3.13.7. Marginal case: $\mu = 4\,t$

Dirac points at k=(π,π). Not an insulator. No topological index.

3.13.8. case IV: $\mu > 4\,t$

All the four special points has $\mathcal{H}_z < 0$. We just use u^I for the whole BZ. No singularity. C=0

3.13.9. case IV: $\mu > 4\,t$

All the four special points has $\mathcal{H}_z < 0$. We just use u^I for the whole BZ. No singularity. C=0

3.13.10. the top band?

The top band has the opposite Chern number $C_+ = -C_-$.

In fact, one can prove that for any tight-binding models, the total Chern number for all the bands is always 0.

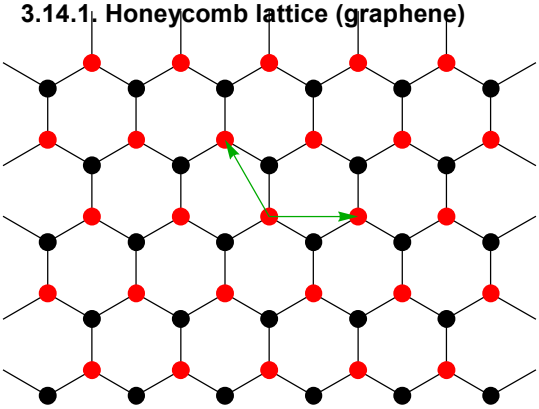
So here, we have $C_+ + C_- = 0$.

3.13.11. Summary

- This model has four phases. Two topological phases with C=+1 and two trivial insulator phase with C=0.
- A topological phase and the trivial insulator phase are separated by a phase transition point, which is known as a topological phase transition.
  - Across the topological phase transition, the topological index changes its value
  - Across a topological transition, the insulating gap closes and then reopens (generically true)
  - This is actually a generic statement: A band can only change its Chern number by crossing with another band. i.e. At the topological transition point, the system must be a metal or a semi-metal (with no insulating gap).
- Gap closing is a necessary condition for a topological transition, but it is not a sufficient one. One may close and reopen the gap without changing the topological index. e.g. the μ=0 point here.

3.14. The model of Haldane on a honeycomb lattice

3.14.1. Honeycomb lattice (graphene)



Two sites per unit cell (two sublattices) a and b (red and black respectively). The green arrow indicates the lattice vectors $\vec{v}_1$ and $\vec{v}_2$. If we shift the lattices by $m\ \vec{v}_1 + n\,\vec{v}_2$ with m and n being integers, the lattice is invariant.

$$V\left(\vec{r}\right) = V\left(\vec{r} + m\ \vec{v}_1 + n\,\vec{v}_2\right) \tag{3.307}$$

Define a to the length of the nearest-neighbor (NN) bonds, $\vec{v}_1 = \left(\sqrt{3}\ a,\ 0\right)$ and $\vec{v}_2 = \left(-\sqrt{3}\ \big/ 2\,a,\ \ 3/2\,a\right)$

If we only consider hoppings between the nearest-neighbor (NN) sites, the Hamiltonian is

$$H = -t \sum_{<i,j>} a_i^\dagger\, b_j - t \sum_{<i,j>} b_i^\dagger\, a_j \tag{3.308}$$

where ⟨i,j⟩ means nearest neighbors.

3.14.2. Band structures

There are three type of NN bonds: (1) along the y axis with $\theta=\pi/2$, (2) along $\theta=\pi/2+2\pi/3=7\pi/6$, (3) along $\theta=\pi/2+4\pi/3=11\pi/6$.

We need to write them out separately.

$$H = -t \sum_i a_{\vec{r}_i}^\dagger b_{r_i+\vec{e}_1} - t \sum_i a_{\vec{r}_i}^\dagger b_{r_i+\vec{e}_2} - t \sum_i a_{\vec{r}_i}^\dagger b_{r_i+\vec{e}_3} + h.c. \tag{3.309}$$

with

$$\vec{e}_1 = (0,\, a) \tag{3.310}$$

$$\vec{e}_2 = \left(-\frac{\sqrt{3}}{2} a,\, -\frac{a}{2}\right) \tag{3.311}$$

$$\vec{e}_3 = \left(\frac{\sqrt{3}}{2} a\,,\, -\frac{a}{2}\right) \tag{3.312}$$

Here the sum $\sum_i$ sums over all unit cells (or say all red sites).

Go to the momentum space using a 2D Fourier transformation

$$a_k = \frac{1}{\sqrt{N}} \sum_i a_i\, e^{i \vec{k}\cdot\vec{r}} \tag{3.313}$$

$$a_i = \frac{1}{\sqrt{N}} \sum_k a_k\, e^{-i \vec{k}\cdot\vec{r}} \tag{3.314}$$

$$b_k = \frac{1}{\sqrt{N}} \sum_i a_i\, e^{i \vec{k}\cdot\vec{r}} \tag{3.315}$$

$$b_i = \frac{1}{\sqrt{N}} \sum_k a_k\, e^{-i \vec{k}\cdot\vec{r}} \tag{3.316}$$

The first term in the Hamiltonian

$$\begin{aligned} -t \sum_i a_{r_i}^\dagger b_{r_i+e_1} &= -\frac{t}{N} \sum_i \sum_k \sum_{k'} a_k^\dagger\, e^{i \vec{k}\cdot\vec{r}_i}\, b_{k'}\, e^{-i \vec{k}'\cdot\left(\vec{r}_i+\vec{e}_1\right)} = \\ -t \sum_k \sum_{k'} a_k^\dagger\, b_{k'}\, e^{-i \vec{k}'\cdot\vec{e}_1} \frac{1}{N} \sum_i e^{i\left(\vec{k}-\vec{k}'\right)\cdot\vec{r}_i} &= -t \sum_k \sum_{k'} a_k^\dagger\, b_{k'}\, e^{-i \vec{k}'\cdot\vec{e}_1}\, \delta_{k,k'} = -t \sum_k a_k^\dagger\, b_k\, e^{-i \vec{k}\cdot\vec{e}_1} \end{aligned} \tag{3.317}$$

This is generically true. By going to the k space, one just need to change $a_{r_i}^\dagger\, b_{r_i+e_1}$ into $a_k^\dagger\, b_k$ and change $\sum_i$ (sum over all unit cells) into $\sum_k$ (sum over all momentum points), and the coefficient is $-t \exp\left[i \vec{k}\cdot\left(\vec{r}_a - \vec{r}_b\right)\right]$ with $\vec{r}_a$ and $\vec{r}_b$ being the coordinates of site a and b.

$$\begin{aligned} H &= -t \sum_i a_{r_i}^\dagger b_{r_i+e_1} - t \sum_i a_{r_i}^\dagger b_{r_i+e_2} - t \sum_i a_{r_i}^\dagger b_{r_i+e_2} + h.c. \\ &= -t \sum_k a_k^\dagger\, b_k \left(e^{-i \vec{k}\cdot\vec{e}_1} + e^{-i \vec{k}\cdot\vec{e}_2} + e^{-i \vec{k}\cdot\vec{e}_3}\right) - t \sum_k b_k^\dagger\, a_k \left(e^{i \vec{k}\cdot\vec{e}_1} + e^{i \vec{k}\cdot\vec{e}_2} + e^{i \vec{k}\cdot\vec{e}_3}\right) \\ &= \sum_k \begin{pmatrix} a_k^\dagger & b_k^\dagger \end{pmatrix} \begin{pmatrix} 0 & \mathcal{H}_{12}\left(\vec{k}\right) \\ \mathcal{H}_{21}\left(\vec{k}\right) & 0 \end{pmatrix} \begin{pmatrix} a_k \\ b_k \end{pmatrix} \end{aligned} \tag{3.318}$$

$$\mathcal{H}_{12}\left(\vec{k}\right) = -t\left[\exp\left(-i \vec{k}\cdot\vec{e}_1\right) + \exp\left(-i \vec{k}\cdot\vec{e}_2\right) + \exp\left(-i \vec{k}\cdot\vec{e}_3\right)\right] \tag{3.319}$$

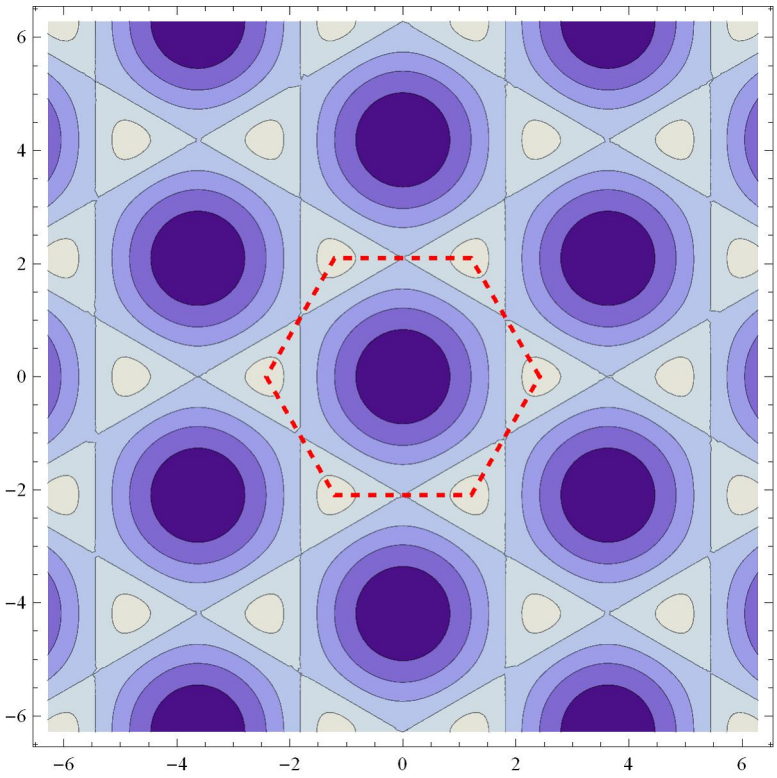
$$\mathcal{H}_{21}\left(\vec{k}\right) = \mathcal{H}_{12}\left(\vec{k}\right)^* = -t\left[\exp\left(i \vec{k}\cdot\vec{e}_1\right) + \exp\left(i \vec{k}\cdot\vec{e}_2\right) + \exp\left(i \vec{k}\cdot\vec{e}_3\right)\right] \tag{3.320}$$

The kernel of the Hamiltonian:

$$\mathcal{H}\left(\vec{k}\right) = \begin{pmatrix} 0 & \mathcal{H}_{12}\left(\vec{k}\right) \\ \mathcal{H}_{21}\left(\vec{k}\right) & 0 \end{pmatrix} \tag{3.321}$$

The eigenvalues of $\mathcal{H}$(k) gives the dispersion relation.

$$\epsilon_{\pm}\left(\vec{k}\right) = \pm \left|\mathcal{H}_{12}\left(\vec{k}\right)\right| = \pm \left|t\right| \sqrt{3 + 2\cos\left(\sqrt{3}\ k_x a\right) + 4\cos\left(\frac{\sqrt{3}}{2} k_x a\right) \mathrm{Cos}\left(\frac{3}{2} k_y a\right)} \tag{3.322}$$



The contour plot of the energy dispersion for the lower band (ϵ_- as a function of k_x and k_y). The red dash lines mark the first BZ, which is a hexagon.

The dispersion $\epsilon_{\pm}$ is a periodic function of $\vec{k}$ space (the hexagon repeats itself in the figure shown above). For the lower band, its energy minimum is located at $k = 0$. The maximum of ϵ_- is reached at the corners of the BZ. The first BZ is a hexagon. It has six corners. However, due to the periodic structure in k-space, the three corner points with θ=0, θ=2π/3 and θ=4π/3 are the same point (their momenta differ by precisely one periodicity). Similarly, the three corners with θ=π, θ=π+2π/3 and θ=π+4π/3 are the same points. Therefore, there are only two different corner points and they are known as the K and K' points, where

$$K = \left(\frac{4\pi}{3\sqrt{3}\ a}, 0\right) \tag{3.323}$$

and

$$K' = \left(-\frac{4\pi}{3\sqrt{3}\ a}, 0\right) \tag{3.324}$$

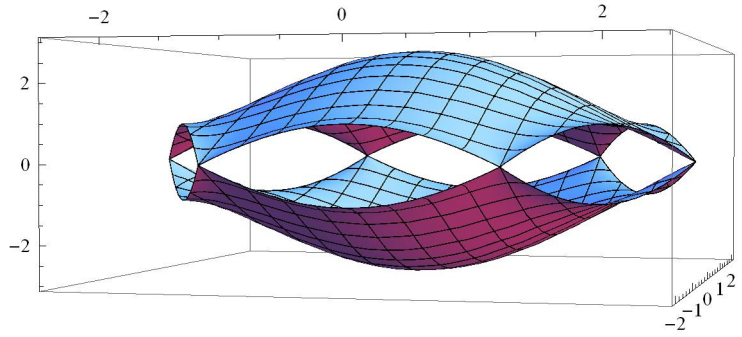
For most momentum points, one of the two bands has positive energy $\epsilon_+ > 0$ and the other one has negative energy $\epsilon_- < 0$. However at the corner of the BZ, K and K', the two bands are degenerate $\epsilon_+ = \epsilon_- = 0$.

$$\epsilon_{\pm}\left(\vec{K}\right) = \pm \left|\mathcal{H}_{12}\left(\vec{K}\right)\right| = \pm \left|t\right| \sqrt{3 + 2\cos\left(\sqrt{3}\ k_x a\right) + 4\cos\left(\frac{\sqrt{3}}{2} k_x a\right) \mathrm{Cos}\left(\frac{3}{2} k_y a\right)} =$$

$$\pm \left|t\right| \sqrt{3 + 2\cos\left(\sqrt{3}\ \frac{4\pi}{3\sqrt{3}\ a} a\right) + 4\cos\left(\frac{\sqrt{3}}{2}\ \frac{4\pi}{3\sqrt{3}\ a} a\right) \mathrm{Cos}\left(\frac{3}{2} \times 0\right)} =$$

$$\pm \left|t\right| \sqrt{3 + 2\cos\left(\frac{4\pi}{3}\right) + 4\cos\left(\frac{2\pi}{3}\right)} = \pm \left|t\right| \sqrt{3 + 2 \times \left(-\frac{1}{2}\right) + 4 \times \left(-\frac{1}{2}\right)} = \sqrt{3 - 3} = 0$$

Two bands have the same energy at K and K': band crossing points.



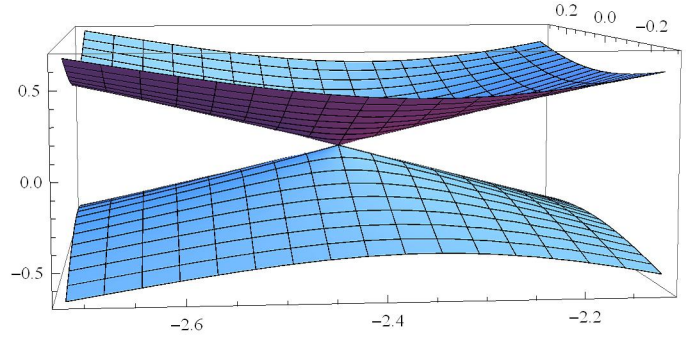
The energy dispersion for both bands ($\epsilon_{\pm}$ as a function of k_x and k_y) in the first BZ (within the red dash lines mark in the figure above).

Near K or K' points, the dispersion for the two bands are linear $\epsilon_{\pm} \propto \pm(k - K)$. To see this, we expand $\epsilon_{\pm}\left(\vec{k}\right)$ near $\vec{k} \sim \vec{K}$ and $\vec{k} \sim \vec{K}'$

$$\epsilon_{\pm}\left(\vec{k}\right) = \epsilon_{\pm}\left(\vec{K} + \vec{q}\right) = \pm \left|t\right| \sqrt{3 + 2\cos\left[\sqrt{3}\ \left(\frac{4\pi}{3\sqrt{3}\ a} + q_x\right) a\right] + 4\cos\left[\frac{\sqrt{3}}{2}\ \left(\frac{4\pi}{3\sqrt{3}\ a} + q_x\right) a\right] \mathrm{Cos}\left(\frac{3}{2} q_y a\right)} = \tag{3.326}$$

$$\pm \frac{3}{2} \left|t\right|\ a \sqrt{{q_x}^2 + {q_y}^2} + O\left(q^2\right) = \pm \frac{3}{2} \left|t\right|\ a\ q + O\left(q^2\right)$$

$$\epsilon_{\pm}\left(\vec{k}\right) = \epsilon_{\pm}\left(\vec{K}' + \vec{q}\right) = \pm \frac{3}{2} \left|t\right|\ a\ q + O\left(q^2\right) \tag{3.327}$$



Zoom in near the K' points.

Q: Fermions with linear dispersion $\epsilon \propto k$, what is that?

A: A Massless Dirac fermion.

$$\mathcal{H}(k) = \mathcal{H}(K+q) = \frac{3}{2} t\, a \begin{pmatrix} 0 & q_x - i\, q_y \\ q_x + i\, q_y & 0 \end{pmatrix} + O(q^2) \approx \frac{3}{2} t\, a \left(q_x \sigma_x + q_y \sigma_y\right) = c\, \vec{q} \cdot \vec{\sigma} \tag{3.328}$$

$$\mathcal{H}(k) = \mathcal{H}(K'+q) = -\frac{3}{2} t\, a \begin{pmatrix} 0 & q_x + i\, q_y \\ q_x - i\, q_y & 0 \end{pmatrix} + O(q^2) \approx -\frac{3}{2} t\, a \left(q_x \sigma_x - q_y \sigma_y\right) = -c\, \vec{q} \cdot \left(\sigma_x\, \vec{\sigma}\, \sigma_x\right) \tag{3.329}$$

where c is the speed of light. Each of them is a Weyl fermion. These two Weyl fermions with opposite chirality forms a Dirac fermion.

Dirac fermions we learned in quantum mechanics:

$$i\, \partial_t \psi = \begin{pmatrix} 0 & c\, \vec{q} \cdot \vec{\sigma} \\ c\, \vec{q} \cdot \vec{\sigma} & 0 \end{pmatrix} \psi \tag{3.330}$$

If one make an unitary transformation (changing the basis, which doesn't change any physics)

$$\psi' = \begin{pmatrix} 0 & \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & 0 \\ \frac{1}{\sqrt{2}} & 0 & 0 & \frac{1}{\sqrt{2}} \\ 0 & -\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & 0 \\ -\frac{1}{\sqrt{2}} & 0 & 0 & \frac{1}{\sqrt{2}} \end{pmatrix} \psi \tag{3.331}$$

The equation turns into

$$i\, \partial_t \psi' = \begin{pmatrix} -c\, \vec{q} \cdot \left(\sigma_x\, \vec{\sigma}\, \sigma_x\right) & 0 \\ 0 & c\, \vec{q} \cdot \vec{\sigma} \end{pmatrix} \psi' \tag{3.332}$$

The Dirac point (band crossing points) in a honeycomb lattice is stable as long as the space inversion symmetry $r \to -r$ and the time reversal symmetry $t \to -t$ are preserved. We will come back to this point latter. No matter how one perturb the systems (e.g. adding longer-range hoppings), the Dirac point is always there as long as the two symmetries mentioned above are preserved.

For graphene, the lower band is filled and the upper band is empty, which is known as "half-filling". The "half" here means that the number of electrons N_e over the number of sites N_s is $N_e / N_S = 1/2$. However, it is worthwhile to notice that the ratio between N_e and the number of unit cells N is 1, because there are two sites in each unit cell. So one of the two bands are totally filled.

By gating, one can turn the energy level slightly away from the middle point.

3.14.3. Aharonov–Bohm effect and complex hopping

Q: Can hopping strength t be complex?

A: Yes, and the phase can come from the Aharonov–Bohm effect in the presence of a magnetic field or spin-orbital couplings.

The Aharonov–Bohm effect:if one moves a particle around a closed contour. The phase difference between the final and initial states is proportional to the magnetic flux enclosed by the contour $\phi = e/\hbar \int\int B \cdot d\vec{S} = e/\hbar \oint A . d\vec{l}$

Discrete version on a lattice: Consider three sites a, b and c. The hopping strength between these three sites are t_{ab} t_{bc} and t_{ca} respectively. If a particle hops from a to b and then to c, the hopping strength around this loop is:

$$t_{ab}\, t_{bc}\, t_{ca} = \left| t_{ab} \right| e^{i \phi_{ab}} * \left| t_{bc} \right| e^{i \phi_{bc}} * \left| t_{ca} \right| e^{i \phi_{ca}} = \left| t_{ab}\, t_{bc}\, t_{ca} \right| e^{i (\phi_{ab} + \phi_{bc} + \phi_{ca})} \tag{3.333}$$

The phase picked up by the electron is:

$$\phi_{ab} + \phi_{bc} + \phi_{ca} = \frac{e}{\hbar} \int\int B \cdot d\vec{S} \tag{3.334}$$

If B is nonzero inside the triangle formed by these three sites, the phase for these hoppings are nonzero.

Please notice that:

t_{ab} and t_{ba} has opposite phase, due to the Hermitian condition (One can also prove this using the Fermi's golden rule, which says that the tunneling amplitude from the state |f> to |i> is the complex conjugate of the tuning amplitude from |i> to |f>).

$$t_{ab} = t_{ba}^{*} \tag{3.335}$$

The individual phases for t_{ab}, t_{bc} and t_{ca} have no physical meaning and they are in fact gauge dependent. Only the total phase on a loop has physical meanings.

$$\phi_{ab} = e/\hbar \int_a^b A \cdot dl \tag{3.336}$$

Underage transformation: $A \to A + \nabla \chi$

$$\phi_{ab} \to \phi_{ab}' = e/\hbar \int_a^b (A + \nabla \chi) \cdot dl = e/\hbar \int_a^b A \cdot dl + e/\hbar \int_a^b \nabla \chi \cdot dl = \phi_{ab} + (\chi_b - \chi_a) \frac{e}{\hbar} \tag{3.337}$$

Obviously, ϕ_{ab} is not a physical observables, since it relies on the gauge choice. However, the total phase around a loop is different. It is a loop integral of A, which is gauge independent and the physics meaning of this Integral is the magnetic flux.

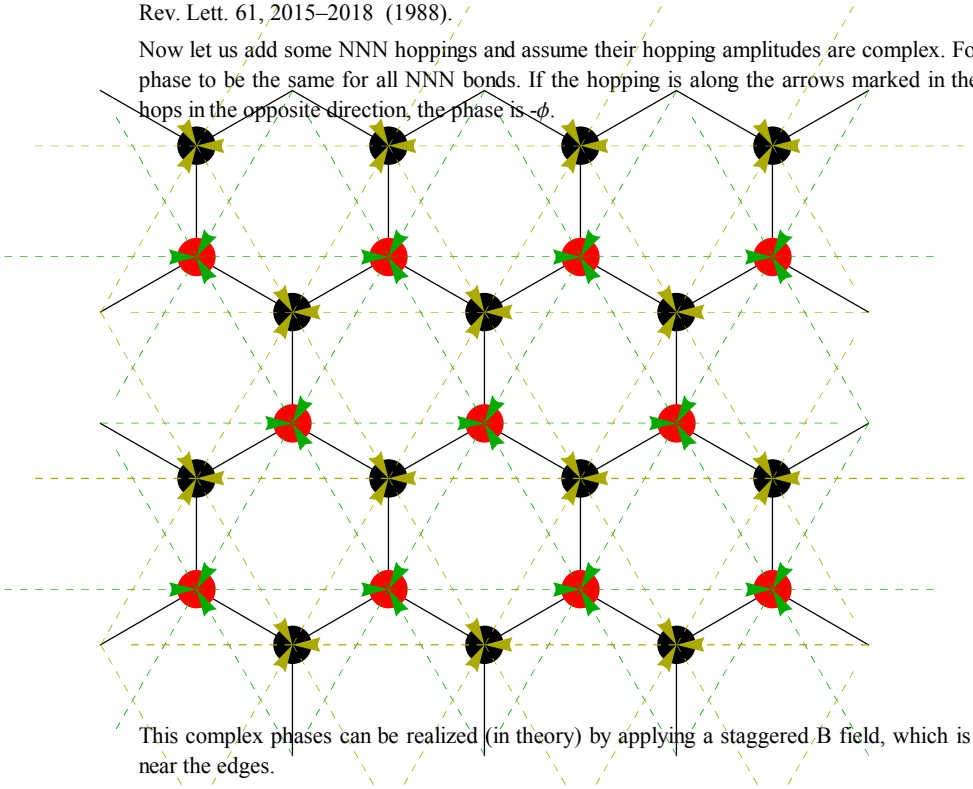
$$\phi_{ab} + \phi_{bc} + \phi_{ca} = e/\hbar \oint A \cdot dl \to \phi_{ab}' + \phi_{bc}' + \phi_{ca}' = e/\hbar \oint (A + \nabla \chi) \cdot dl = e/\hbar \oint A \cdot dl + e/\hbar \oint \nabla \chi \cdot dl = e/\hbar \oint A \cdot dl = \phi_{ab} + \phi_{bc} + \phi_{ca} \tag{3.338}$$

The complex hopping strength induced by B fields breaks the time-reversal symmetry because $B \to -B$ under time reversal. (in other words, under time-reversal one need to flip the sign of all these phases).

3.14.4. Complex next-nearest-neighbor (NNN) hoppings (breaking T-symmetry using *B* fields)

Ref: F. D. M. Haldane, Model for a Quantum Hall Effect without Landau Levels: Condensed-Matter Realization of the "Parity Anomaly", Phys. Rev. Lett. 61, 2015–2018 (1988).

Now let us add some NNN hoppings and assume their hopping amplitudes are complex. For simplicity, we choose the amplitude and the complex phase to be the same for all NNN bonds. If the hopping is along the arrows marked in the figure, the phase of the hopping strength is ϕ. If one hops in the opposite direction, the phase is $-\phi$.



This complex phases can be realized (in theory) by applying a staggered B field, which is positive near the center of each hexagon and negative near the edges.

The NNN hoppings are from an *a*-site to an *a*-site (and from a *b*-site to a *b*-site). For a-to-a hoppings, there are three different types of NNN bonds, along θ=0, $2\pi/3$ and $4\pi/3$. Same is true for b-to-b hoppings. So the Hamiltonian is:

$$H_{NNN} = -t' e^{i\phi} \sum_i a_{r_i}^\dagger a_{r_i+v_1} - t' e^{i\phi} \sum_i a_{r_i+v_1}^\dagger a_{r_i-v_3} - t' e^{i\phi} \sum_i a_{r_i-v_3}^\dagger a_{r_i} + h.c. + (a \to b \text{ and } \phi \to -\phi) \tag{3.339}$$

Here, v_1 and v_2 are marked on the first figure of this section with $\vec{v}_1 = \left(\sqrt{3}\, a,\ 0\right)$ and $\vec{v}_2 = \left(-\sqrt{3}/2\, a,\ \ 3/2\, a\right)$. $\vec{v}_2 = \left(-\sqrt{3}/2\, a,\ \ -3/2\, a\right)$

$$\begin{aligned} H_{\text{NNN}} &= -t' e^{i\phi} \sum_i a_{r_i}{}^\dagger a_{r_i+v_1} - t' e^{i\phi} \sum_i a_{r_i+v_1}{}^\dagger a_{r_i-v_3} - t' e^{i\phi} \sum_i a_{r_i-v_3}{}^\dagger a_{r_i} + h.c. + (a \to b \text{ and } \phi \to -\phi) \\ &= -t' e^{i\phi} \sum_k a_k{}^\dagger a_k \left(e^{-i k\cdot v_1} + e^{-i k\cdot v_2} + e^{-i k\cdot v_3}\right) + h.c. + (a \to b \text{ and } \phi \to -\phi) \\ &= -2\, t' \sum_k a_k{}^\dagger a_k \left[\cos(k\cdot v_1 - \phi) + \cos(k\cdot v_2 - \phi) + \cos(k\cdot v_3 - \phi)\right] - \\ &\quad 2\, t' \sum_k b_k{}^\dagger b_k \left[\cos(k\cdot v_1 + \phi) + \cos(k\cdot v_2 + \phi) + \cos(k\cdot v_3 + \phi)\right] \end{aligned} \tag{3.340}$$

$$H = H_{\text{NN}} + H_{\text{NNN}} = \sum_k \begin{pmatrix} a_k{}^\dagger & b_k{}^\dagger \end{pmatrix} \begin{pmatrix} \mathcal{H}_{11}(k) & \mathcal{H}_{12}(k) \\ \mathcal{H}_{21}(k) & \mathcal{H}_{22}(k) \end{pmatrix} \begin{pmatrix} a_k \\ b_k \end{pmatrix} \tag{3.341}$$

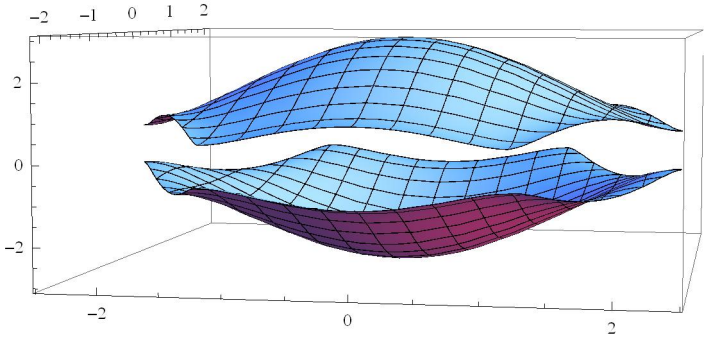
$$\mathcal{H}_{12}(k) = -t\left(e^{-i\vec{k}\cdot\vec{e}_1} + e^{-i\vec{k}\cdot\vec{e}_2} + e^{-i\vec{k}\cdot\vec{e}_3}\right) \tag{3.342}$$

$$\mathcal{H}_{21}(k) = \mathcal{H}_{12}(k)^* = -t\left(e^{i\vec{k}\cdot\vec{e}_1} + e^{i\vec{k}\cdot\vec{e}_2} + e^{i\vec{k}\cdot\vec{e}_3}\right) \tag{3.343}$$

$$\mathcal{H}_{11}(k) = -2\, t' \left[\cos(k\cdot v_1 - \phi) + \cos(k\cdot v_2 - \phi) + \cos(k\cdot v_3 - \phi)\right] \tag{3.344}$$

$$\mathcal{H}_{22}(k) = -2\, t' \left[\cos(k\cdot v_1 + \phi) + \cos(k\cdot v_2 + \phi) + \cos(k\cdot v_3 + \phi)\right] \tag{3.345}$$

If one computes the eigenvalues of $\mathcal{H}$(k), one find that the two bands never cross with each other for any k (if t' is non-zero and ϕ is NOT an integer times π).



The energy dispersion for both bands ($\epsilon_\pm$ as a function of k_x and k_y) in the first BZ (within the red dash lines mark in the figure above).

Using Pauli matrices:

$$\mathcal{H} = \mathcal{H}_0(k)\, I + \mathcal{H}_x(k)\, \sigma_x + \mathcal{H}_y(k)\, \sigma_y + \mathcal{H}_z(k)\, \sigma_z \tag{3.346}$$

$$\mathcal{H}_0 = \frac{\mathcal{H}_{11}(k) + \mathcal{H}_{22}(k)}{2} = -2\, t' \cos\phi \left[\cos(k\cdot v_1) + \cos(k\cdot v_2) + \cos(k\cdot v_3)\right] \tag{3.347}$$

$$\mathcal{H}_z = \frac{\mathcal{H}_{11}(k) - \mathcal{H}_{22}(k)}{2} = -2\, t' \sin\phi \left[\sin(k\cdot v_1) + \sin(k\cdot v_2) + \sin(k\cdot v_3)\right] \tag{3.348}$$

$$\mathcal{H}_x = \text{Re}[\mathcal{H}_{21}(k)] = -t\left[\cos\left(\vec{k}\cdot\vec{e}_1\right) + \cos\left(\vec{k}\cdot\vec{e}_2\right) + \cos\left(\vec{k}\cdot\vec{e}_3\right)\right] \tag{3.349}$$

$$\mathcal{H}_y = \text{Im}[\mathcal{H}_{21}(k)] = -t\left[\sin\left(\vec{k}\cdot\vec{e}_1\right) + \sin\left(\vec{k}\cdot\vec{e}_2\right) + \sin\left(\vec{k}\cdot\vec{e}_3\right)\right] \tag{3.350}$$

The energy dispersions:

$$\epsilon_\pm\left(\vec{k}\right) = \mathcal{H}_0\left(\vec{k}\right) \pm \sqrt{\mathcal{H}_x\left(\vec{k}\right)^2 + \mathcal{H}_y\left(\vec{k}\right)^2 + \mathcal{H}_z\left(\vec{k}\right)^2} \tag{3.351}$$

Without the complex NNN hoppings, $\mathcal{H}_0 = \mathcal{H}_z = 0$, so the dispersion

$$\epsilon_\pm\left(\vec{k}\right) = \pm\sqrt{\mathcal{H}_x\left(\vec{k}\right)^2 + \mathcal{H}_y\left(\vec{k}\right)^2} \tag{3.352}$$

At K and K', $\mathcal{H}_x = \mathcal{H}_y = 0$, so the two bands degenerate (without the complex NNN hoppings)

$$\epsilon_{\pm}\left(\vec{k}\right) = 0 \tag{3.353}$$

which gives the Dirac points.

Now, with these complex NNN hoppings, At K and K' points, $\mathcal{H}_x = \mathcal{H}_y = 0$, but $\mathcal{H}_z \neq 0$. The gap between the two bands:

$$\epsilon_{+}\left(\vec{k}\right) - \epsilon_{-}\left(\vec{k}\right) = 2\sqrt{\mathcal{H}_x\left(\vec{k}\right)^2 + \mathcal{H}_y\left(\vec{k}\right)^2 + \mathcal{H}_z\left(\vec{k}\right)^2} \tag{3.354}$$

At K or K', the gap is:

$$\epsilon_{+}\left(\vec{k}\right) - \epsilon_{-}\left(\vec{k}\right) = 2\sqrt{\mathcal{H}_x\left(\vec{k}\right)^2 + \mathcal{H}_y\left(\vec{k}\right)^2 + \mathcal{H}_z\left(\vec{k}\right)^2} = 2\left|\mathcal{H}_z\left(\vec{k} = K\right)\right| = 6\sqrt{3}\, t' \sin\phi \tag{3.355}$$

In fact, at the K point,

$$\mathcal{H}_z = -3\sqrt{3}\, t' \sin\phi \tag{3.356}$$

at the K' point

$$\mathcal{H}_z = 3\sqrt{3}\, t' \sin\phi \tag{3.357}$$

They have opposite signs (as long as ϕ is not n π).

Based on what we learned last time, this means that one cannot define the wavefunction in the whole BZ. We need to cut the systems into two regions. The region I contains the K point, the region II contains the K' points. And we need to use different eigenvectors for these two regions. Using the same method we learned in the last lecture, one finds that the Chern number here is ±1.

If one choose the boundary between region I and II to be very close to the K or K' points, one find that:

$$e^{i\,\phi(k)} = \frac{\frac{\mathcal{H}_z + \left|\vec{\mathcal{H}}(k)\right|}{\mathcal{H}_x(k) + i\,\mathcal{H}_y(k)}}{\left|\frac{\mathcal{H}_z + \left|\vec{\mathcal{H}}(k)\right|}{\mathcal{H}_x(k) + i\,\mathcal{H}_y(k)}\right|} = \frac{\left|\mathcal{H}_x(k) + i\,\mathcal{H}_y(k)\right|}{\mathcal{H}_x(k) + i\,\mathcal{H}_y(k)} = \frac{\left|q_x + i\,q_y\right|}{q_x + i\,q_y} = \frac{1}{e^{i\,\theta}} = e^{-i\,\theta} \tag{3.358}$$

3.14.5. Potential energy (breaking inversion symmetry)

Let's keep NNN hoppings to be zero for now and add some potential energy to the Hamiltonian to see whether we can open a gap to get an insulator.

$$H_{\text{Potential}} = (V + M)\sum_i a_i^{\dagger} a_i + (V - M)\sum_i b_i^{\dagger} b_i = V\,N + M\sum_i a_i^{\dagger} a_i - M\sum_i b_i^{\dagger} b_i \tag{3.359}$$

The V part (average potential between a and b sites) just adds a constant term to the energy, since the total particle number N is conserved. So we can drop the V term and only consider the difference between the potential energies at a and b sites (M).

In k-space

$$H_{\text{Potential}} = M\sum_i a_i^{\dagger} a_i - M\sum_i b_i^{\dagger} b_i = M\sum_k a_k^{\dagger} a_k - M\sum_k b_k^{\dagger} b_k = \sum_k \begin{pmatrix} a_k^{\dagger} & b_k^{\dagger} \end{pmatrix} M\,\sigma_z \begin{pmatrix} a_k \\ b_k \end{pmatrix} \tag{3.360}$$

It adds a σ_z component to the Hamiltonian. Same as the NNN complex hopping, this term also opens a gap at the Dirac point. If we add this term to the Hamiltonian without the complex NNN hoppings, the gap is 2M at K and K', and the system is a trivia insulator at half-filling.

Q: What will happen if we have both $H_{\text{Potential}}$ and H_{NNN}?

A: We just need to look at the signs of $\mathcal{H}_z$ at K and K' points. If they have the same sign, we can use one wavefunction to cover the whole BZ, so C=0 (trivial insulator). If they have opposite signs, the system is a topological insulator with C=±1

At the K point,

$$\mathcal{H}_z = M - 3\sqrt{3}\, t' \sin\phi \tag{3.361}$$

at the K' point

$$\mathcal{H}_z = M + 3\sqrt{3}\, t' \sin\phi \tag{3.362}$$

Therefore, as long as $|M| < |3\sqrt{3}\, t' \sin\phi|$, the system is an topological insulator ($\mathcal{H}_z$ flips sign). If $|M| > |3\sqrt{3}\, t' \sin\phi|$, $\mathcal{H}_z$ is always positive (or negative) and thus the system is topologically trivial.

The marginal case $|M| = |3\sqrt{3}\, t' \sin\phi|$ is a topological transition. Here, $\mathcal{H}_z = 0$ at either the K point or the K' point. Because $\mathcal{H}_x = \mathcal{H}_y = 0$ at these two points, the gap must be zero at one of the two points. So there is a band crossing in the system (either at K o K', depending on the sign of M ant t sin ϕ) and the system is not an insulator.

The insulating gap is closed at the topological transition point.

Remarks:

The model of Haldane is the first example of a topological insulator beyond quantum Hall effect.

It demonstrates that topological insulator is a generic concept, which may appear in any insulating systems (NOT just quantum Hall).

It also demonstrates that as long as the topological index is nonzero, one will observe all the topological phenomena expected for a quantum Hall state, including the quantized Hall conductivity and the existence of the edge states.

The key differences between the model of Haldane and the quantum Hall effects are (1) the B field is on average zero in the model of Haldane while the QHE has a uniform B field and (2) there is a very strong lattice background in the model of Haldane while the QHE requires weak lattice potential.

Systems similar to the Haldane's model are known as topological Chern insulators or Chern insulators (average B is 0 and have a strong lattice potential). But sometimes, Chern insulator are also used to refer to the quantum Hall effect.

The model of Haldane is also the foundation to explore more complicated and exotic topological states. For example, the time-reversal invariant topological insulators was first proposed using a modified Haldane's models, which we will study latter in the semester.