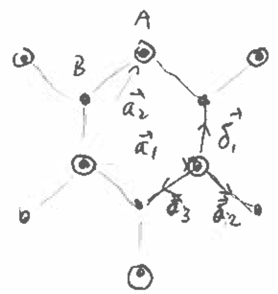
LECTURE 6

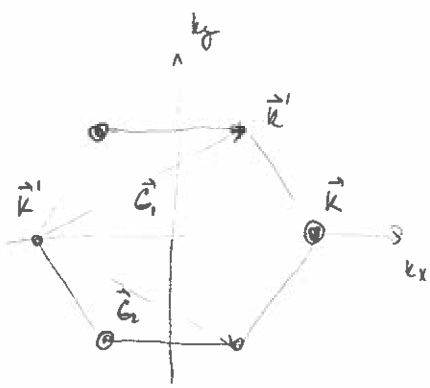
GRAPHENE



$$\vec{\delta}_1 = a(0,1)$$
$$\vec{\delta}_{2,3} = a\left(\pm\frac{\sqrt{3}}{2}, -\frac{1}{2}\right)$$
} n.n. vectors

Primitive vectors of the Bravais lattice

$$\vec{a}_1 = \vec{\delta}_2 - \vec{\delta}_3 = a(\sqrt{3}, 0)$$
$$\vec{a}_2 = \vec{\delta}_1 - \vec{\delta}_3 = a\left(\frac{\sqrt{3}}{2}, \frac{3}{2}\right)$$



$$\vec{K} = \frac{4\pi}{a}\left(\frac{1}{3\sqrt{3}}, 0\right) \qquad \vec{K}' = -\vec{K}$$

$\vec{G}_1, \vec{G}_2$ - Rec. lattice vectors

C: $Z = 6$ $\quad 1s^2 2s^2 2p^2$ $\quad$ 2s2p (8 states) $\Big\{$ σ^* ; π : p_z ; σ : s, p_x, p_y

N.N. Tight-binding model (neglect spin) π band

$$H_0 = -t\sum_{\langle ij\rangle} c_i^\dagger c_j = \sum_{\vec{k}} \mathcal{H}_0^{\alpha\beta}(\vec{k})\, c_{k\alpha}^\dagger c_{k\beta} \qquad \alpha,\beta = A, B$$

$$\mathcal{H}_0(\vec{k}) = \vec{d}(\vec{k})\cdot\vec{\sigma}$$

$$d_x(k) = -t\sum_{p=1}^{3}\cos(\vec{k}\cdot\vec{\delta}_p)$$
$$d_y(k) = -t\sum_{p=1}^{3}\sin(\vec{k}\cdot\vec{\delta}_p)$$
$$d_z(k) = 0$$

$$E_0(\vec{k}) = \pm|\vec{d}(\vec{k})| = \pm\sqrt{d_x^2(\vec{k}) + d_y^2(\vec{k})}$$

$E_0(\vec{k})$ has point zeros at $\vec{k} = \pm\vec{K}$ (two bands touch)

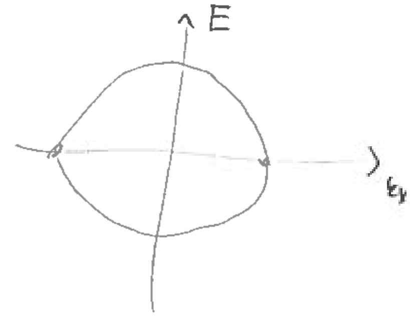
$\rightarrow$ semimetal

lower band filled, upper band empty.

$$E_0(k_x,0) = \pm t\sqrt{\left[1+2\cos\left(k_x a \tfrac{\sqrt{3}}{2}\right)\right]^2} = \pm t\left|1+2\cos\left(k_x a \tfrac{\sqrt{3}}{2}\right)\right|$$

$$\cos\varphi = -\frac{1}{2} \qquad \varphi = \pm\frac{2\pi}{3}$$

$$k_x a \frac{\sqrt{3}}{2} = \pm\frac{2\pi}{3} \quad \Rightarrow \quad k_x = \frac{4\pi}{3\sqrt{3}a}$$



Low-E Hamiltonian

- expand $\mathcal{H}_0(\vec{k})$ around $\vec{K} = \left(\frac{4\pi}{3\sqrt{3}a}, 0\right)$ (take $a=1$)

$$\vec{k} = \vec{K} + \vec{q}$$

$$d_x(\vec{k}) = -t\left[\cos(k_y) + \cos\left(\tfrac{\sqrt{3}}{2}k_x - \tfrac{1}{2}k_y\right) + \cos\left(-\tfrac{\sqrt{3}}{2}k_x - \tfrac{1}{2}k_y\right)\right]$$

$$= -t\left[\cos q_y + \cos\left(\tfrac{2\pi}{3} + \tfrac{\sqrt{3}}{2}q_x - \tfrac{1}{2}q_y\right) + \cos\left(-\tfrac{2\pi}{3} - \tfrac{\sqrt{3}}{2}q_x - \tfrac{1}{2}q_y\right.$$

$$\simeq -t\left[1 - \tfrac{1}{2} + \tfrac{\sqrt{3}}{2}\left(\tfrac{\sqrt{3}}{2}q_x - \tfrac{1}{2}q_y\right) - \tfrac{\sqrt{3}}{2}\left(-\tfrac{\sqrt{3}}{2}q_x - \tfrac{1}{2}q_y\right)\right]$$

$$= -t\,\frac{3}{2}q_x$$

$$d_y(\vec{k}) \simeq -t\,\frac{3}{2}q_y$$

$$\mathcal{H}^{K}_{eff}(\vec{q}) = v_F\left(q_x\sigma_x + q_y\sigma_y\right) \quad \Big| \; v_F = -\frac{3}{2}ta$$

$$\mathcal{H}^{-K}_{eff}(\vec{q}) = v_F\left(-q_x\sigma_x + q_y\sigma_y\right)$$

Two massless Dirac Hamiltonians.

Combine them into 4x4 structure

$$\boxed{\begin{aligned}\mathcal{H}_{eff}(\vec{q}) &= v_F(\sigma_x \tau_z q_x + \sigma_y q_y) \\ &\to -i\hbar v_F(\sigma_x \tau_z \partial_x + \sigma_y \partial_y)\end{aligned}}$$

$\vec{\sigma}$, $\vec{\tau}$ are Pauli matrices in sublattice and "valley" spaces, respectively.

$$\boxed{E(\vec{q}) = v_F|\vec{q}|}$$

<u>The point zeros of $E(\vec{q})$ are protected by symmetries.</u>

SYMMETRIES

① Time reversal $\mathcal{T}$ (spinless particles)

$\mathcal{T}$: $t \to -t$: $\hat{x} \to \hat{x}$, $\hat{p} \to -\hat{p}$

$$\left.\begin{aligned} \mathcal{T}: &\quad \theta \hat{x} \theta^{-1} = \hat{x} \\ \mathcal{T}: &\quad \theta \hat{p} \theta^{-1} = -\hat{p} \end{aligned}\right\} \quad \mathcal{T}: \theta [\hat{x}, \hat{p}] \theta^{-1} = \theta i\hbar \theta^{-1}$$

$$= -[\hat{x}, \hat{p}] = -i\hbar$$

$$\Rightarrow \quad \theta i \theta^{-1} = -i$$

$\theta = K$ complex conjugation
$\theta^{-1} = K$

$\boxed{\theta \text{ is an antilinear, antiunitary operator}}$

- Antilinear: $U|\lambda\psi\rangle = \lambda^* U|\psi\rangle$
- Antiunitary $\langle U\psi_1 | U\psi_2\rangle = \langle \psi_1|\psi_2\rangle^* = \langle \psi_2|\psi_1\rangle$

- Time reversal in crystals (spinless particles)

$$H = \sum_k c_k^+ \mathcal{H}(k)\, c_k \qquad \left(\text{Bloch ham.}, \quad c_k = \begin{pmatrix} c_{k1} \\ c_{k2} \\ \vdots \\ c_{kN} \end{pmatrix}\right)$$

$\boxed{\theta c_j \theta = c_j}$

$$\theta \frac{1}{\sqrt{N}} \sum_k e^{i\vec{k}\cdot\vec{r}_j} c_k \, \theta =$$

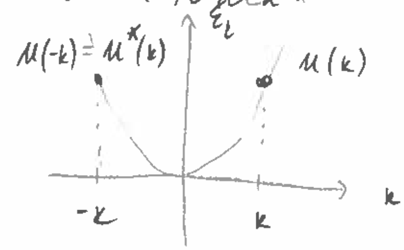
$$\left.\begin{aligned} &= \frac{1}{\sqrt{N}} \sum_k e^{-i\vec{k}\cdot\vec{r}_j}\, \theta c_k \theta \\ &= \frac{1}{\sqrt{N}} \sum_k e^{i\vec{k}\cdot\vec{r}_j}\, c_{-k} \end{aligned}\right\} \quad \text{satisfied if} \quad \boxed{\theta c_k \theta = c_{-k}}$$

$$\theta c_k^+ \theta = c_{-k}^+$$

Hamiltonian: $\quad \theta H \theta^{-1} = H$

$$\Rightarrow \quad \sum_k c^\dagger_{-k}\, \theta \mathcal{H}(\vec{k}) \theta^{-1} c_{-k} = \sum_k c^\dagger_k \mathcal{H}(\vec{k})\, c_k$$

$$\boxed{\mathcal{H}^*(\vec{k}) = \mathcal{H}(-\vec{k})}$$ $\leftarrow$ T-invariance condition for the Bloch Hamiltonian



Eigenstates:

$$\overset{\theta}{} \mathcal{H}(k)\, u(k) = \varepsilon_k\, u(k)$$

$$\mathcal{H}(-k)\, u^*(k) = \varepsilon_k\, u^*(k) \quad \rightarrow \quad \mathcal{H}(k)\, u^*(-k) = \varepsilon_{-k}\, u^*(-k)$$

- For a T-invariant Hamiltonian for each eigenstate $u(k)$ at energy ε_k there is an eigenstate $u(-k) = u^*(k)$ at the same energy.

- Vanishing Hall conductivity for T-invariant systems.

Berry curvature:

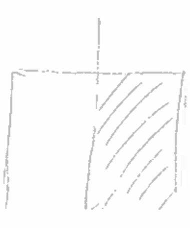
$$\mathcal{F}_{ij}(-\vec{k}) = -i\left\{\langle \partial_i u(-k) | \partial_j u(-k)\rangle - (i \leftrightarrow j)\right\}$$

$$= -i\left\{\langle \partial_i u^*(k) | \partial_j u^*(k)\rangle - (i \leftrightarrow j)\right\}$$

$$= -i\left\{\langle \partial_j u(k) | \partial_i u(k)\rangle - (i \leftrightarrow j)\right\}$$

$$= -\mathcal{F}_{ij}(\vec{k})$$

$$1 = \frac{1}{2\pi}\int_{BZ} \mathcal{F}_{ij}(\vec{k})\, d^2k = 0$$ $\leftarrow$ Chern # vanishes in a T-invariant system



② Inversion

$\mathcal{P}: \ \vec{r} \to -\vec{r}, \quad \vec{p} \to -\vec{p}$

Unitary symmetry: $\mathcal{P}\,[\vec{r}, \vec{p}]\,\mathcal{P} = [\vec{r}, \vec{p}]$ no complex conjugation!

In graphene $\mathcal{P}$ interchanges A and B sublattices

$$\mathcal{P}: \quad c_{\vec{r}} \to \sigma_x c_{-\vec{r}}$$

$$\mathcal{P}: \quad c_k \to \sigma_x c_{-k}$$

$$\mathcal{P}: \quad \sigma_x \mathcal{H}(\vec{k}) \sigma_x \to \mathcal{H}(-\vec{k})$$

Graphene:

$$\mathcal{H}(\vec{k}) = \vec{d}(\vec{k}) \cdot \vec{\sigma}$$

Combination of $\mathcal{T}\mathcal{P}$: $\boxed{\sigma_x \mathcal{H}^*(\vec{k}) \sigma_x = \mathcal{H}(\vec{k})}$

σ_1, σ_3 are real:

$$d_1(\vec{k}) = d_1(\vec{k})$$

$$d_2(\vec{k}) = +d_2(\vec{k})$$

$$\boxed{d_3(\vec{k}) = -d_3(\vec{k})} \Rightarrow d_3(\vec{k}) = 0$$

As long a $\mathcal{T}$ an $\mathcal{P}$ are maintained, $d_3(\vec{k}) = 0$, and graphene has gapless spectrum near $\vec{k} = \pm\vec{K}$.

C_3 rotational symmetry further restricts the Dirac nodes to be EXACTLY at $\pm\vec{K}$.