset{\text{top, bottom}}{2} \times \underset{\text{valley}}{2} \times \underset{\text{spin}}{2}$

- wave function

$$\left[\left(-i\partial_x - \frac{y}{2l_B^2} \right) \sigma_x + \left(-i\partial_y + \frac{x}{2l_B^2} \right) \sigma_y \right] \begin{pmatrix} 0 \\ e^{-r^2/4l_B^2} \end{pmatrix} = 0$$

$$\begin{cases} \psi_0(r) = e^{-r^2/4l_B^2} \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix} \\ \psi_0'(r) = e^{-r^2/4l_B^2} \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \end{pmatrix} \end{cases}$$

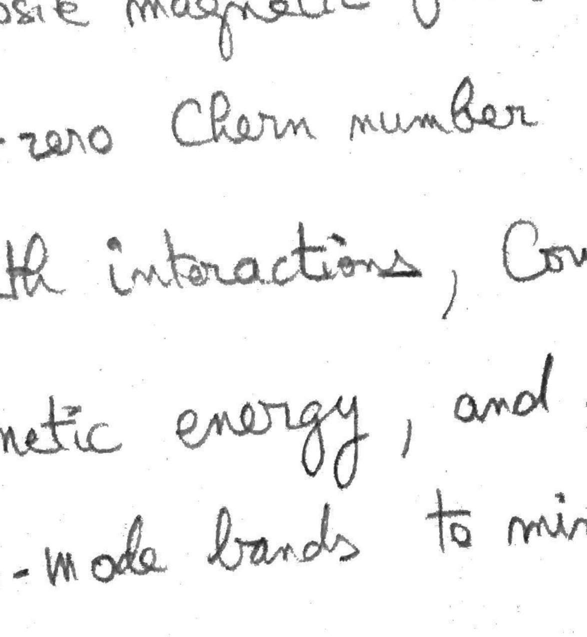
the zero-energy modes have a sublattice polarization, they are not coupled to first-order by $3 t_K \tau_x$

$\longrightarrow$ explains the flatness of bands

D] Interactions

The two zero-modes - corresponding to opposite magnetic fields - have quantized and non-zero Chern number $C = \pm 1$

With interactions, Coulomb energy dominates kinetic energy, and splits the eight zero-mode bands to minimize exchange energy.



at $\nu = 3$, the unoccupied band has a Chern number (and a spin polarizat° $\}$ so one expects

(A) anomalous Hall effect - chiral edge states

(B) ferromagnetism