Topological models on Honeycomb lattice (1)

Hamiltonian: $H = \vec{\tau}\cdot\vec{d}(k) + \vec{\tau}\cdot\vec{\tilde{d}}(\vec{k})$

$\vec{\tau}\cdot\vec{d}(k)$: NN hopping + onsite term

$\vec{\tau}\cdot\vec{\tilde{d}}(\vec{k})$: NNN hopping + onsite term.

$\vec{d}(\vec{k}) = \Bigg(t\left[\sin(k_x$ [redacted] $) + 2\sin\left(\frac{k_x}{2}\right)\cos(\pi/3)\cos\left(\frac{\sqrt{3}}{2}k_y\right)\right]$, $t\left[-2\cos(k_x/2)\sin(\pi/3)\sin(\sqrt{3}/2\, k_y)\right]$, $M - 2B\left[2 - \cos k_x - 2\cos\left(\frac{k_x}{2}\right)\cos\left(\frac{\sqrt{3}}{2}k_y\right)\right] \Bigg)$

$\Rightarrow$

$$d_1(\vec{k}) = t\left[\sin(k_x) + 2\sin\left(\frac{k_x}{2}\right)\underbrace{\cos(\pi/3)}_{=1/2}\cos\left(\frac{\sqrt{3}}{2}k_y\right)\right]$$

$$= \frac{t}{2i}\left(e^{ik_x} - e^{-ik_x}\right) + t\sin\frac{k_x}{2}\cos\frac{\sqrt{3}}{2}k_y$$

$$= \frac{t}{2i}\left(e^{ik_x} - e^{-ik_x}\right) + \frac{t}{4i}\left(e^{ik_x/2} - e^{-ik_x/2}\right) \times \left(e^{i\sqrt{3}k_y/2} + e^{-i\sqrt{3}k_y/2}\right)$$

$$= \frac{t}{2i}\left(e^{ik_x} - e^{-ik_x}\right) + \frac{t}{4i}\left[e^{i\left(\frac{k_x}{2} + \frac{\sqrt{3}}{2}k_y\right)} - e^{-i\left(\frac{k_x}{2} + \frac{\sqrt{3}}{2}k_y\right)} + e^{i\left(\frac{k_x}{2} - \frac{\sqrt{3}}{2}k_y\right)} - e^{-i\left(\frac{k_x}{2} + \frac{\sqrt{3}}{2}k_y\right)}\right]$$

$$d_2(\vec{k}) = -2t\cos\left(\frac{k_x}{2}\right)\underbrace{\sin(\pi/3)}_{=\sqrt{3}/2}\sin\left(\frac{\sqrt{3}}{2}k_y\right)$$

$= -\sqrt{3}t\,\frac{1}{4i}$ [redacted] $\left(e^{ik_x/2} + e^{-ik_x/2}\right)\left(e^{i\frac{\sqrt{3}}{2}k_y} - e^{-i\frac{\sqrt{3}}{2}k_y}\right)$.

(2)

$$= -t\frac{\sqrt{3}}{4i}\Big[e^{i\left(\frac{k_x}{2}+\frac{\sqrt{3}}{2}k_y\right)} - e^{-i\left(\frac{k_x}{2}+\frac{\sqrt{3}}{2}k_y\right)} - e^{+i\left(\frac{k_x}{2}-\frac{\sqrt{3}}{2}k_y\right)} + e^{-i\left(\frac{k_x}{2}-\frac{\sqrt{3}}{2}k_y\right)} \Big].$$

$$d_3(\vec{k}) = M - 2B\left[2 - \cos k_x - 2\cos(k_x/2)\cos\left(\frac{\sqrt{3}}{2}k_y\right)\right].$$

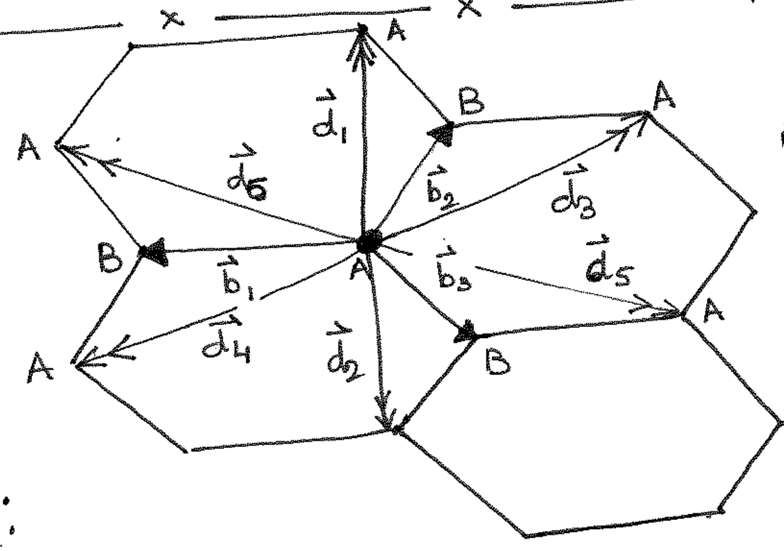
$$= (M-4B) + 2B\cos k_x + 4B\cos(k_x/2)\cos\left(\frac{\sqrt{3}k_y}{2}\right)$$

$$= (M-4B) + B\left(e^{ik_x} + e^{-ik_x}\right) + B\left(e^{ik_x/2} + e^{-ik_x/2}\right) \times \left(e^{i\sqrt{3}k_y/2} + e^{-i\sqrt{3}k_y/2}\right)$$

$$= (M-\cancel{4}4B) + B\left(e^{ik_x} + e^{-ik_x}\right) + B\Big[e^{i\left(\frac{k_x}{2}+\frac{\sqrt{3}}{2}k_y\right)} + e^{-i\left(\frac{k_x}{2}+\frac{\sqrt{3}}{2}k_y\right)} + e^{i\left(\frac{k_x}{2}-\frac{\sqrt{3}}{2}k_y\right)} + e^{-i\left(\frac{k_x}{2}-\frac{\sqrt{3}}{2}k_y\right)} \Big].$$

—— x —— x —— x —— x —— x ——

Geometry:



NNN vectors.

i) $\vec{d}_1 = a(0, \sqrt{3}\,\hat{y})$.
$\vec{d}_2 = -\vec{d}_1$.

ii) $\vec{d}_3 = a\left(\frac{3}{2}\hat{x}, \frac{\sqrt{3}}{2}\hat{y}\right)$
$\vec{d}_4 = -\vec{d}_3$

iii) $\vec{d}_5 = a\left(\frac{3}{2}\hat{x}, -\frac{\sqrt{3}}{2}\hat{y}\right)$
$\vec{d}_6 = -\vec{d}_5$

$|\vec{d}_1| = |\vec{d}_2| = |\vec{d}_3| = |\vec{d}_4| = |\vec{d}_5| = |\vec{d}_6| = \sqrt{3}a = \sqrt{3}$

NN vectors:

$\vec{b}_1 = a(-\hat{x}, 0)$

$\vec{b}_2 = a\left(\frac{1}{2}\hat{x}, \frac{\sqrt{3}}{2}\hat{y}\right)$ and $\vec{b}_3 = a\left(+\frac{1}{2}\hat{x}, -\frac{\sqrt{3}}{2}\hat{y}\right)$. $\Rightarrow |\vec{b}_1| = |\vec{b}_2| = |\vec{b}_3| = a = 1$.

In terms of the NN vectors, the components of $\vec{d}(\vec{k})$ can be written as

$$d_1(\vec{k}) = t\left[\frac{i}{2}\left(e^{i\vec{k}\cdot\vec{b}_1} - e^{-i\vec{k}\cdot\vec{b}_1}\right) - \frac{i}{4}\left(e^{i\vec{k}\cdot\vec{b}_2} - e^{-i\vec{k}\cdot\vec{b}_2}\right) - \frac{i}{4}\left(e^{i\vec{k}\cdot\vec{b}_3} - e^{-i\vec{k}\cdot\vec{b}_3}\right)\right]$$

$$d_2(\vec{k}) = t\left[\frac{\sqrt{3}\,i}{4}\left(e^{i\vec{k}\cdot\vec{b}_2} - e^{-i\vec{k}\cdot\vec{b}_2}\right) - \frac{\sqrt{3}\,i}{4}\left(e^{i\vec{k}\cdot\vec{b}_3} - e^{-i\vec{k}\cdot\vec{b}_3}\right)\right]$$

$$d_3(\vec{k}) = (M-4B) + B\left(e^{i\vec{k}\cdot\vec{b}_1} + e^{-i\vec{k}\cdot\vec{b}_1}\right) + B\left(e^{i\vec{k}\cdot\vec{b}_2} + e^{-i\vec{k}\cdot\vec{b}_2}\right) + B\left(e^{i\vec{k}\cdot\vec{b}_3} + e^{i\vec{k}\cdot\vec{b}_3}\right)$$

<u>Note:</u> <u>Hopping</u> in the direction of $\vec{b}_1$ is the coefficient of the term $e^{i\vec{k}\cdot\vec{b}_1}$, whereas <u>hopping</u> in the opposite direction, i.e., along $-\vec{b}_1$ is the coefficient of the term $e^{-i\vec{k}\cdot\vec{b}_1}$. This way the hermiticity of the Hamiltonian is preserved.

The same convention is true for the hopping along $\vec{b}_2$ and $\vec{b}_3$, and in the opposite direction.

Note that each site of the honeycomb lattice has 3 NN sites. NN sites belong to A & B sublattices. Hopping from any A sublattice site to its 3 NN are captured by the coefficients of $e^{i\vec{k}\cdot\vec{b}_1}$, $e^{i\vec{k}\cdot\vec{b}_2}$ and $e^{i\vec{k}\cdot\vec{b}_3}$, whereas the hopping from B to A sites are coefficients of $e^{-i\vec{k}\cdot\vec{b}_1}$, $e^{-i\vec{k}\cdot\vec{b}_2}$ and $e^{-i\vec{k}\cdot\vec{b}_3}$ which also ensures hermiticity of the Hamiltonian.

d-vector [redacted] with NNN hopping on honeycomb lattice:

$$\tilde{d}(\bar{k}) = \begin{pmatrix} \tilde{A}\sin\left(k_x \frac{3}{2}\right)\cos(\pi/6)\cos\left(\frac{\sqrt{3}}{2}k_y\right) \\ -\tilde{A}\left[\sin(\sqrt{3}k_y) - 2\cos\left(\frac{3}{2}k_x\right)\sin(\pi/6)\sin\left(\frac{\sqrt{3}}{2}k_y\right)\right] \\ -2\tilde{B}\left[3-\cos(\sqrt{3}k_y) - 2\cos\left(\frac{3}{2}k_x\right)\cos\left(\frac{\sqrt{3}}{2}k_y\right)\right] \end{pmatrix}$$

$\Rightarrow$

$$\tilde{d}_1(\bar{k}) = \tilde{A}\sin\left(\frac{3k_x}{2}\right)\underbrace{\cos(\pi/6)}_{=\sqrt{3}/2}\cos\left(\frac{\sqrt{3}k_y}{2}\right).$$

$$= \frac{\sqrt{3}}{2}\tilde{A}\,\frac{1}{2i}\left(e^{i\frac{3k_x}{2}} - e^{-i\frac{3k_x}{2}}\right)\frac{1}{2}\left(e^{i\frac{\sqrt{3}}{2}k_y} + e^{-i\frac{\sqrt{3}}{2}k_y}\right).$$

$$= \tilde{A}\left(\frac{\sqrt{3}}{8i}\right)\left[e^{i\left(\frac{3k_x}{2}+\frac{\sqrt{3}}{2}k_y\right)} - e^{-i\left(\frac{3k_x}{2}+\frac{\sqrt{3}}{2}k_y\right)} + e^{i\left(\frac{3k_x}{2}-\frac{\sqrt{3}}{2}k_y\right)} - e^{-i\left(\frac{3k_x}{2}-\frac{\sqrt{3}}{2}k_y\right)}\right].$$

$$\tilde{d}_2(\bar{k}) = -\tilde{A}\left[\sin(\sqrt{3}k_y) - 2\cos\left(\frac{3}{2}k_x\right)\underbrace{\sin\left(\frac{\pi}{6}\right)}_{=1/2}\sin\left(\frac{\sqrt{3}}{2}k_y\right)\right]$$

$$= -\tilde{A}\left(\frac{1}{2i}\right)\left(e^{i\sqrt{3}k_y} - e^{-i\sqrt{3}k_y}\right)$$

$$+\tilde{A}\cos\left(\frac{3}{2}k_x\right)\sin\left(\frac{\sqrt{3}}{2}k_y\right).$$

$$= -\tilde{A}\left(\frac{1}{2i}\right)\left[e^{i\sqrt{3}k_y} - e^{-i\sqrt{3}k_y}\right]$$ [redacted]

$$+\tilde{A}\left(\frac{1}{4i}\right)\left(e^{i\frac{3k_x}{2}} + e^{-i\frac{3k_x}{2}}\right)\left(e^{i\frac{\sqrt{3}}{2}k_y} - e^{-i\frac{\sqrt{3}}{2}k_y}\right).$$

$$= \tilde{A}\left(-\frac{1}{2i}\right)\left[e^{i\sqrt{3}k_y} - e^{-i\sqrt{3}k_y}\right]$$ [redacted]

$$+\tilde{A}\left(\frac{1}{4i}\right)\left[e^{i\left(\frac{3k_x}{2}+\frac{\sqrt{3}}{2}k_y\right)} - e^{-i\left(\frac{3k_x}{2}+\frac{\sqrt{3}}{2}k_y\right)} - e^{i\left(\frac{3k_x}{2}-\frac{\sqrt{3}}{2}k_y\right)} + e^{-i\left(\frac{3k_x}{2}-\frac{\sqrt{3}}{2}k_y\right)}\right].$$

$$\tilde{d}_3(\vec{k}) = -2\tilde{B}\left[3 - \cos(\sqrt{3}\,k_y) - 2\cos\left(\tfrac{3}{2}k_x\right)\cos\left(\tfrac{\sqrt{3}}{2}k_y\right)\right].$$ ⑤

$$= -6\tilde{B} + 2\tilde{B}\cos(\sqrt{3}\,k_y) + 4\tilde{B}\cos\left(\tfrac{3}{2}k_x\right)\cos\left(\tfrac{\sqrt{3}}{2}k_y\right).$$

$$= -6\tilde{B} + \tilde{B}\left(e^{i\sqrt{3}k_y} + e^{-i\sqrt{3}k_y}\right)$$
$$+ \tilde{B}\left(e^{i\frac{3}{2}k_x} + e^{-i\frac{3}{2}k_x}\right)\left(e^{i\frac{\sqrt{3}}{2}k_y} + e^{-i\frac{\sqrt{3}}{2}k_y}\right).$$

$$= -6\tilde{B} + \tilde{B}\left(e^{i\sqrt{3}k_y} + e^{-i\sqrt{3}k_y}\right).$$
$$+ \tilde{B}\left(e^{i\left(\frac{3}{2}k_x + \frac{\sqrt{3}}{2}k_y\right)} + e^{-i\left(\frac{3}{2}k_x + \frac{\sqrt{3}}{2}k_y\right)}\right.$$
$$\left. + e^{i\left(\frac{3}{2}k_x - \frac{\sqrt{3}}{2}k_y\right)} + e^{-i\left(\frac{3}{2}k_x - \frac{\sqrt{3}}{2}k_y\right)}\right).$$

Next we express $\tilde{d}_1(\vec{k})$, $\tilde{d}_2(\vec{k})$ and $\tilde{d}_3(\vec{k})$ in terms of the NNN vectors $\vec{d}_1, \dots, \vec{d}_6$:

$$\tilde{d}_1(\vec{k}) = \tilde{A}\left[\left(-\frac{\sqrt{3}}{8}i\right)\left(e^{i\vec{k}\cdot\vec{d}_3} - e^{-i\vec{k}\cdot\vec{d}_3}\right) + \left(-\frac{\sqrt{3}}{8}i\right)\left(e^{i\vec{k}\cdot\vec{d}_5} - e^{-i\vec{k}\cdot\vec{d}_5}\right)\right]$$

$$\equiv \tilde{A}\left[\left(-\frac{\sqrt{3}}{8}i\right)\left(e^{i\vec{k}\cdot\vec{d}_3} - e^{i\vec{k}\cdot\vec{d}_4}\right) + \left(-\frac{\sqrt{3}}{8}i\right)\left(e^{i\vec{k}\cdot\vec{d}_5} - e^{i\vec{k}\cdot\vec{d}_6}\right)\right]$$

as $\vec{d}_2 = -\vec{d}_1$, $\vec{d}_4 = -\vec{d}_3$ and $\vec{d}_6 = -\vec{d}_5$

$$\tilde{d}_2(\vec{k}) = \tilde{A}\left[\left(\frac{i}{2}\right)\left(e^{i\vec{k}\cdot\vec{d}_1} - e^{-i\vec{k}\cdot\vec{d}_1}\right) + \left(-\frac{i}{4}\right)\left(e^{i\vec{k}\cdot\vec{d}_3} - e^{-i\vec{k}\cdot\vec{d}_3}\right)\right.$$
$$\left. + \left(\frac{i}{4}\right)\left(e^{i\vec{k}\cdot\vec{d}_5} - e^{-i\vec{k}\cdot\vec{d}_5}\right)\right].$$

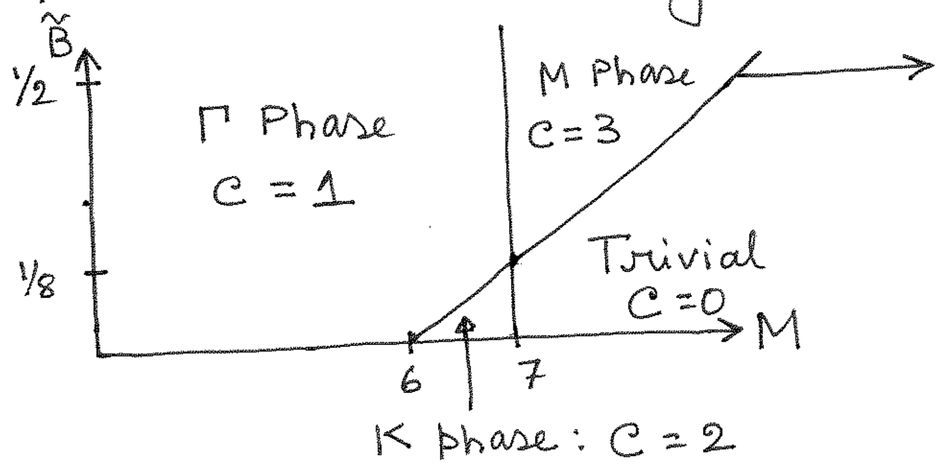
$$\equiv \tilde{A}\left[\left(\frac{i}{2}\right)\left(e^{i\vec{k}\cdot\vec{d}_1} - e^{i\vec{k}\cdot\vec{d}_2}\right) + \left(-\frac{i}{4}\right)\left(e^{i\vec{k}\cdot\vec{d}_3} - e^{i\vec{k}\cdot\vec{d}_4}\right)\right.$$
$$\left. + \left(\frac{i}{4}\right)\left(e^{i\vec{k}\cdot\vec{d}_5} - e^{i\vec{k}\cdot\vec{d}_6}\right)\right].$$

$$\tilde d_3(\vec k) = -6\tilde B + \tilde B\left(e^{i\vec k\cdot\vec d_4} + e^{-i\vec k\cdot\vec d_1}\right) + \tilde B\left(e^{i\vec k\cdot\vec d_3} + e^{-i\vec k\cdot\vec d_3}\right) + \tilde B\left(e^{i\vec k\cdot\vec d_5} - e^{-i\vec k\cdot\vec d_5}\right)$$

$$= -6\tilde B + \tilde B\left(e^{i\vec k\cdot\vec d_1} + e^{i\vec k\cdot\vec d_2} + e^{i\vec k\cdot\vec d_3} + e^{i\vec k\cdot\vec d_4} + e^{i\vec k\cdot\vec d_5} + e^{i\vec k\cdot\vec d_6}\right)$$

Note that each site of the honeycomb lattice is accompa-nied by SIX NNN sites. For any site the NNN vectors are identical: $\vec d_1, \vec d_2, \vec d_3, \vec d_4, \vec d_5$ and $\vec d_6$. Also the SIX NNN belong to the same sublattice as the original site. Therefore, I expressed all the NNN hopping terms in terms of SIX NNN vectors: $\vec d_1, \ldots, \vec d_6$. These hoppings can be implemented by selecting ONE site at a time & then connecting its SIX NNN sites. Then this procedure needs to be repeated for all the sites to ensure hermiticity.

All the numerical simulations & phase diagrams will be constructed for $t = 1$, $\tilde A = 1$, $B = 1$. Then we have the following tuning parameters: M and $\tilde B$. The resulting phase diagram reads as



Equation of this line.

$$\boxed{\tilde B = \frac{M}{8} - \frac{3}{4}}.$$

See, Nat. Phys. 9, 98 (2013).