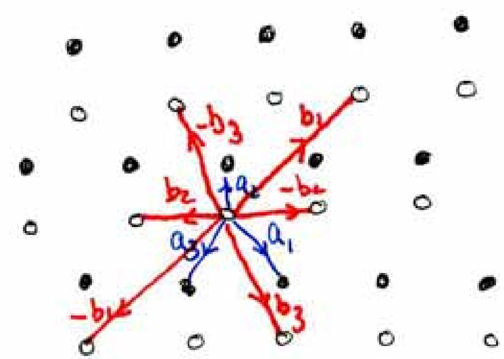
Lecture 14: Graphene, Parity Anomaly, (→ Spin Quantum Hall Effect)

14.1 Graphene Band Structure (including Haldane terms)

Haldane PRL 61 2015 (1988)

14.1.1 Geometry



Honeycomb lattice (bipartite)

○ B

● A

$\vec{a}_i$: nearest neighbor hops

$\pm\vec{b}_i$: NNN hops

* $\vec{b}_i$ define lattice translation symmetries ($\vec{a}$s do not)

$$\vec{b}_1 = \vec{a}_2 - \vec{a}_3$$

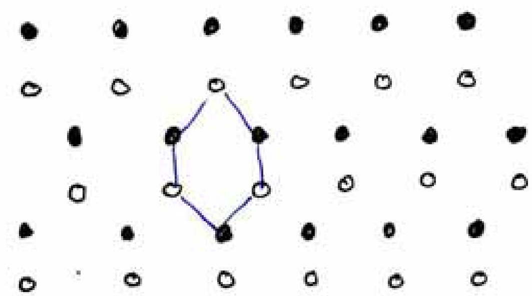
$$\vec{b}_2 = \vec{a}_3 - \vec{a}_1$$

$$\vec{b}_3 = \vec{a}_1 - \vec{a}_2$$

$$\vec{a}_1 + \vec{a}_2 + \vec{a}_3 = 0$$

C_{6v} symmetry

14.1.2 Hamiltonian, with commensurate flux



 = unit cell

~~6 vertices / plaquette / 3 cells~~

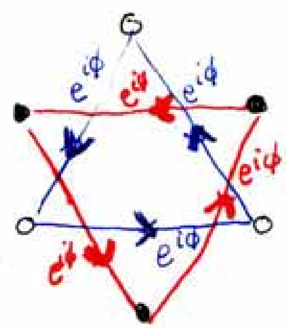
6 vertices / cell, but each vertex ~~and~~ intersects 3 cells

$\Rightarrow 2\ (A+B)$ ✓

t_1: nearest neighbor hopping

t_2: next-nearest neighbor hopping

We associate phases with the t_2, but not with the t_1



On A sublattice, $+b_i$ get $e^{i\phi}$

on B sublattice, $-b_i$ get $e^{i\phi}$

M: Symmetry-breaking energy $+M$ on A sites
$-M$ on B sites

This phase-assignment is appropriate if each cell sees the same (symmetric) flux distribution with zero total flux

It could be realized by aligned magnetic dipoles - pointing out of plane, of course - at centers of each plaquette.

[note: for magnetic, as opposed to electric, dipoles, the total flux vanishes! (Fermi correction)

]

Start from B point. Use spinor notation $\begin{pmatrix} \psi_A \\ \psi_B \end{pmatrix}$

nearest neighbor terms (multiplying $c_k^+ c_k$)

$$t_1 \left(e^{i\vec{k}\cdot\vec{a}_1} + e^{i\vec{k}\cdot\vec{a}_2} + e^{i\vec{k}\cdot\vec{a}_3} \right) \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}$$

mates: $$t_1 \left(e^{-i\vec{k}\cdot\vec{a}_1} + e^{-i\vec{k}\cdot\vec{a}_2} + e^{-i\vec{k}\cdot\vec{a}_3} \right) \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}$$

next nearest neighbor terms (B)

$$t_2 \left(e^{i\vec{k}\cdot\vec{b}_1} e^{-i\phi} + e^{i\vec{k}\cdot\vec{b}_2} e^{-i\phi} + e^{i\vec{k}\cdot\vec{b}_3} e^{-i\phi} + e^{-i\vec{k}\cdot\vec{b}_1} e^{+i\phi} + e^{-i\vec{k}\cdot\vec{b}_2} e^{+i\phi} + e^{-i\vec{k}\cdot\vec{b}_3} e^{+i\phi} \right)$$

$$H(\vec{k}) = t_1 \left(\sum_i \cos k a_i \, \sigma_1 - \sum_i \sin k a_i \, \sigma_2 \right)$$

$$+ 2 t_2 \cos\phi \sum_i \cos k b_i \, \mathbb{1} + \left(M - 2 t_2 \sin\phi \sum_i \sin k b_i \right) \sigma_3$$

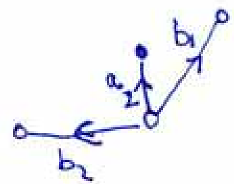
14.1.3 Brillouin zone

Translation basis

$$b_1 = \left(\frac{\sqrt{3}}{2}, \frac{3}{2}\right)$$

(where $a_2 = (0,1)$)

$$b_2 = (-\sqrt{3}, 0)$$



$$\left(b_3 = \left(\frac{\sqrt{3}}{2}, -\frac{3}{2}\right) \right)$$

90° rotations of b's; normalize

Dual lattice

$$k_1 = \frac{2\pi\,(0, \sqrt{3})}{3\sqrt{3}/2} \qquad k_2 = \frac{2\pi\,\left(\frac{3}{2}, -\frac{\sqrt{3}}{2}\right)}{3\sqrt{3}/2}$$

$$k_1 \cdot b_1 = 2\pi \qquad k_2 \cdot b_1 = 0$$

$$k_1 \cdot b_2 = 0 \qquad k_2 \cdot b_2 = 2\pi$$

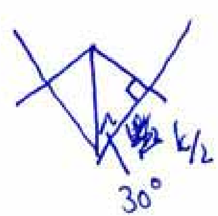
$$\left(k_3 \equiv -k_1 - k_2 = \frac{2\pi}{3\sqrt{3}/2}\left(-\frac{3}{2}, -\frac{\sqrt{3}}{2}\right) \right)$$

Wigner-Seitz construction: bisect translation vectors from $\vec{G}$ to make unit cell (Br. zone)

Here it will give us a hexagon with corners defined by

$$k_\alpha \cdot k_1 = k_\alpha \cdot k_2 = \frac{1}{2} k_1^2 \left(= \frac{1}{2} k_2^2\right)$$ and rotations thereof.

Alternatively, by calculation or geometry



$k_{\text{corners}} = \frac{k_1}{\sqrt{3}}$ through $30, 90, \underset{180-30}{\underset{\downarrow}{150}}, \underset{180+30}{\underset{\downarrow}{210}}, \underset{180+90}{\underset{\downarrow}{270}}, \underset{-30}{\underset{\downarrow}{330}}$ degrees

Corner 1: $\frac{2\pi}{\sqrt{3}}\,\frac{2}{3}\begin{pmatrix}\frac{\sqrt{3}}{2} & \frac{1}{2}\\ -\frac{1}{2} & \frac{\sqrt{3}}{2}\end{pmatrix}\begin{pmatrix}0\\1\end{pmatrix} = \frac{4\pi}{3\sqrt{3}}\begin{pmatrix}\frac{1}{2}\\ \frac{\sqrt{3}}{2}\end{pmatrix}$

Corner 2: $\frac{4\pi}{3\sqrt{3}}\begin{pmatrix}1\\0\end{pmatrix}$

Corner 3: $\frac{4\pi}{3\sqrt{3}}\begin{pmatrix}\frac{1}{2}\\ -\frac{\sqrt{3}}{2}\end{pmatrix}$

Corner 4: $\frac{4\pi}{3\sqrt{3}}\begin{pmatrix}-\frac{1}{2}\\ -\frac{\sqrt{3}}{2}\end{pmatrix}$

Corner 5: $\frac{4\pi}{3\sqrt{3}}\begin{pmatrix}-1\\0\end{pmatrix}$

Corner 6: $\frac{4\pi}{3\sqrt{3}}\begin{pmatrix}-\frac{1}{2}\\ +\frac{\sqrt{3}}{2}\end{pmatrix}$

$$k^{(1)}\cdot a_1 = \frac{4\pi}{3\sqrt{3}}\left(\frac{1}{2},\frac{\sqrt{3}}{2}\right)\left(\frac{\sqrt{3}}{2},-\frac{1}{2}\right) = 0$$

$$k^{(1)}\cdot a_2 = \frac{4\pi}{3\sqrt{3}}\left(\frac{1}{2},\frac{\sqrt{3}}{2}\right)\cdot\begin{pmatrix}0\\1\end{pmatrix} = \frac{2\pi}{3}$$

$$k^{(1)}_3\cdot a_3 = \frac{4\pi}{3\sqrt{3}}\left(\frac{1}{2},\frac{\sqrt{3}}{2}\right)\begin{pmatrix}-\sqrt{3}/2\\-1/2\end{pmatrix} = -\frac{2\pi}{3}$$

$$k_1\cdot b_1 = k_1(a_2-a_3) = \frac{4\pi}{3}$$

$\vdots$ other bs

$$k^{(2)}\cdot a_1 = \frac{4\pi}{3\sqrt{3}}(1,0)\cdot\begin{pmatrix}\sqrt{3}/2\\-1/2\end{pmatrix} = \frac{2\pi}{3}$$

$$k^{(2)}\cdot a_2 = \frac{4\pi}{3\sqrt{3}}(1,0)\begin{pmatrix}0\\1\end{pmatrix} = 0$$

$$k^{(2)}\cdot a_3 = -\frac{2\pi}{3}$$ ~~etc.~~

$$k^{(3)}\cdot a_1 = \frac{4\pi}{3\sqrt{3}}\left(\frac{1}{2},-\frac{\sqrt{3}}{2}\right)\begin{pmatrix}\frac{\sqrt{3}}{2}\\-\frac{1}{2}\end{pmatrix} = \frac{2\pi}{3}$$

$$k^{(3)}\cdot a_2 = \frac{4\pi}{3\sqrt{3}}\left(\frac{1}{2},-\frac{\sqrt{3}}{2}\right)\begin{pmatrix}0\\1\end{pmatrix} = -\frac{2\pi}{3}$$

$$k^{(3)}\cdot a_3 = 0$$

$$k^{(j+3)} = -k^{(j)}$$

$\Longrightarrow$

$$k^{(1)} \cdot b_1 = \frac{4\pi}{3} \approx -\frac{2\pi}{3}$$

$$k^{(1)} \cdot b_2 = -\frac{2\pi}{3}$$

$$k^{(1)} \cdot b_3 = -\frac{2\pi}{3}$$

$$k^{(2)} \cdot b_1 = \frac{2\pi}{3}$$

$$k^{(2)} \cdot b_2 = -\frac{4\pi}{3} \approx \frac{2\pi}{3}$$

$$k^{(4)} \cdot b_3 = \frac{2\pi}{3}$$

$$k^{(3)} \cdot b_1 = -\frac{2\pi}{3}$$

$$k^{(3)} \cdot b_2 = -\frac{2\pi}{3}$$

$$k^{(3)} \cdot b_3 = \frac{4\pi}{3} \approx -\frac{2\pi}{3}$$

etc.

$$\boxed{\begin{array}{l} k_1, k_3, k_5 \text{ identical} \\ \quad\quad = \\ -k_2, -k_4, -k_6 \end{array}}$$

$\nwarrow$ C_{3v} residual symmetry

14.1.4 The gap closes where the coefficients of all three σ_i vanish

$$\sum_i \cos ka_i = \sum_i \sin ka_i = 0$$

$$\left[M - 2t_2 \sin\phi \sum_i \sin kb_i = 0 \right]$$

$$ka_1 \equiv A \quad ka_2 \equiv B \Rightarrow ka_3 = -A-B$$

$$\sin A + \sin B = \sin A+B$$

$$2\sin\frac{A+B}{2}\cos\frac{A-B}{2} = 2\sin\frac{A+B}{2}\cos\frac{A+B}{2}$$

$$\Downarrow$$

$$\sin\frac{A+B}{2} = 0$$

$$\frac{A+B}{2} = 0 \text{ or } \pi$$

$$\cos\frac{A-B}{2} = -\frac{1}{2}$$

$$A = \pm\frac{2\pi}{3} = -B$$

or

$$\cos\frac{A+B}{2} = \cos\frac{A-B}{2}$$

$$\frac{A+B}{2} \equiv \pm\frac{A-B}{2} \quad (2\pi)$$

$$A \equiv 0 \text{ or } B \equiv 0 \quad (2\pi)$$

$$4\cos^2\frac{A}{2} = 1$$

$$A = \frac{2\pi}{3} \text{ or } \frac{4\pi}{3}$$

$$\cos A + \cos B + \cos(A+B) = 0$$

$$2\cos\frac{A+B}{2}\cos\frac{A-B}{2} + 2\cos^2\frac{A+B}{2} = 1$$

Upshot: Gap vanishes $(M = \phi_2 = 0)$ at corners, and only there! Deep reason: 2d rep. of C_{3v}

Parity-violating terms take $C_{3v} \to C_3$, and remove gap.

14.1.5 Expanding around these points, $k = k^0_\alpha + \delta k$, $\delta k \to \Pi$, we get

$$H = \underbrace{\tfrac{3}{2} t_1 |a_i|}_{\text{"}c\text{"}} \left(\Pi^1_\alpha \sigma_1 - \Pi^2_\alpha \sigma_2 \right) + \underbrace{m_\alpha \underbrace{\left(\tfrac{3}{2} t_1 |a_i|\right)^2}_{c^2}}_{M - 3\sqrt{3}\,\alpha\, t_2 \sin\phi} \sigma_3$$

$\alpha = \pm 1$
(2 corners)

[coeff. of $\Pi^1 \sigma_1$: $-\sum_i t_1 a^i_1 \sin k \cdot a_i$ (work at $k^{(2)}, k^{(5)}$)

$\Pi^1 \sigma_2$: $t_1 \sum_i a^i_1 \cos k \cdot a_i$

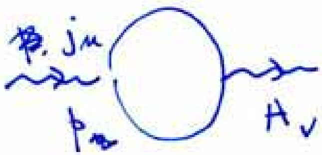
etc.]

This is the Dirac Hamiltonian!

2 2-component fermions

opposite sign of mass (opposite P, T)

14.2 Parity anomaly



$\gamma_0 = \sigma_2 \quad \gamma_1 = i\sigma_3 \quad \gamma_2 = i\sigma_1$

["Majorana" - not that it matters for a charged field]

$$\langle j_\mu \rangle = \int \frac{d^3k}{(2\pi)^3} \frac{\mathrm{tr}\, \gamma_\mu (\not{p} + \not{k} + m) \gamma_\nu (\not{k} + m)}{[(p+k)^2 + m^2][k^2 + m^2]}$$

← Euclideanized

superficially linearly divergent

regulate with large M boson loop (Pauli-Villars)

$$\int_0^1 d\alpha \int \frac{d^3k}{(2\pi)^3} \,\mathrm{tr}\, \frac{\gamma_\mu (\not{p} + \not{k} + m) \gamma_\nu (\not{k} + m)}{[\alpha(p+k)^2 + (1-\alpha)k^2 + m^2]^2} \quad - \quad (m \to M)$$

$k + \alpha p \to \tilde{k}$, write as k (in computer code: $k = L + \alpha p$)

small p $\quad (p^2 \ll m^2)$

numerator $\rightarrow m\underbrace{\left(\mathrm{tr}\,\gamma_\mu \not{p} \gamma_\nu (1-\alpha) + \mathrm{tr}\,\gamma_\mu \gamma_\nu \not{p} (-\alpha)\right)}_{-2\epsilon_{\mu\nu\rho} p_\rho \, m}$

$$\underbrace{2m\,\epsilon_{\mu\nu\rho} \int \frac{d^3k}{(2\pi)^3} \frac{1}{(k^2+m^2)^2}}$$

$$\hookrightarrow \frac{1}{|m|} \int_0^\infty dk\, k^2 \frac{4\pi}{8\pi^3} \frac{1}{(k^2+1)^2}$$

k^2+1-1

$$\hookrightarrow \frac{1}{2\pi^2} \frac{1}{|m|} \int_0^\infty dk \left\{ \underset{\pi/2}{\frac{1}{k^2+1}} - \underset{\pi/4}{\frac{1}{(k^2+1)^2}} \right\}$$

$$= \frac{1}{8\pi |m|}$$

Altogether: $\frac{1}{4\pi} \frac{m}{|m|} \epsilon_{\mu\nu\rho} p_\rho \qquad (-(m \to M))$

$$j_1 = \left(\frac{m}{|m|} - \frac{M}{|M|}\right) \frac{1}{4\pi} E_2 \quad = (0 \text{ or } \pm 1) \frac{E_2}{4\pi}$$ for various choices of signs!

Will find: opposite $\frac{m}{|m|}$ at two nodal points

$\frac{M}{|M|}$ determined by external B.