Honeycomb Lattice Model

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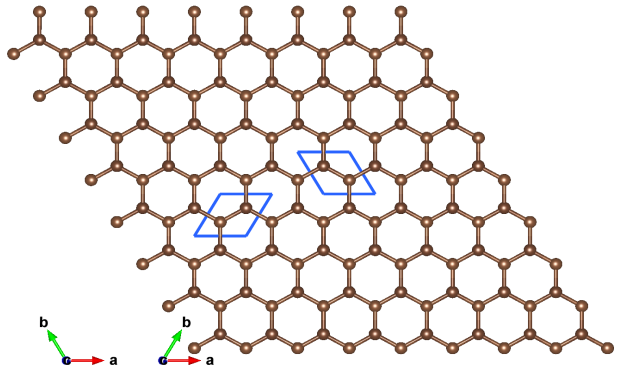

Figure 1: the structure of the honeycomb lattice and the corresponding unite vectors(basis) in the real space, there are two kinds of choice for the unite cell.

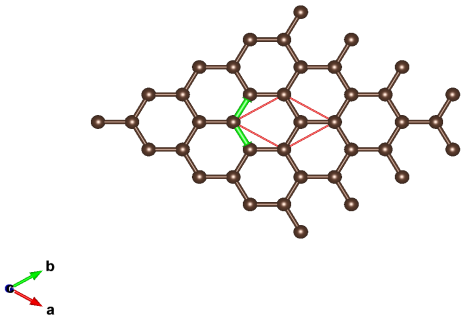

Figure 2: the basis for the unite cell in real space and the corresponding reciprocal space

§1 General Honeycomb Lattice and Its Properties

ℜ.1 Basic Lattice Structure

Honeycomb lattice is a very important system, many important models are constructed from it, so in this part, we make some efforts to think about this model in more details. as the Figure 1 shows.

this lattice consists of regular hexagon, these regular hexagons fill the whole two dimensional real space.

there are two kinds of choice for the unite cell, suppose the side length of the regular hexagon is a, this is also the distance for the nearest carbon atoms. then one choice of the unite cell consists of the following two basis

$$\vec{a}_1 = 2 \times a\cos\frac{\pi}{6}\hat{x} = \sqrt{3}a\hat{x} \quad \vec{a}_2 = R_z(\frac{2\pi}{3})\vec{a}_1 = -\frac{\sqrt{3}}{2}a\hat{x} + \frac{3}{2}a\hat{y}$$

these two unite vectors are related to each other by a rotation of $\frac{2\pi}{3}$ along the z direction.if we define $a_3 = \hat{z}$, then we can calculate the basis for the reciprocal space

$$b_1 = 2\pi\frac{\vec{a_2}\times\vec{a_3}}{\vec{a_1}\cdot\vec{a_2}\times\vec{a_3}} = 2\pi\frac{\frac{3}{2}a\hat{x} + \frac{\sqrt{3}}{2}a\hat{y}}{\frac{3\sqrt{3}}{2}a^2} = \frac{2\pi}{\sqrt{3}a}(\hat{x} + \frac{\sqrt{3}}{3}\hat{y})$$

$$b_2 = 2\pi\frac{\vec{a_3}\times\vec{a_1}}{\vec{a_1}\cdot\vec{a_2}\times\vec{a_3}} = 2\pi\frac{\sqrt{3}a\hat{y}}{\frac{3\sqrt{3}}{2}a^2} = \frac{2\pi}{\sqrt{3}a}(\frac{2\sqrt{3}}{3}\hat{y})$$

another kind choice of the unite vectors in the real space is

$$\vec{a}_1 = 2 \times a\cos\frac{\pi}{6}\hat{x} = \sqrt{3}a\hat{x} \quad \vec{a}_2 = R_z(\frac{\pi}{3})\vec{a}_1 = \frac{\sqrt{3}}{2}a\hat{x} + \frac{3}{2}a\hat{y}$$

these two unite vectors are related to each other by a rotation of $\frac{\pi}{3}$ along the z direction. and the corresponding basis in the reciprocal space is

$$b_1 = 2\pi\frac{\vec{a_2}\times\vec{a_3}}{\vec{a_1}\cdot\vec{a_2}\times\vec{a_3}} = 2\pi\frac{\frac{3}{2}a\hat{x} - \frac{\sqrt{3}}{2}a\hat{y}}{\frac{3\sqrt{3}}{2}a^2} = \frac{2\pi}{\sqrt{3}a}(\hat{x} - \frac{\sqrt{3}}{3}\hat{y})$$

$$b_2 = 2\pi\frac{\vec{a_3}\times\vec{a_1}}{\vec{a_1}\cdot\vec{a_2}\times\vec{a_3}} = 2\pi\frac{\sqrt{3}a\hat{y}}{\frac{3\sqrt{3}}{2}a^2} = \frac{2\pi}{\sqrt{3}a}(\frac{2\sqrt{3}}{3}\hat{y})$$

since these two kinds of choice are related to each other by a rotation(rotate the whole system $\frac{\pi}{3}$ along the z axes), and we often use the latter one.

in order to make the whole system looks more symmetric, we can rotate the whole system along the z axes $\frac{\pi}{6}$ counterclockwise, then the corresponding lattice vectors are

$$\vec{a}_1 \to R_z(-\frac{\pi}{6})\vec{a}_1 = \frac{3}{2}a\hat{x} - \frac{\sqrt{3}}{2}a\hat{y} \tag{1}$$

$$\vec{a}_2 \to R_z(-\frac{\pi}{6})\vec{a}_2 = \frac{3}{2}a\hat{x} + \frac{\sqrt{3}}{2}a\hat{y} \tag{2}$$

the reciprocal lattice vectors are

$$\vec{b}_1 \to R_z(-\frac{\pi}{6})\vec{b}_1 = \frac{2\pi}{\sqrt{3}a}(\frac{\sqrt{3}}{3}\hat{x} - \hat{y}) \tag{3}$$

$$\vec{b}_2 \to R_z(-\frac{\pi}{6})\vec{b}_2 = \frac{2\pi}{\sqrt{3}a}(\frac{\sqrt{3}}{3}\hat{x} + \hat{y}) \tag{4}$$

we can see these basis vectors transform to a more symmetric way as in the Figure 2. then using these lattice vectors in the reciprocal space, we can plot the first BZ and indicate some important symmetric points of the honeycomb system.

ℜ.2 Honeycomb lattice derivation from FCC lattice

for fcc lattice, the eight vortex coordinates are (in the basis $e_x = (1,0,0)^T$,$e_y = (0,1,0)^T$,$e_z = (0,0,1)^T$)

$$\begin{aligned} V_1 &= (0,0,0)^T & V_8 &= (1,1,1)^T & \\ V_2 &= (1,0,0)^T & V_3 &= (0,1,0)^T & V_4 &= (0,0,1)^T \\ V_5 &= (1,1,0)^T & V_6 &= (1,0,1)^T & V_7 &= (0,1,1)^T \end{aligned}$$

and coordinates for the six face center are:

$$\begin{aligned} F_1 &= (\frac{1}{2},\frac{1}{2},0)^T & F_6 &= (\frac{1}{2},\frac{1}{2},1)^T \\ F_2 &= (\frac{1}{2},0,\frac{1}{2})^T & F_5 &= (\frac{1}{2},1,\frac{1}{2})^T \\ F_3 &= (0,\frac{1}{2},\frac{1}{2})^T & F_6 &= (1,\frac{1}{2},\frac{1}{2})^T \end{aligned}$$

if we look from the [1,1,1] direction, where should these sites locate? in order to figure out this, we should at first put V_1V_8 direction as the new $\vec{e}_z{}'$ direction and use it to create new basis $\vec{e}_x{}'$ and $\vec{e}_y{}'$. then check the coordinates for these points in this new basis. so we establish that

$$\begin{aligned} \vec{e}_z{}' &= (e_x,e_y,e_z)\frac{1}{\sqrt{3}}(1,1,1)^T \\ \vec{e}_x{}' &= (e_x,e_y,e_z)\frac{1}{\sqrt{6}}(1,1,-2)^T \\ \vec{e}_y{}' &= \vec{e}_z{}' \times \vec{e}_x{}' = (e_x,e_y,e_z)\frac{1}{\sqrt{2}}(-1,1,0)^T \end{aligned}$$

or equivalently

$$(\vec{e}_x', \vec{e}_y', \vec{e}_z') = (e_x, e_y, e_z)U$$

where

$$U = \begin{pmatrix} \frac{1}{\sqrt{6}} & \frac{-1}{\sqrt{2}} & \frac{1}{\sqrt{3}} \\ \frac{1}{\sqrt{6}} & \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{3}} \\ \frac{-2}{\sqrt{6}} & 0 & \frac{1}{\sqrt{3}} \end{pmatrix} \tag{5}$$

and we have

$$U^{-1} = U^{\dagger} = \begin{pmatrix} \frac{1}{\sqrt{6}} & \frac{1}{\sqrt{6}} & \frac{-2}{\sqrt{6}} \\ \frac{-1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & 0 \\ \frac{1}{\sqrt{3}} & \frac{1}{\sqrt{3}} & \frac{1}{\sqrt{3}} \end{pmatrix} \tag{6}$$

since the vector $V = (e_x, e_y, e_z)X = (\vec{e}_x', \vec{e}_y', \vec{e}_z')U^{-1}X$,so the new coordinate in the new frame $(\vec{e}_x', \vec{e}_y', \vec{e}_z')$ is

$$X' = U^{-1}X = U^{\dagger}X$$

so the new coordinate for V_1 is $(0,0,0)^T$ for V_8 is

$$X_8' = U^{\dagger}(1,1,1)^T = \begin{pmatrix} \frac{1}{\sqrt{6}} & \frac{1}{\sqrt{6}} & \frac{-2}{\sqrt{6}} \\ \frac{-1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & 0 \\ \frac{1}{\sqrt{3}} & \frac{1}{\sqrt{3}} & \frac{1}{\sqrt{3}} \end{pmatrix} \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix} = (0,0,\sqrt{3})^T$$

so if we look from the [1,1,1] direction, V_1, V_8 are both located at the origin $(0,0)^T$. similarly, for V_2, we have

$$X_2' = U^{\dagger}(1,0,0)^T = \begin{pmatrix} \frac{1}{\sqrt{6}} & \frac{1}{\sqrt{6}} & \frac{-2}{\sqrt{6}} \\ \frac{-1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & 0 \\ \frac{1}{\sqrt{3}} & \frac{1}{\sqrt{3}} & \frac{1}{\sqrt{3}} \end{pmatrix} \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} = (\frac{1}{\sqrt{6}}, -\frac{1}{\sqrt{2}}, \frac{1}{\sqrt{3}})^T$$

for V_3, we have

$$X_3' = U^{\dagger}(0,1,0)^T = \begin{pmatrix} \frac{1}{\sqrt{6}} & \frac{1}{\sqrt{6}} & \frac{-2}{\sqrt{6}} \\ \frac{-1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & 0 \\ \frac{1}{\sqrt{3}} & \frac{1}{\sqrt{3}} & \frac{1}{\sqrt{3}} \end{pmatrix} \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} = (\frac{1}{\sqrt{6}}, \frac{1}{\sqrt{2}}, \frac{1}{\sqrt{3}})^T$$

for V_4, we have

$$X_4' = U^{\dagger}(0,0,1)^T = \begin{pmatrix} \frac{1}{\sqrt{6}} & \frac{1}{\sqrt{6}} & \frac{-2}{\sqrt{6}} \\ \frac{-1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & 0 \\ \frac{1}{\sqrt{3}} & \frac{1}{\sqrt{3}} & \frac{1}{\sqrt{3}} \end{pmatrix} \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} = (\frac{-2}{\sqrt{6}}, 0, \frac{1}{\sqrt{3}})^T$$

for V_5, we have

$$X_5' = U^{\dagger}(1,1,0)^T = \begin{pmatrix} \frac{1}{\sqrt{6}} & \frac{1}{\sqrt{6}} & \frac{-2}{\sqrt{6}} \\ \frac{-1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & 0 \\ \frac{1}{\sqrt{3}} & \frac{1}{\sqrt{3}} & \frac{1}{\sqrt{3}} \end{pmatrix} \begin{pmatrix} 1 \\ 1 \\ 0 \end{pmatrix} = (\frac{2}{\sqrt{6}}, 0, \frac{2}{\sqrt{3}})^T$$

for V_6, we have

$$X_6' = U^{\dagger}(1,0,1)^T = \begin{pmatrix} \frac{1}{\sqrt{6}} & \frac{1}{\sqrt{6}} & \frac{-2}{\sqrt{6}} \\ \frac{-1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & 0 \\ \frac{1}{\sqrt{3}} & \frac{1}{\sqrt{3}} & \frac{1}{\sqrt{3}} \end{pmatrix} \begin{pmatrix} 1 \\ 0 \\ 1 \end{pmatrix} = (\frac{-1}{\sqrt{6}}, \frac{-1}{\sqrt{2}}, \frac{2}{\sqrt{3}})^T$$

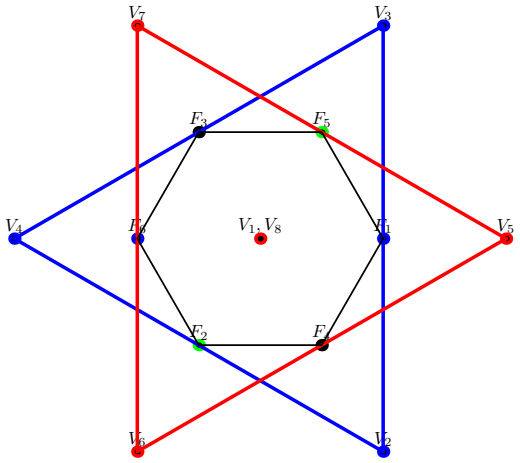

Figure 3: fcc lattice look from [111] direction

for V_7, we have

$$X_7' = U^\dagger(0,1,1)^T = \begin{pmatrix} \frac{1}{\sqrt{6}} & \frac{1}{\sqrt{6}} & \frac{-2}{\sqrt{6}} \\ \frac{-1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & 0 \\ \frac{1}{\sqrt{3}} & \frac{1}{\sqrt{3}} & \frac{1}{\sqrt{3}} \end{pmatrix} \begin{pmatrix} 0 \\ 1 \\ 1 \end{pmatrix} = (\frac{-1}{\sqrt{6}}, \frac{1}{\sqrt{2}}, \frac{2}{\sqrt{3}})^T$$

similarly, for the face center, we have

$$X_{F1}' = \frac{1}{2}(X_2' + X_3') = (\frac{1}{\sqrt{6}}, 0, \frac{1}{\sqrt{3}})^T$$

$$X_{F6}' = \frac{1}{2}(X_6' + X_7') = (\frac{-1}{\sqrt{6}}, 0, \frac{2}{\sqrt{3}})^T$$

$$X_{F2}' = \frac{1}{2}(X_2' + X_4') = (\frac{-1}{2\sqrt{6}}, -\frac{1}{2\sqrt{2}}, \frac{1}{\sqrt{3}})^T$$

$$X_{F5}' = \frac{1}{2}(X_5' + X_7') = (\frac{1}{2\sqrt{6}}, \frac{1}{2\sqrt{2}}, \frac{2}{\sqrt{3}})^T$$

$$X_{F3}' = \frac{1}{2}(X_3' + X_4') = (\frac{-1}{2\sqrt{6}}, \frac{1}{2\sqrt{2}}, \frac{1}{\sqrt{3}})^T$$

$$X_{F6}' = \frac{1}{2}(X_5' + X_6') = (\frac{1}{2\sqrt{6}}, -\frac{1}{2\sqrt{2}}, \frac{2}{\sqrt{3}})^T$$

so, when we look from [1,1,1] direction, the whole graph looks as Figure 3.

§2 Graphene and Its Properties

ℜ.1 Basic Configuration

as for graphene, it‘s just the honeycomb lattice with two different atoms in each unite cell, we can draw its structure and the corresponding BZ as the Figure 4 illustration.

The lattice vectors for the graphene structure are:

$$\vec{a}_1 = \frac{a}{2}(3, -\sqrt{3}) \quad \vec{a}_2 = \frac{a}{2}(3, \sqrt{3})$$

and the vectors connecting the nearest coupling are:

$$\delta_1 = \frac{a}{2}(1, \sqrt{3}) \quad \delta_2 = \frac{a}{2}(1, -\sqrt{3}) \quad \delta_3 = -a(1, 0)$$

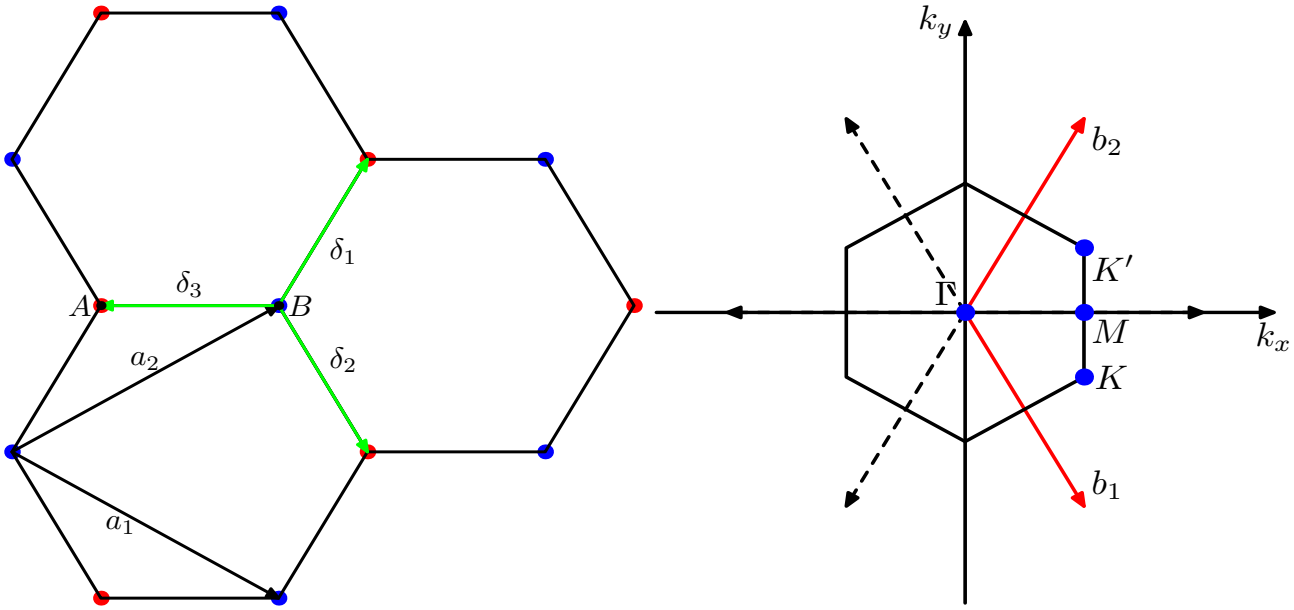

Figure 4: the lattice structure of the graphene and the corresponding Brillouin Zone. Left: the lattice structure, $a_1 = \frac{a}{2}(3, -\sqrt{3})$ and $a_2 = \frac{a}{2}(3, \sqrt{3})$ are the lattice vectors and $\delta_1 = \frac{1}{3}(-a_1 + 2a_2) = \frac{a}{2}(1, \sqrt{3})$,$\delta_2 = \frac{1}{3}(2a_1 - a_2) = \frac{a}{2}(1, -\sqrt{3})$,$\delta_3 = -\frac{1}{3}(a_1 + a_2) = -a(1, 0)$ are the vectors connecting the nearest couplings. Right: the first BZ for the graphene, $b_1 = \frac{2\pi}{\sqrt{3}a}(\frac{\sqrt{3}}{3}, -1)$ and $b_2 = \frac{2\pi}{\sqrt{3}a}(\frac{\sqrt{3}}{3}, 1)$ are the lattice vector for the reciprocal lattice. $\Gamma = (0, 0)$, $K = \frac{2}{3}b_1 + \frac{1}{3}b_2 = \frac{2\pi}{\sqrt{3}a}(\frac{\sqrt{3}}{3}, -\frac{1}{3})$,$K' = \frac{2}{3}b_2 + \frac{1}{3}b_1 = \frac{2\pi}{\sqrt{3}a}(\frac{\sqrt{3}}{3}, \frac{1}{3})$, $M = \frac{1}{2}(b_1 + b_2) = \frac{2\pi}{\sqrt{3}a}(\frac{\sqrt{3}}{3}, 0)$ are the high symmetric points in the Brillouin Zone. and a is the length of the nearest bond.

the lattice vectors for the reciprocal lattice are:

$$\vec{b}_1 = \frac{2\pi}{\sqrt{3}a}(\frac{\sqrt{3}}{3}, -1) \quad \vec{b}_2 = \frac{2\pi}{\sqrt{3}a}(\frac{\sqrt{3}}{3}, 1)$$

and there are many high symmetric points in the BZ which read as

$$\Gamma = (0, 0) \quad K = \frac{2\pi}{\sqrt{3}a}(\frac{\sqrt{3}}{3}, -\frac{1}{3}) \quad K' = \frac{2\pi}{\sqrt{3}a}(\frac{\sqrt{3}}{3}, \frac{1}{3}) \quad M = \frac{2\pi}{\sqrt{3}a}(\frac{\sqrt{3}}{3}, 0)$$

ℜ.2 Bulk Properties

as for graphene, we can write down the lattice tight binding model which read as

$$H = -t \sum_{<i,j>,\sigma} (a^\dagger_{i,\sigma} b_{j,\sigma} + H.c) - t' \sum_{<<i,j>>,\sigma} (a^\dagger_{i,\sigma} a_{j,\sigma} + b^\dagger_{i,\sigma} b_{j,\sigma} + H.c)$$

the first term is the nearest coupling term for different kinds of atoms and the second term is the next nearest coupling of the same kind of atoms for both A and B atoms.

since when we translate the unite cell with integer combination of the lattice unite vectors we can fill the whole space and in each such translated unite cell, there are only one of each A and B atoms, so we can use $r_{m,n}$ to label the position of the translated unite cell with respect to the original one, which means that

$$r_{m,n} = m\vec{a}_1 + n\vec{a}_2$$

and the position of the A and B atom in the primary unite cell is r_A and r_B. then we can find that

$$r_{A(B),m,n} = r_{A(B)} + m\vec{a}_1 + n\vec{a}_2$$

in order to derive the properties in the bulk, we should choose the periodic boundary condition and in each direction there are N_1 and N_2 sites.then the Fourier transform is($k_1 = \frac{b_1}{N_1} l_1$ and $k_2 = \frac{b_2}{N_2} l_2$ is along the b_1 and b_2 namely, $(k_1, k_2) = k_1\hat{b}_1 + k_2\hat{b}_2$)

$$c_{A(B),k_1,k_2,\sigma} = \frac{1}{\sqrt{N_1 N_2}} \sum_{m,n} e^{-i(k_1,k_2)\cdot r_{A(B),m,n}} c_{A(B),m,n,\sigma}$$

$$c_{A(B),m,n,\sigma} = \frac{1}{\sqrt{N_1 N_2}} \sum_{k_1,k_2} e^{i(k_1,k_2)\cdot r_{A(B),m,n}} c_{A(B),k_1,k_2,\sigma}$$

then we have

$$\begin{aligned}
&\sum_{<i,j>,\sigma} (a^\dagger_{i,\sigma} b_{j,\sigma} + H.c) \\
&= \sum_{<(m,n),(l,s)>,\sigma} \frac{1}{N_1 N_2} \sum_{(k_1,k_2),(k_1',k_2')} a^\dagger_{k_1,k_2,\sigma} b_{k_1',k_2',\sigma} e^{-i(k_1,k_2)\cdot r_{A,m,n}} e^{i(k_1',k_2')\cdot r_{B,l,s}} + H.c \\
&= \sum_{(l,s),\sigma} \frac{1}{N_1 N_2} \sum_{(k_1,k_2),(k_1',k_2')} a^\dagger_{k_1,k_2,\sigma} b_{k_1',k_2',\sigma} e^{i(k_1,k_2)\cdot r_{B,l,s}} (\sum_{i=1}^{3} e^{-i(k_1,k_2)\cdot\delta_i}) e^{-i(k_1',k_2')\cdot r_{B,l,s}} + H.c \\
&= \sum_{(k_1,k_2),(k_1',k_2'),\sigma} a^\dagger_{k_1,k_2,\sigma} b_{k_1',k_2',\sigma} \delta_{k_1,k_1'} \delta_{k_2,k_2'} (\sum_{i=1}^{3} e^{-i(k_1,k_2)\cdot\delta_i}) + H.c \\
&= \sum_{(k_1,k_2),\sigma} (\sum_{i=1}^{3} e^{-i(k_1,k_2)\cdot\delta_i}) a^\dagger_{k_1,k_2,\sigma} b_{k_1,k_2,\sigma} + H.c
\end{aligned}$$

similarly, we have

$$\begin{aligned}
&\sum_{<<i,j>>,\sigma} (a^\dagger_{i,\sigma} a_{j,\sigma} + H.c) \\
&= \sum_{<(m,n),(l,s)>,\sigma} \frac{1}{N_1 N_2} \sum_{(k_1,k_2),(k_1',k_2')} a^\dagger_{k_1,k_2,\sigma} a_{k_1',k_2',\sigma} e^{-i(k_1,k_2)\cdot r_{A,m,n}} e^{i(k_1',k_2')\cdot r_{B,l,s}} + H.c \\
&= \frac{1}{2} \sum_{(l,s),\sigma} \frac{1}{N_1 N_2} \sum_{(k_1,k_2),(k_1',k_2')} a^\dagger_{k_1,k_2,\sigma} a_{k_1',k_2',\sigma} e^{-i(k_1,k_2)\cdot r_{B,l,s}} e^{i(k_1',k_2')\cdot r_{B,l,s}} (\cdots) + H.c \\
&(\cdots) = (e^{-i(k_1,k_2)\cdot a_1} + e^{-i(k_1,k_2)\cdot a_2} + e^{-i(k_1,k_2)\cdot(a_2-a_1)} + e^{-i(k_1,k_2)\cdot -a_1} + e^{-i(k_1,k_2)\cdot -a_2} + e^{-i(k_1,k_2)\cdot -(a_2-a_1)}) \\
&= \frac{1}{2} \sum_{(k_1,k_2),\sigma} (\cdots) a^\dagger_{k_1,k_2,\sigma} a_{k_1,k_2,\sigma} + H.c \\
&= \sum_{(k_1,k_2),\sigma} (\cdots) a^\dagger_{k_1,k_2,\sigma} a_{k_1,k_2,\sigma}
\end{aligned}$$

where the extra factor of $\frac{1}{2}$ comes from that when we counts the next nearest bonds, we have count each bond for twice when we sum over all the cells(because there is H.c means that the bond is un-directional), besider $(\cdots) = (e^{-i(k_1,k_2)\cdot a_1} + e^{-i(k_1,k_2)\cdot a_2} + e^{-i(k_1,k_2)\cdot(a_2-a_1)} + e^{-i(k_1,k_2)\cdot -a_1} + e^{-i(k_1,k_2)\cdot -a_2} + e^{-i(k_1,k_2)\cdot -(a_2-a_1)})$ in the above equation. with the same calculation, we know that

$$\begin{aligned}
&\sum_{<<i,j>>,\sigma} (b^\dagger_{i,\sigma} b_{j,\sigma} + H.c) \\
&= \sum_{(k_1,k_2),\sigma} (\cdots) b^\dagger_{k_1,k_2,\sigma} b_{k_1,k_2,\sigma}
\end{aligned}$$

so after collecting all the terms, we know that the hamiltonian in momentum space is

$$H = \sum_{(k_1,k_2),\sigma} \{(-t(\sum_{i=1}^{3} e^{i(k_1,k_2)\cdot\delta_i}) a^\dagger_{k_1,k_2,\sigma} b_{k_1,k_2,\sigma} + H.c) - t'((\cdots) a^\dagger_{k_1,k_2,\sigma} a_{k_1,k_2,\sigma} + (\cdots) b^\dagger_{k_1,k_2,\sigma} b_{k_1,k_2,\sigma})\}$$

since the spin degree of freedom is degeneracy and we can use the the following basis

$$\gamma_{k_1,k_2,\sigma} = (a_{k_1,k_2,\sigma}, b_{k_1,k_2,\sigma})^T$$

then we have

$$H = \sum_{(k_1,k_2),\sigma} \gamma^\dagger_{k_1,k_2,\sigma} H_{(k_1,k_2)} \gamma_{k_1,k_2,\sigma}$$

where the metrics H read as

$$H_{(k_1,k_2)} = \begin{pmatrix} -t'(\cdots) & -t\sum_{i=1}^3 e^{-i(k_1,k_2)\cdot\delta_i} \\ -t\sum_{i=1}^3 e^{i(k_1,k_2)\cdot\delta_i} & -t'(\cdots) \end{pmatrix} \tag{7}$$

the energy spectrum is

$$E_{(k_1,k_2)} = -t'(\cdots) \pm t|\sum_{i=1}^3 e^{i(k_1,k_2)\cdot\delta_i}|$$

since we know that

$$\vec{b}_1 = \frac{2\pi}{\sqrt{3}a}(\frac{\sqrt{3}}{3}, -1) \quad \vec{b}_2 = \frac{2\pi}{\sqrt{3}a}(\frac{\sqrt{3}}{3}, 1)$$

so $\hat{b}_1 = \frac{1}{2}(1, -\sqrt{3})$ and $\hat{b}_2 = \frac{1}{2}(1, \sqrt{3})$ and $\hat{b}_1 \cdot a_1 = \frac{2\pi}{|\vec{b_1}|} = \frac{3}{2}a$, $\hat{b}_2 \cdot a_2 = \frac{2\pi}{|\vec{b_2}|} = \frac{3}{2}a$ and $\hat{b}_2 \cdot a_1 = \hat{b}_1 \cdot a_2 = 0$,so we have

$$E_{k_x,k_y} = E_{(k_x - \frac{k_y}{\sqrt{3}}, k_x + \frac{k_y}{\sqrt{3}})}$$

and we can calculate the spectrum in E_{k_x,k_y} as$(k_1 = (k_x - \frac{k_y}{\sqrt{3}})\hat{b}_1, k_2 = (k_x + \frac{k_y}{\sqrt{3}})\hat{b}_2)$

$$\begin{aligned} -t'(\cdots) &= -t'(e^{-i(k_x - \frac{k_y}{\sqrt{3}})\frac{3}{2}a} + e^{-i(k_x + \frac{k_y}{\sqrt{3}})\frac{3}{2}a} + e^{i(k_x - \frac{k_y}{\sqrt{3}})\frac{3}{2}a} e^{-i(k_x + \frac{k_y}{\sqrt{3}})\frac{3}{2}a} + c.c) \\ &= -t'(e^{-i(k_x - \frac{k_y}{\sqrt{3}})\frac{3}{2}a} + e^{-i(k_x + \frac{k_y}{\sqrt{3}})\frac{3}{2}a} + e^{-i\sqrt{3}ak_y} + c.c) \\ &= -t'(2\cos(\sqrt{3}ak_y) + 4\cos(\frac{3}{2}ak_x)\cos(\frac{\sqrt{3}}{2}ak_y)) \\ &= -t'f(\mathbf{k}) \end{aligned}$$

where we have defined $f(\mathbf{k}) = 2\cos(\sqrt{3}ak_y) + 4\cos(\frac{3}{2}ak_x)\cos(\frac{\sqrt{3}}{2}ak_y)$

$$-t\sum_{i=1}^3 e^{-i(k_1,k_2)\cdot\delta_i} = -t(e^{-i(\frac{1}{2}ak_x + \frac{\sqrt{3}}{2}ak_y)} + e^{-i(\frac{1}{2}ak_x - \frac{\sqrt{3}}{2}ak_y)} + e^{-i(-ak_x)})$$

which means that

$$\begin{aligned} |-t\sum_{i=1}^3 e^{-i(k_1,k_2)\cdot\delta_i}| &= t\sqrt{3 + (e^{i\sqrt{3}ak_y} + c.c) + (e^{i(-\frac{3}{2}ak_x - \frac{\sqrt{3}}{2}ak_y)} + c.c) + (e^{i(-\frac{3}{2}ak_x + \frac{\sqrt{3}}{2}ak_y)} + c.c)} \\ &= t\sqrt{3 + f(\mathbf{k})} \end{aligned}$$

collecting all these terms, we can find that the spectrum of the graphene is

$$E_{\mathbf{k}} = -t'f(\mathbf{k}) \pm t\sqrt{3 + f(\mathbf{k})}$$

since we have

$$f(R_z(\frac{\pi}{3})\vec{k}) = 2\cos(\sqrt{3}a(\frac{\sqrt{3}}{2}k_x + \frac{1}{2}k_y)) + 4\cos(\frac{3}{2}a(\frac{1}{2}k_x - \frac{\sqrt{3}}{2}k_y))\cos(\frac{\sqrt{3}}{2}a(\frac{\sqrt{3}}{2}k_x + \frac{1}{2}k_y))$$

$$
\begin{aligned}
&= 2\cos(\frac{3}{2}ak_x + \frac{\sqrt{3}}{2}ak_y) + 4 \times \frac{1}{2}(\cos(\frac{3}{2}ak_x - \frac{\sqrt{3}}{2}ak_y) + \cos(\sqrt{3}ak_y)) \\
&= 2\cos(\sqrt{3}ak_y) + 2(cos(\frac{3}{2}ak_x + \frac{\sqrt{3}}{2}ak_y) + cos(\frac{3}{2}ak_x - \frac{\sqrt{3}}{2}ak_y)) \\
&= 2\cos(\sqrt{3}ak_y) + 4\cos(\frac{3}{2}ak_x)\cos(\frac{\sqrt{3}}{2}ak_y) = f(\vec{k})
\end{aligned}
$$

which means that the energy band of the graphene has a six-fold rotation symmetry, so we can try to find the energy minima just in one sixth region of the first Brillouin Zone. namely in the triangle spanned by Γ, K, K' since we have in the triangle Γ, K, K' region, $\frac{3}{2}ak_x \in (0, \frac{3}{2}a\frac{2\pi}{\sqrt{3}a}\frac{\sqrt{3}}{3}) = (0, \pi)$ and $\frac{\sqrt{3}}{2}ak_y \in (-\frac{\sqrt{3}}{2}a\frac{2\pi}{\sqrt{3}a}\frac{1}{3}, \frac{\sqrt{3}}{2}a\frac{2\pi}{\sqrt{3}a}\frac{1}{3}) = (-\frac{\pi}{3}, \frac{\pi}{3})$ so we have

$$
\partial_{k_x} f(k) = 4\cos(\frac{\sqrt{3}}{2}ak_y)(-\frac{3}{2}a\sin(\frac{3}{2}ak_x)) < 0
$$

and when $k_x = \frac{2\pi}{\sqrt{3}a}\frac{\sqrt{3}}{3}$, we have

$$
f(\frac{2\pi}{3a}, k_y) = 2\cos(\sqrt{3}ak_y) - 4\cos(\frac{\sqrt{3}}{2}ak_y) = 4(\cos(\frac{\sqrt{3}}{2}ak_y) - \frac{1}{2})^2 - 3
$$

so as k_y goes from 0 to $\pm\frac{2\pi}{\sqrt{3}a}\frac{1}{3}$ the function $f(\frac{2\pi}{3a}, k_y)$ decrease from -2 to -3

when $k_y = \frac{\sqrt{3}}{3}k_x$, we have

$$
\begin{aligned}
f(k_x, \frac{\sqrt{3}}{3}k_x) &= 2\cos(ak_x) + 4\cos(\frac{3}{2}ak_x)\cos(\frac{1}{2}ak_x) \\
&= 2\cos(\frac{2}{3}t) + 4\cos(t)\cos(\frac{1}{3}t) \;\; (t = \frac{3}{2}ak_x \in (0, \pi)) \\
&= 2\cos(\frac{2}{3}t) + 2(\cos(\frac{2}{3}t) + \cos(\frac{4}{3}t)) \\
&= 4(\cos(\frac{2}{3}t) + \frac{1}{2})^2 - 3
\end{aligned}
$$

which means that as k_x goes from 0 to $\frac{2\pi}{\sqrt{3}a}\frac{\sqrt{3}}{3}$,then $(k_x, \frac{\sqrt{3}}{3}k_x)$ goes from Γ point to K' and f(k) decrease from 6 to -3

collecting all the discussion above together the six-fold rotation symmetry, we can have the behavior of $f(k)$ in the whole BZ which is illustrated in Figure 5. since for the energy band we have

$$
E_{k,+} - E_{k,-} = 2t\sqrt{3 + f(k)}
$$

so we can clearly see the whole upper band and the lower band touch at $f(k) = -3$, which is just the K and K' point. so the bulk is gapped except for the K and K' points which is called the Dirac points. if we expand the f(k) near this two Dirac points, we have

$$
\begin{aligned}
f(K + \vec{k}) &= 2\cos(-\frac{2\pi}{3} + \sqrt{3}ak_y) + 4\cos(\pi + \frac{3}{2}ak_x)\cos(-\frac{\pi}{3} + \frac{\sqrt{3}}{2}ak_y) \\
&= 2(-\frac{1}{2}\cos(\sqrt{3}ak_y) + \frac{\sqrt{3}}{2}\sin(\sqrt{3}ak_y)) - 4\cos(\frac{3}{2}ak_x)(\frac{1}{2}\cos(\frac{\sqrt{3}}{2}ak_y) + \frac{\sqrt{3}}{2}\sin(\frac{\sqrt{3}}{2}ak_y)) \\
&= -(1 - \frac{1}{2}3a^2k_y^2) + 3ak_y - 4(1 - \frac{1}{2}\frac{9}{4}a^2k_x^2)(\frac{1}{2}(1 - \frac{1}{2}\frac{3}{4}a^2k_y^2) + \frac{3}{4}ak_y) \\
&= -3 + \frac{9}{4}a^2k_x^2 + \frac{9}{4}a^2k_y^2
\end{aligned}
$$

so the leader term in the energy spectrum near the Dirac Points are

$$
E_{K+\vec{k},\pm} = -t'(-3) \pm \sqrt{3 - 3 + \frac{9}{4}a^2k_x^2 + \frac{9}{4}a^2k_y^2} = 3t' \pm \frac{3at}{2}|\vec{k}|
$$

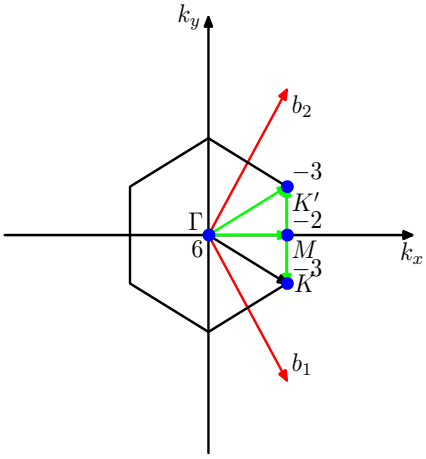

Figure 5: the behavior of f(k) in the Brillouin zone, the arrow means monotonous decreasing direction of the value.the behavior of f(k) in other regions can be obtain from the triangle $\Gamma KK'$ by the six-fold rotation symmetry

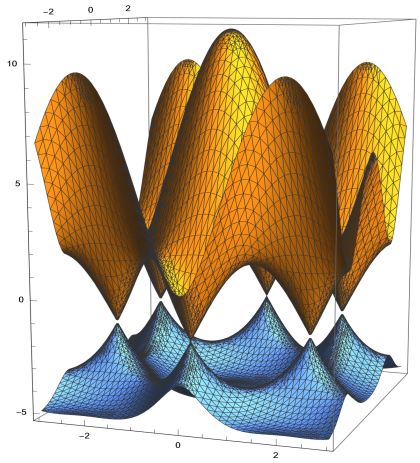

Figure 6: the band structure of the graphene,where we have chosen the parameter a=1 $t = 2.7$ and $t' = -0.2t$

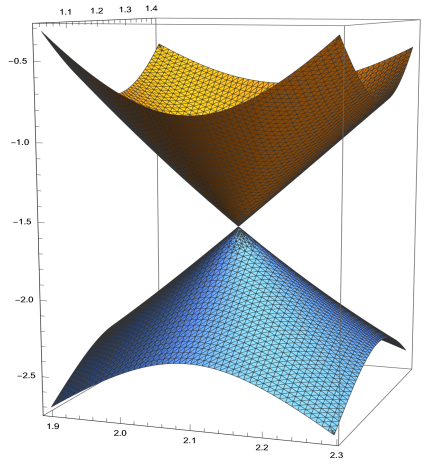

Figure 7: the Dirac Cone near the Dirac Points K and K'

we can see that the dispersion relation is linear on $|\vec{k}|$,which means that this is a cone, called the Dirac Cone near the Dirac points K and K'. This linear relation means that the fermi velocity $\frac{\partial E}{\partial k}$ remains constant and does not rely on the energy. with all these knowledge in mind, we can draw the band structure of the graphene (Figure 6).

ℜ.3 The Boundary Modes

as for the graphene, there are two kinds of boundary, one is called the Zigzag boundary and other one is called armchair boundary, which is illustrated as in Figure 8

§3 Haldane model and its properties

ℜ.1 General Configuration

another important model constructed from honeycomb lattice is the famous Haldane model. Haldane use this model to argue that the critical point for the integer quantum hall effect is not the existence of the magnetic field but the breaking of the time reversal symmetry of the whole system. The quantum hall effect without external magnetic field is called the anomalous quantum hall effect.

the model and it's flux configuration is illustrated in the Figure 9. in this model, in each Lattice site A and B, he introduced the onsite energy of M and $-M$

$$\sum_{i\in A} M c_i^\dagger c_i + \sum_{j\in B} (-M) c_j^\dagger c_j$$

so that the inversion symmetry of the whole system is breaking. if M=0 the symmetry group is $C_{6,v}$ and if $M \neq 0$, the symmetry group is $C_{3,v}$.

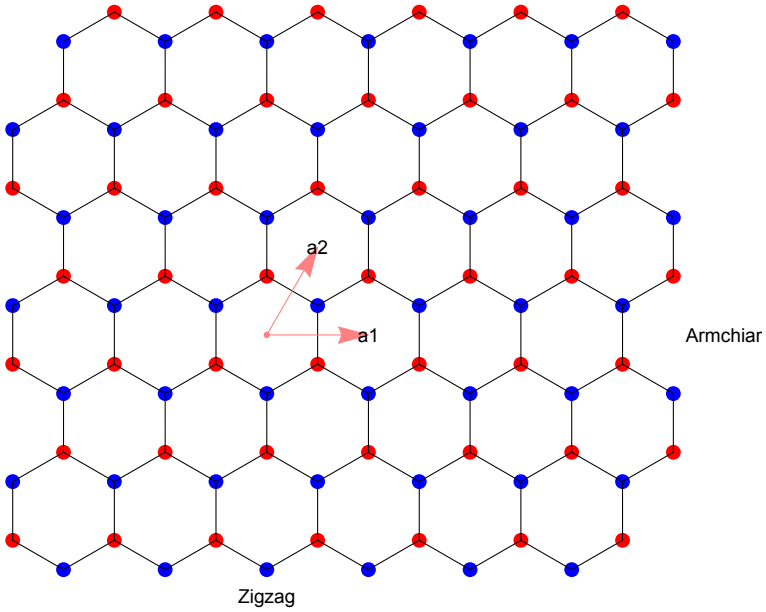

Figure 8: two kinds of boundary for graphene system, one is called the Zigzag boundary and other one is called the Armchair boundary

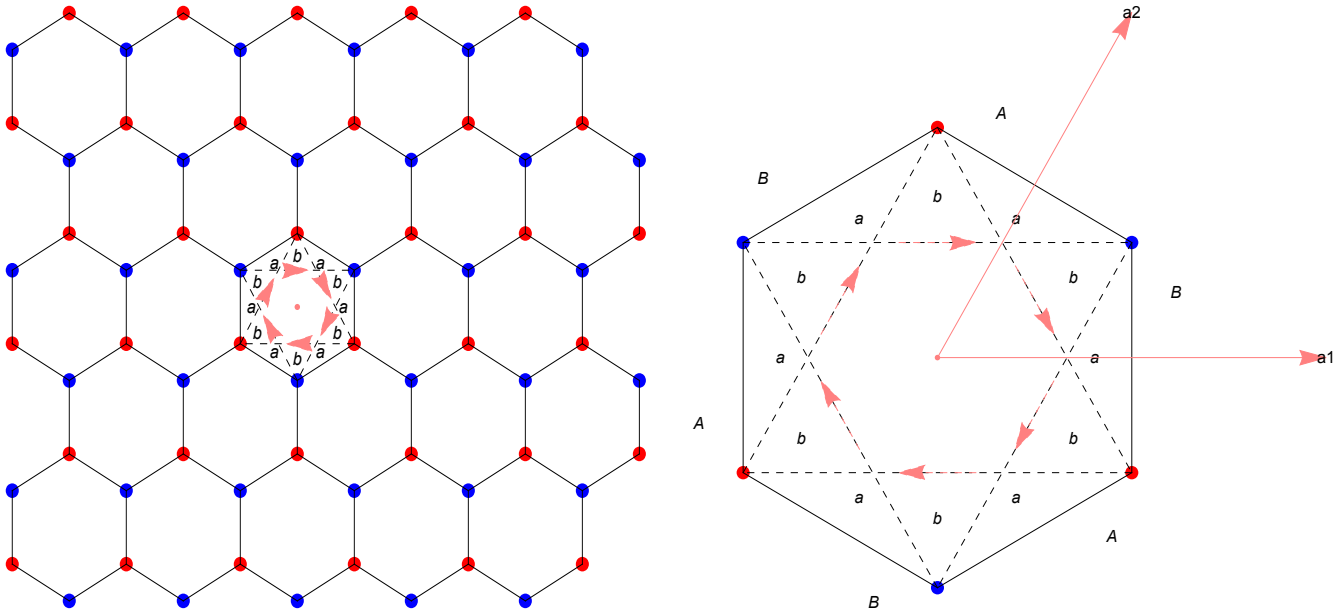

Figure 9: Left: the overall lattice tight binding model of the Haldane model, it's the honeycomb lattice. Right: the flux configuration in each regular hexagons

besides the onsite term, there is also a nearest coupling term just like the honeycomb lattice

$$\sum_{<i,j>} t_1(c_i^\dagger c_j + c_j^\dagger c_i)$$

the most important part of this model is that to break time-reversal invariance, he also add a periodic local magnetic-flux density B(r) in the z direction normal to the 2D plane, with the full symmetry of the lattice, and with zero total flux through the unit cell.

since closed paths of first-neighbor hops enclose complete unit cells (and hence no net flux),the extra phases we gain for the parameter t_1 from Peierls Substitution due to the periodic magnetic filed is

$$\frac{ie}{\hbar}\int_{A\to B}\vec{A}\cdot d\vec{l} = \frac{1}{6}\frac{ie}{\hbar}\oint_{\partial(\text{Cell})}\vec{A}\cdot d\vec{l} = \frac{1}{6}\frac{ie}{\hbar}\int_{\text{Cell}}\vec{B}\cdot d\vec{S} = \frac{1}{6}\frac{ie}{\hbar}\Phi_{\text{total}} = 0$$

which means that the t_1 matrix elements for the nearest coupling are unaffected.

since the phase is path related, we can consider the extra phases we gain for the next nearest couplings along the straight line which is indicated as arrow in Figure 9. so the extra phases for the t_2 hopping is

$$\frac{ie}{\hbar}\int_{A_1\to A_2}\vec{A}\cdot d\vec{l} = \frac{ie}{\hbar}\int_{A_1\to A_2}\vec{A}\cdot d\vec{l} + \frac{ie}{\hbar}\int_{A_2\to B}\vec{A}\cdot d\vec{l} + \frac{ie}{\hbar}\int_{B\to A_2}\vec{A}\cdot d\vec{l} = i\frac{e}{\hbar}(2\Phi_a+\Phi_b) = i2\pi\frac{2\Phi_a+\Phi_b}{\Phi_0}$$

where $\Phi_0 = \frac{h}{e}$ is the fundamental flux. so we have $t_2 \to t_2 e^{i2\pi\frac{2\Phi_a+\Phi_b}{\Phi_0}}$ if the next nearest hopping is along the direction as the arrow shows in Figure 9.define $\phi = 2\pi\frac{2\Phi_a+\Phi_b}{\Phi_0}$, then $t_2 \to t_2 e^{i\phi}$ and the total flux in the minor hexagons inside the unite cell is $-6(\Phi_a+\Phi_b)$ so as to maintain the net flux in the entire unite cell to be zero.

with this in mind, we can see that for atoms A ,if the next nearest hopping in the a_1 direction, the extra phase for the term $c_{i,A}^\dagger c_{i+a_1,A}$ is $e^{i\phi}$, since it annihilates a electron at $i+a_1$ and create an electron at i sites, which means the electron moves from $i+a_1$ to i along a_1, which is just the same direction of these arrows. and if the next nearest hopping is along the a_2 direction, the extra phase is $e^{-i\phi}$, since the electron moves just opposite the direction of these arrows, But as for atom B, if the next nearest hopping is along the a_1 direction, the extra phase is $e^{-i\phi}$, since the electron moves just opposite the direction of these arrows. and if the next nearest hopping is along the a_2 direction, the extra phase is $e^{i\phi}$, since electron moves just along the opposite direction of these arrows. with this in mind we can write down the next nearest hopping term of this model (we use (m,n) to replace the site i since it's two dimensional) and write $a_3 = a_2 - a_1$,

$$\begin{aligned}\sum_{(m,n)\in A} t_2(&e^{i\phi}c_{(m,n)}^\dagger c_{(m,n)+a_1} + e^{-i\phi}c_{(m,n)}^\dagger c_{(m,n)+a_2} + e^{i\phi}c_{(m,n)}^\dagger c_{(m,n)+a_2-a_1}\\ &+ e^{-i\phi}c_{(m,n)}^\dagger c_{(m,n)-a_1} + e^{i\phi}c_{(m,n)}^\dagger c_{(m,n)-a_2} + e^{-i\phi}c_{(m,n)}^\dagger c_{(m,n)-(a_2-a_1)})\end{aligned}$$

$$\begin{aligned}\sum_{(m,n)\in B} t_2(&e^{-i\phi}c_{(m,n)}^\dagger c_{(m,n)+a_1} + e^{i\phi}c_{(m,n)}^\dagger c_{(m,n)+a_2} + e^{-i\phi}c_{(m,n)}^\dagger c_{(m,n)+a_2-a_1}\\ &+ e^{i\phi}c_{(m,n)}^\dagger c_{(m,n)-a_1} + e^{-i\phi}c_{(m,n)}^\dagger c_{(m,n)-a_2} + e^{i\phi}c_{(m,n)}^\dagger c_{(m,n)-(a_2-a_1)})\end{aligned}$$

note that the above one has no H.c, since we think that this term is for one specific atoms connection to the next nearest ones. similarly we can use the Fourier Transform to move on to the momentum space

$$c_{A(B),k_1,k_2,\sigma} = \frac{1}{\sqrt{N_1N_2}}\sum_{m,n} e^{-i(k_1,k_2)\cdot r_{A(B),m,n}} c_{A(B),m,n,\sigma}$$

$$c_{A(B),m,n,\sigma} = \frac{1}{\sqrt{N_1 N_2}} \sum_{k_1,k_2} e^{i(k_1,k_2)\cdot r_{A(B),m,n}} c_{A(B),k_1,k_2,\sigma}$$

the onsite term is just simply:

$$\begin{aligned}
\sum_{(m,n)} \pm M c^\dagger_{(m,n)} c_{(m,n)} &= \sum_{(m,n)} \pm M \sum_{(k_1,k_2)} \sum_{(k_1',k_2')} \frac{1}{N_1 N_2} a^\dagger_{k_1,k_2} a_{k_1',k_2'} e^{-i(k_1,k_2)\cdot r_{m,n}} e^{i(k_1',k_2')\cdot r_{m,n}} \\
&= \pm M \sum_{(k_1,k_2)} \sum_{(k_1',k_2')} a^\dagger_{k_1,k_2} a_{k_1',k_2'} \delta_{k_1,k_1'} \delta_{k_2,k_2'} \\
&= \pm M \sum_{(k_1,k_2)} a^\dagger_{k_1,k_2} a_{k_1,k_2}
\end{aligned}$$

which means that the onsite terms is

$$M \sum_{(k_1,k_2)} a^\dagger_{k_1,k_2,A} a_{k_1,k_2,A} - M \sum_{(k_1,k_2)} a^\dagger_{k_1,k_2,B} a_{k_1,k_2,B}$$

since t_1 is unaffected, so the nearest hopping term is the same as the graphene

$$\begin{aligned}
&\sum_{<i,j>,\sigma} (a^\dagger_{i,\sigma} b_{j,\sigma} + H.c) \\
&= \sum_{<(m,n),(l,s)>,\sigma} \frac{1}{N_1 N_2} \sum_{(k_1,k_2),(k_1',k_2')} a^\dagger_{k_1,k_2,\sigma} b_{k_1',k_2',\sigma} e^{-i(k_1,k_2)\cdot r_{A,m,n}} e^{i(k_1',k_2')\cdot r_{B,l,s}} + H.c \\
&= \sum_{(l,s),\sigma} \frac{1}{N_1 N_2} \sum_{(k_1,k_2),(k_1',k_2')} a^\dagger_{k_1,k_2,\sigma} b_{k_1',k_2',\sigma} e^{-i(k_1,k_2)\cdot r_{B,l,s}} (\sum_{i=1}^{3} e^{-i(k_1,k_2)\cdot \delta_i}) e^{i(k_1',k_2')\cdot r_{B,l,s}} + H.c \\
&= \sum_{(k_1,k_2),(k_1',k_2'),\sigma} a^\dagger_{k_1,k_2,\sigma} b_{k_1',k_2',\sigma} \delta_{k_1,k_1'} \delta_{k_2,k_2'} (\sum_{i=1}^{3} e^{-i(k_1,k_2)\cdot \delta_i}) + H.c \\
&= \sum_{(k_1,k_2),\sigma} (\sum_{i=1}^{3} e^{-i(k_1,k_2)\cdot \delta_i}) a^\dagger_{k_1,k_2,\sigma} b_{k_1,k_2,\sigma} + H.c
\end{aligned}$$

finally, we consider the next nearest coupling term. at first, we consider a more general case

$$\begin{aligned}
\sum_{(m,n)} a^\dagger_{(m,n)} a_{(m,n)+(t,s)} &= \sum_{(m,n)} \sum_{k_1,k_2} \sum_{k_1',k_2'} \frac{1}{N_1 N_2} a^\dagger_{k_1,k_2} a_{k_1',k_2'} e^{-i(k_1,k_2)\cdot(m,n)} e^{i(k_1',k_2')\cdot[(m,n)+(t,s)]} \\
&= \sum_{k_1,k_2} \sum_{k_1',k_2'} e^{i(k_1',k_2')\cdot(t,s)} \sum_{(m,n)} \frac{1}{N_1 N_2} a^\dagger_{k_1,k_2} a_{k_1',k_2'} e^{-i(k_1,k_2)\cdot(m,n)} e^{i(k_1',k_2')\cdot(m,n)} \\
&= \sum_{k_1,k_2} \sum_{k_1',k_2'} e^{i(k_1',k_2')\cdot(t,s)} a^\dagger_{k_1,k_2} a_{k_1',k_2'} \delta_{k_1,k_1'} \delta_{k_2,k_2'} \\
&= \sum_{k_1,k_2} e^{i(k_1,k_2)\cdot(t,s)} a^\dagger_{k_1,k_2} a_{k_1,k_2}
\end{aligned}$$

so finally, collecting all the terms, we have the whole hamiltonian in momentum space read as

$$\begin{aligned}
H = &M \sum_{(k_1,k_2)} a^\dagger_{k_1,k_2,A} a_{k_1,k_2,A} - M \sum_{(k_1,k_2)} a^\dagger_{k_1,k_2,B} a_{k_1,k_2,B} \\
&+ t_1 \sum_{(k_1,k_2)} (\sum_{i=1}^{3} e^{-i(k_1,k_2)\cdot\delta_i}) a^\dagger_{k_1,k_2,A} a_{k_1,k_2,B} + H.c \\
&+ \sum_{(k_1,k_2)} t_2 (e^{i\phi} e^{i(k_1,k_2)\cdot a_1} + e^{-i\phi} e^{i(k_1,k_2)\cdot a_2} + e^{i\phi} e^{i(k_1,k_2)\cdot a_3} + h.c) a^\dagger_{k_1,k_2,A} a_{k_1,k_2,A}
\end{aligned}$$

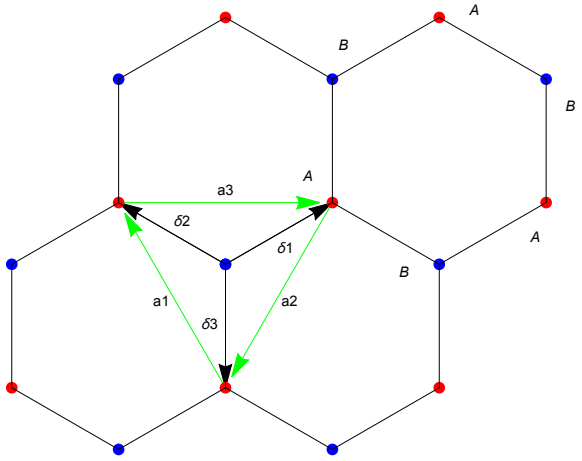

Figure 10: the redefined vectors

$$+\sum_{(k_1,k_2)} t_2(e^{-i\phi}e^{i(k_1,k_2)\cdot a_1}+e^{i\phi}e^{i(k_1,k_2)\cdot a_2}+e^{-i\phi}e^{i(k_1,k_2)\cdot a_3}+h.c)a^\dagger_{k_1,k_2,B}a_{k_1,k_2,B}$$

if we write (k_1,k_2) as k and use the the basis $\gamma_k=(a_{k,A},a_{k,B})^T$, then we have

$$H=\sum_k \gamma_k^\dagger H_k \gamma_k$$

and the diagonal part in the momentum space is

$$H_k=\begin{pmatrix} M+t_2(e^{i\phi}e^{ik\cdot a_1}+e^{-i\phi}e^{ik\cdot a_2}+e^{i\phi}e^{ik\cdot a_3}+h.c) & t_1\sum_{i=1}^3 e^{-ik\cdot\delta_i} \\ t_1\sum_{i=1}^3 e^{ik\cdot\delta_i} & -M+t_2(e^{-i\phi}e^{ik\cdot a_1}+e^{i\phi}e^{ik\cdot a_2}+e^{-i\phi}e^{ik\cdot a_3}+h.c)\end{pmatrix} \tag{8}$$

in order to make full the expression more symmetric, we can redefine the vetor so that $a_1+a_2+a_3=0$

$$a_1\to -a_2$$
$$a_2\to a_1$$
$$a_3\to -a_3$$

we can see this change in the Figure 10. after this new redefinition, the hamiltonian becomes($\phi\to-\phi$ this because different paper use different sign convention for Peierls Substitution, this is a difference from $\phi\to-\phi$ and in this notes I want to follow Haldane's original paper)

$$H_k=\begin{pmatrix} M+t_2(e^{-i\phi}e^{ik\cdot -a_2}+e^{i\phi}e^{ik\cdot a_1}+e^{-i\phi}e^{ik\cdot -a_3}+h.c) & t_1\sum_{i=1}^3 e^{-ik\cdot\delta_i} \\ t_1\sum_{i=1}^3 e^{ik\cdot\delta_i} & -M+t_2(e^{i\phi}e^{ik\cdot -a_2}+e^{-i\phi}e^{ik\cdot a_1}+e^{i\phi}e^{ik\cdot -a_3}+h.c)\end{pmatrix}$$
$$=\begin{pmatrix} M+t_2(\sum_{i=1}^3 e^{i\phi}e^{ik\cdot a_i}+h.c) & t_1\sum_{i=1}^3 e^{-ik\cdot\delta_i} \\ t_1\sum_{i=1}^3 e^{ik\cdot\delta_i} & -M+t_2(\sum_{i=1}^3 e^{-i\phi}e^{ik\cdot a_i}+h.c)\end{pmatrix}$$

since

$$\sum_{i=1}^3 e^{-ik\cdot\delta_i}=\sum_{k=1}^3\cos(k\cdot\delta_i)-i\sin(k\cdot\delta_i)$$
$$\sum_{i=1}^3 e^{i\phi}e^{ik\cdot a_i}+h.c=2\sum_{i=1}^3\cos(\phi+k\cdot a_i)=2\sum_{i=1}^3\cos(\phi)\cos(k\cdot a_i)-\sin(\phi)\sin(k\cdot a_i)$$

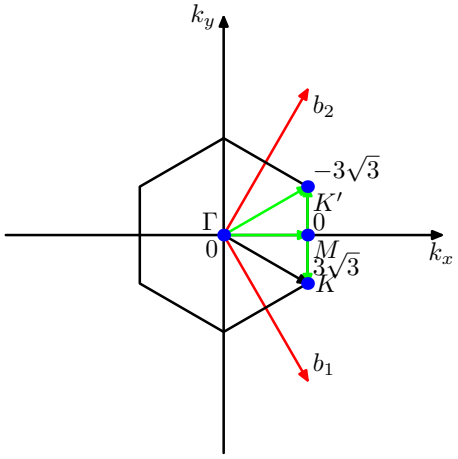

Figure 11: the behavior of the function $g(k)$

$$\sum_{i=1}^{3} e^{-i\phi}e^{ik\cdot a_i} + h.c = 2\sum_{i=1}^{3}\cos(\phi - k\cdot a_i) = 2\sum_{i=1}^{3}\cos(\phi)\cos(k\cdot a_i) + \sin(\phi)\sin(k\cdot a_i)$$

so finally, we have that the block diagonal hamiltonian in momentum space is

$$H_k = 2t_2\sum_{i=1}^{3}\cos(\phi)\cos(k\cdot a_i)I + t_1\sum_{i=1}^{3}\cos(k\cdot\delta_i)\sigma_x + t_1\sum_{k=1}^{3}\sin(k\cdot\delta_i)\sigma_y + (M - 2t_2\sum_{i=1}^{3}\sin(\phi)\sin(k\cdot a_i))\sigma_z$$

which is the same as the formula given in Haldane's original paper[1].

ℜ.2 The band structure and phase diagram

next we need to consider the energy spectrum and the corresponding topological phases in this system. since when $M = 0$ and $\phi = 0$, this model is just the graphene model, so we can use the previous result that

$$\sum_i 2\cos(k\cdot a_i) = f(k) = 2\cos(\sqrt{3}ak_y) + 4\cos(\frac{3}{2}ak_x)\cos(\frac{\sqrt{3}}{2}ak_y)$$

and

$$|\sum_i \cos(k\cdot\delta_i)|^2 + |\sum_i \sin(k\cdot\delta_i)|^2 = 3 + f(k)$$

on the other hand, we know that

$$a_1 = \delta_2 - \delta_3 = \frac{a}{2}(3,\sqrt{3})\ \ a_1 = \delta_3 - \delta_1 = \frac{a}{2}(-3,\sqrt{3})\ \ a_3 = \delta_1 - \delta_2 = \frac{a}{2}(0,-2\sqrt{3})$$

so we know that

$$2\sum_i \sin(k\cdot a_i) = 2\sin(\frac{a}{2}(3k_x + \sqrt{3}k_y)) + 2\sin(\frac{a}{2}(-3k_x + \sqrt{3}k_y)) + 2\sin(\frac{a}{2}(-2\sqrt{3}k_y))$$

$$= 4\sin(\frac{\sqrt{3}}{2}ak_y)\cos(\frac{3}{2}ak_x) - 2\sin(\sqrt{3}ak_y) = g(k)$$

fallowing the same discussion about the function f(k), we can find that from Γ to K, $g(k)$ increasingly from 0 to $3\sqrt{3}$, from K to K', it then deceasing from $3\sqrt{3}$ to $-3\sqrt{3}$, and for fixed k_x, it decrease as k_y increase, which are illustrated in Figure 11. then the spectrum is just

$$E_{k,\pm} = t_2\cos(\phi)f(k) \pm \sqrt{t_1^2(3 + f(k)) + (M - t_2\sin(\phi)g(k))^2}$$

then we examine some special points, we can find that at the K and K' points, we have (since in Haldane's original paper, he labelled δ_1, δ_2 in such a way that $z \cdot (\delta_1 \times \delta_2)$ is positive, so we should replace $\delta_1 \to \delta_2, \delta_2 \to \delta_1$ from the notation in the section Honeycomb lattice in previous one.)

$$K \cdot \delta_1 = \frac{2\pi}{\sqrt{3}}(\frac{\sqrt{3}}{3}, -\frac{1}{3}) \cdot \frac{a}{2}(1, -\sqrt{3}) = \frac{2\pi}{3}$$
$$K \cdot \delta_2 = \frac{2\pi}{\sqrt{3}}(\frac{\sqrt{3}}{3}, -\frac{1}{3}) \cdot \frac{a}{2}(1, \sqrt{3}) = 0$$
$$K \cdot \delta_3 = \frac{2\pi}{\sqrt{3}}(\frac{\sqrt{3}}{3}, -\frac{1}{3}) \cdot a(-1, 0) = -\frac{2\pi}{3}$$

$$K' \cdot \delta_1 = \frac{2\pi}{\sqrt{3}}(\frac{\sqrt{3}}{3}, \frac{1}{3}) \cdot \frac{a}{2}(1, -\sqrt{3}) = 0$$
$$K' \cdot \delta_2 = \frac{2\pi}{\sqrt{3}}(\frac{\sqrt{3}}{3}, \frac{1}{3}) \cdot \frac{a}{2}(1, \sqrt{3}) = \frac{2\pi}{3}$$
$$K' \cdot \delta_3 = \frac{2\pi}{\sqrt{3}}(\frac{\sqrt{3}}{3}, \frac{1}{3}) \cdot a(-1, 0) = -\frac{2\pi}{3}$$

since the band close only when the coefficient of Pauli metrics are all vanishing, From the properties of Graphene, we know that this can only happens at the Dirac Points.In these points $\sum_i \cos(K \cdot \delta_i) = 0$ and $\sum_i \sin(K \cdot \delta_i) = 0$ and

$$\sum_i \sin(K \cdot a_i) = \sin(\frac{2\pi}{3}) + \sin(-\frac{4\pi}{3}) + \sin(\frac{2\pi}{3}) = 3\sin(\frac{2\pi}{3}) = \frac{3}{2}\sqrt{3}$$

$$\sum_i \sin(K' \cdot a_i) = \sin(\frac{4\pi}{3}) + \sin(-\frac{2\pi}{3}) + \sin(-\frac{2\pi}{3}) = -3\sin(\frac{2\pi}{3}) = -\frac{3}{2}\sqrt{3}$$

so in order to make the coefficient of σ_z to vanish, the value for M should be

$$K : M = 3\sqrt{3}t_2 \sin(\phi)$$
$$K' : M = -3\sqrt{3}t_2 \sin(\phi)$$

in order to make sure that the energy spectrum never overlap unless they are touched, we can further require that

$$E_{k,-}^{\max} \leq E_{k,+}^{\min}$$

this can be done by choosing small enough t_2 since when $t_2 = 0$, this upper band is always larger than zero and the lower band is always smaller than zero(the spectrum is a continuous function of t_2).

when $M = 0$ and $t_2 \sin\phi = 0$, then at K and K' points, the band gap close at the same time, so this Eigen value of this system has the symmetry of $C_{3,v}$(Inversion interchange the K and K' points). But if one of $M = 0$ and $t_2 \sin\phi = 0$ is violated, the condition $M = 3\sqrt{3}t_2 \sin(\phi), M = -3\sqrt{3}t_2 \sin(\phi)$ can not be satisfied at the same time, so either the tree K points or the three K' points are closing at the same time, and the symmetry group of this system is reduced to C_3 group. And the topological phases of this system is illustrated in Figure 12.

in order to see the low energy level properties of this system, we can expand the hamiltonian near the K and K' points.near the K Points, we have

$$\sum_{i=1}^{3} \cos((K + k) \cdot \delta_i) = \cos(\frac{2\pi}{3} + \frac{1}{2}ak_x - \frac{\sqrt{3}}{2}ak_y) + \cos(0 + \frac{1}{2}ak_x + \frac{\sqrt{3}}{2}ak_y) + \cos(-\frac{2\pi}{3} - ak_x)$$

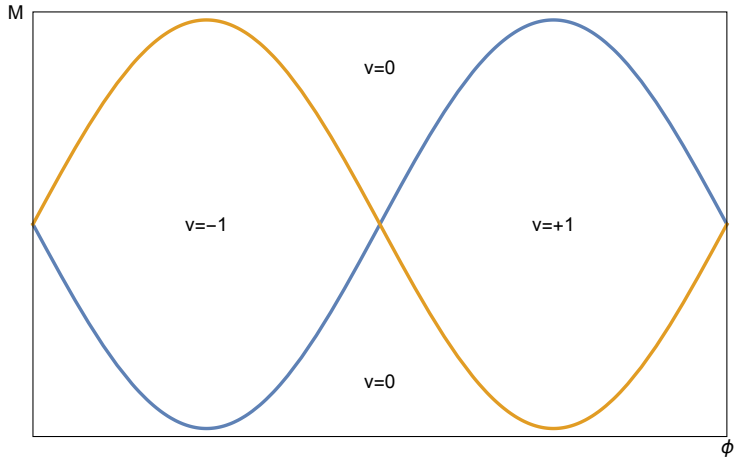

Figure 12: Phase diagram of Haldane Model

$$
\begin{aligned}
&= -\frac{1}{2}\cos(\frac{1}{2}ak_x - \frac{\sqrt{3}}{2}ak_y) - \frac{\sqrt{3}}{2}\sin(\frac{1}{2}ak_x - \frac{\sqrt{3}}{2}ak_y) + \cos(\frac{1}{2}ak_x + \frac{\sqrt{3}}{2}ak_y) \\
&- \frac{1}{2}\cos(ak_x) - \frac{\sqrt{3}}{2}\sin(ak_x) \\
\text{(linear term)} &\sim -\frac{1}{2} - \frac{\sqrt{3}}{2}(\frac{1}{2}ak_x - \frac{\sqrt{3}}{2}ak_y) + 1 - \frac{1}{2} - \frac{\sqrt{3}}{2}ak_x \\
&= \frac{3a}{2}(-\frac{\sqrt{3}}{2}k_x + \frac{1}{2}k_y)
\end{aligned}
$$

similarly, we have

$$
\begin{aligned}
\sum_{i=1}^{3}\sin((K+k)\cdot\delta_i) &= \sin(\frac{2\pi}{3} + \frac{1}{2}ak_x - \frac{\sqrt{3}}{2}ak_y) + \sin(0 + \frac{1}{2}ak_x + \frac{\sqrt{3}}{2}ak_y) + \sin(-\frac{2\pi}{3} - ak_x) \\
&= \frac{\sqrt{3}}{2}\cos(\frac{1}{2}ak_x - \frac{\sqrt{3}}{2}ak_y) - \frac{1}{2}\sin(\frac{1}{2}ak_x - \frac{\sqrt{3}}{2}ak_y) + \sin(\frac{1}{2}ak_x + \frac{\sqrt{3}}{2}ak_y) \\
&- \frac{\sqrt{3}}{2}\cos(ak_x) + \frac{1}{2}\sin(ak_x) \\
\text{(linear term)} &\sim \frac{\sqrt{3}}{2} - \frac{1}{2}(\frac{1}{2}ak_x - \frac{\sqrt{3}}{2}ak_y) + (\frac{1}{2}ak_x + \frac{\sqrt{3}}{2}ak_y) - \frac{\sqrt{3}}{2} + \frac{1}{2}ak_x \\
&= \frac{3a}{2}(\frac{1}{2}k_x + \frac{\sqrt{3}}{2}k_y)
\end{aligned}
$$

if we define

$$h(k) = \sum_{i=1}^{3} e^{ik\cdot\delta_i}$$

we can find that

$$h(R_z(\frac{\pi}{3})k) = \sum_{i=1}^{3} e^{-ik\cdot\delta_i} = h(k)^*$$

and the coefficients of σ_x, σ_y is just

$$\sum_{i=1}^{3}\cos(k\cdot\delta_i) = \mathrm{Re}\{h(k)\} \quad \sum_{i=1}^{3}\sin(k\cdot\delta_i) = \mathrm{Im}\{h(k)\}$$

so using these result we can derive that near $-K$:

$$\sum_{i=1}^{3}\cos((-K+k)\cdot\delta_i) = \frac{3a}{2}(\frac{\sqrt{3}}{2}k_x - \frac{1}{2}k_y)$$

$$\sum_{i=1}^{3}\sin((-K+k)\cdot\delta_i)=\frac{3a}{2}(\frac{1}{2}k_x+\frac{\sqrt{3}}{2}k_y)$$

similarly, near the K' points, we have

$$\begin{aligned}\sum_{i=1}^{3}\cos((K'+k)\cdot\delta_i)&=\cos(0+\frac{1}{2}ak_x-\frac{\sqrt{3}}{2}ak_y)+\cos(\frac{2\pi}{3}+\frac{1}{2}ak_x+\frac{\sqrt{3}}{2}ak_y)+\cos(-\frac{2\pi}{3}-ak_x)\\&=\cos(\frac{1}{2}ak_x-\frac{\sqrt{3}}{2}ak_y)-\frac{1}{2}\cos(\frac{1}{2}ak_x+\frac{\sqrt{3}}{2}ak_y)-\frac{\sqrt{3}}{2}\sin(\frac{1}{2}ak_x+\frac{\sqrt{3}}{2}ak_y)\\&-\frac{1}{2}\cos(ak_x)-\frac{\sqrt{3}}{2}\sin(ak_x)\\(\text{linear term})&\sim 1-\frac{1}{2}-\frac{\sqrt{3}}{2}(\frac{1}{2}ak_x+\frac{\sqrt{3}}{2}ak_y)-\frac{1}{2}-\frac{\sqrt{3}}{2}ak_x\\&=\frac{3a}{2}(-\frac{\sqrt{3}}{2}k_x-\frac{1}{2}k_y)\end{aligned}$$

$$\begin{aligned}\sum_{i=1}^{3}\sin((K'+k)\cdot\delta_i)&=\sin(0+\frac{1}{2}ak_x-\frac{\sqrt{3}}{2}ak_y)+\sin(\frac{2\pi}{3}+\frac{1}{2}ak_x+\frac{\sqrt{3}}{2}ak_y)+\sin(-\frac{2\pi}{3}-ak_x)\\&=\sin(\frac{1}{2}ak_x-\frac{\sqrt{3}}{2}ak_y)+\frac{\sqrt{3}}{2}\cos(\frac{1}{2}ak_x+\frac{\sqrt{3}}{2}ak_y)-\frac{1}{2}\sin(\frac{1}{2}ak_x+\frac{\sqrt{3}}{2}ak_y)\\&-\frac{\sqrt{3}}{2}\cos(ak_x)+\frac{1}{2}\sin(ak_x)\\(\text{linear term})&\sim(\frac{1}{2}ak_x-\frac{\sqrt{3}}{2}ak_y)+\frac{\sqrt{3}}{2}-\frac{1}{2}(\frac{1}{2}ak_x+\frac{\sqrt{3}}{2}ak_y)-\frac{\sqrt{3}}{2}+\frac{1}{2}ak_x\\&=\frac{3a}{2}(\frac{1}{2}k_x-\frac{\sqrt{3}}{2}k_y)\end{aligned}$$

so if we define $(x,y)_K[k]=(\sum_{i=1}^{3}\cos((K+k)\cdot\delta_i),\sum_{i=1}^{3}\sin((K+k)\cdot\delta_i))$ and similarly for $(x,y)_{K'}[k]$, we can find that

$$(x,y)_K[k]=\frac{3}{2}aR_z(-\frac{\pi}{6})(-k_x,k_y)^T=\frac{3}{2}aR_z(\frac{\pi}{3})(k_y,k_x)^T\to(x,y)_K[-\sigma_zR_z(\frac{\pi}{6})\vec{k}]=\frac{3}{2}a\vec{k}$$

$$(x,y)_{K'}[k]=\frac{3}{2}aR_z(\frac{5\pi}{6})(k_x,k_y)^T\to(x,y)_{K'}[R_z(-\frac{5\pi}{6})\vec{k}]=\frac{3}{2}a\vec{k}$$

we can see clearly see that the Energy spectrum of graphene has C_6 symmetry , but the symmetry group for the hamiltonian of graphene is C_3 due to the fact that the nearest coupling term($\sum_i e^{-ik\cdot\delta_i}$) only take C_3 symmetry.

with the above expansion in mind, we can write the effective hamiltonian in this system near the K and K' points as

$$\frac{3a}{2}t_1(k_x\sigma_x+k_y\sigma_y)$$

on the other hand, since the leading term of $2\sum_i\sin((K+k)\cdot a_i)=2\sum_i(\sin(K\cdot a_i)\cos(k\cdot a_i)+\cos(K\cdot a_i)\sin(k\cdot a_i))=2\sum_i\sin(K\cdot a_i)=g(K)$, so we can write down the whole expansion of the Haldane model near the Dirac point:

$$\begin{aligned}K:H&=-6t_2\cos(\phi)I+\frac{3}{2}at_1R_z(-\frac{\pi}{6})(-k_x,k_y)^T\cdot(\sigma_x,\sigma_y)+(M-3\sqrt{3}t_2\sin(\phi))\sigma_z\\K':H&=-6t_2\cos(\phi)I+\frac{3}{2}at_1R_z(\frac{5\pi}{6})(k_x,k_y)^T\cdot(\sigma_x,\sigma_y)+(M+3\sqrt{3}t_2\sin(\phi))\sigma_z\end{aligned}$$

after ignoring the constant term and by redefining the $\vec{k}$ vectors, we can write down the following effective hamiltonian:

$$H = \frac{3}{2}at_1(k_{\alpha,1}, k_{\alpha,2}) \cdot (\sigma_x, \sigma_y) + (M - \alpha 3\sqrt{3}t_2 \sin(\phi))\sigma_z$$

where $\alpha = +$ is for K points and $\alpha = -$ is for K' points.

§4 Quantum Spin Hall Effect in Graphene

ℜ.1 The Bulk Properties

another important model constructed in the honeycomb lattice is the so called model for the quantum spin hall effect, which can be regarded as the extended Haldane model which include the spin degree of freedom in each sites.in this model, we will consider the whole hamiltonian and the low energy effective hamiltonian.

the first term in this model is the onsite energy term, which read as

$$H_\nu = \sum_{i\in A} \lambda_\nu c_i^\dagger c_i + \sum_{i\in B} -\lambda_\nu c_i^\dagger c_i$$

when we transfer to the momentum space, this term is just

$$\sum_k \lambda_\nu c_{k,A}^\dagger c_{k,A} - \sum_k \lambda_\nu c_{k,B}^\dagger c_{k,B}$$

when we consider the low energy effective hamiltonian, we should project this one to the points near the K and K' points, if we use the basis $\Psi = (c_{K,A}, c_{K,B}, c_{K',A}, c_{K',B})^T$,then we can write the effective hamiltonian as $\Psi^\dagger H_{\text{low}} \Psi$ then the above term contribute to H_{low} the following metrics:

$$H_\nu \to \lambda_\nu \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix} = I \otimes \sigma_z$$

where the previous one in the tensor product act on the (K, K') block and the second factor σ_z act on the (A, B) sublattice. the second term in this model is the same nearest coupling term:

$$H_t = t \sum_{<i,j>,\sigma} c_{i,\sigma}^\dagger c_{j,\sigma}$$

using the results in previous section, we know this term in momentum space is just

$$H_{t,k} = t\sum_{i=1}^{3} \cos(k \cdot \delta_i)\sigma_x + t\sum_{k=1}^{3} \sin(k \cdot \delta_i)\sigma_y$$

near the K and K' points, we know that

$$H_{t,K} = \frac{3a}{2}tR_z(-\frac{\pi}{6})(-k_x, k_y)^T \cdot (\sigma_x, \sigma_y)$$
$$H_{t,K'} = \frac{3a}{2}tR_z(\frac{5\pi}{6})(k_x, k_y)^T \cdot (\sigma_x, \sigma_y)$$

since we know that

$$R_z(-\frac{\pi}{6})(-k_x, k_y)^T = R_z(-\frac{\pi}{6}) - \sigma_z(k_x, k_y)^T = -\sigma_z R_z(\frac{\pi}{6})(k_x, k_y)^T$$

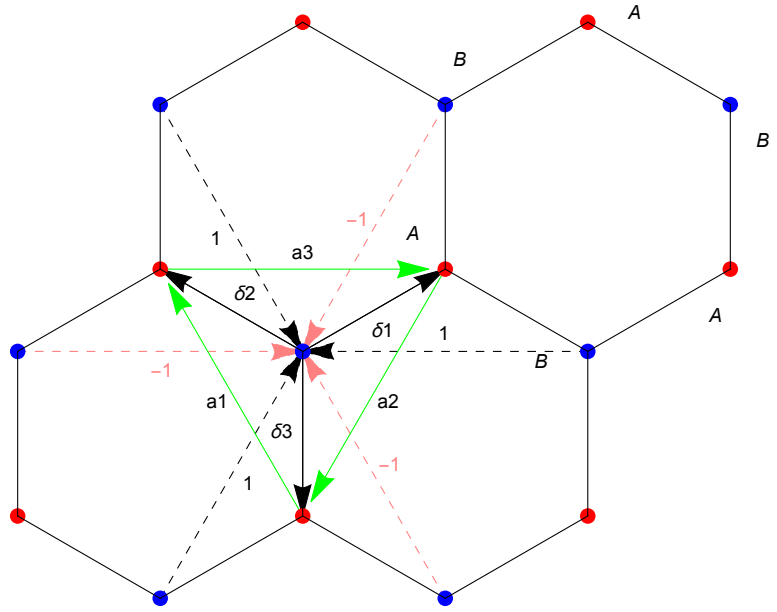

Figure 13: the sign convention for $v_{i,j}$ for the term H_{so} in the QSH model

since the system has a C_3 symmetry and $R_z(\frac{5\pi}{6})(k_x,k_y)^T = R_z(\frac{2\pi}{3})R_z(\frac{\pi}{6})(k_x,k_y)^T$, we can make the increment on (k_x,k_y) near K along the direction $R_z(\frac{\pi}{6})(k_x,k_y)^T$ and near K' along the direction $R_z(\frac{5\pi}{6})(k_x,k_y)^T$, then this term contribute to the low energy effective hamiltonian metrics as

$$H_t \to \frac{3a}{2}t\begin{pmatrix} -k_x\sigma_x + k_y\sigma_y & 0 \\ 0 & k_x\sigma_x + k_y\sigma_y \end{pmatrix} = \frac{3a}{2}t(-\tau_z\otimes\sigma_x + I\otimes\sigma_y)$$

where the Pauli metrics τ_i act on the (K,K') block. if we redefine the $k_x \to -k_x$, then this term is just

$$\frac{3a}{2}t(-\tau_z\otimes\sigma_x + I\otimes\sigma_y) \to \frac{3a}{2}t(\tau_z\otimes\sigma_x + I\otimes\sigma_y) = v_F(\tau_z\otimes\sigma_x + I\otimes\sigma_y)$$

and the third term is not the original one in Haldane's papers, it has the following form instead:

$$H_{\text{so}} = \sum_{<<i,j>>} i\lambda_{\text{so}} v_{i,j} c_i^\dagger s^z c_j$$

where $v_{i,j} = \frac{2}{\sqrt{3}}(\hat{d}_1\times\hat{d}_2)_z = \pm 1$ and d_1, d_2 is are vectors along the two bonds the electron traverse going from site j to i. and the sign of these values is depicted in the Figure 13 with these illustration, we can write down the term for H_{so} explicitly as:

$$\begin{aligned} H_{\text{so}} = i\lambda_{\text{so}} \sum_{(m,n)\in B} & (c^\dagger_{(m,n)} s^z c_{(m,n)+a_1} + c^\dagger_{(m,n)} s^z c_{(m,n)+a_2} + c^\dagger_{(m,n)} s^z c_{(m,n)+a_3} \\ & - c^\dagger_{(m,n)} s^z c_{(m,n)-a_1} - c^\dagger_{(m,n)} s^z c_{(m,n)-a_2} - c^\dagger_{(m,n)} s^z c_{(m,n)-a_3}) \\ & + i\lambda_{\text{so}} \sum_{(m,n)\in A} (-c^\dagger_{(m,n)} s^z c_{(m,n)+a_1} - c^\dagger_{(m,n)} s^z c_{(m,n)+a_2} - c^\dagger_{(m,n)} s^z c_{(m,n)+a_3} \\ & + c^\dagger_{(m,n)} s^z c_{(m,n)-a_1} + c^\dagger_{(m,n)} s^z c_{(m,n)-a_2} + c^\dagger_{(m,n)} s^z c_{(m,n)-a_3}) \end{aligned}$$

so when making Fourier Transform to this term, we have

$$H_{\text{so}} = i\lambda_{\text{so}} \sum_k c^\dagger_{k,B} s^z c_{k,B} (e^{ik\cdot a_1} + e^{ik\cdot a_2} + e^{ik\cdot a_3} - e^{ik\cdot -a_1} - e^{ik\cdot -a_2} - e^{ik\cdot -a_3})$$

$$+ i\lambda_{\text{so}} \sum_k c^\dagger_{k,A} s^z c_{k,A} (-e^{ik\cdot a_1} - e^{ik\cdot a_2} - e^{ik\cdot a_3} + e^{ik\cdot -a_1} + e^{ik\cdot -a_2} - e^{ik\cdot -a_3})$$

define $g(k) = -i(e^{ik\cdot a_1} + e^{ik\cdot a_2} + e^{ik\cdot a_3} - e^{ik\cdot -a_1} - e^{ik\cdot -a_2} - e^{ik\cdot -a_3}) = 2\sum_{i=1}^3 \sin(k\cdot a_i)$ then

$$H_{\text{so}} = \lambda_{\text{so}} \sum_k -g(k) c^\dagger_{k,B} s^z c_{k,B} + g(k) c^\dagger_{k,A} s^z c_{k,A}$$

since from Haldane's model we know that $g(K) = 3\sqrt{3}$ and $g(K') = -3\sqrt{3}$, so this term contribute to the low energy effective hamiltonian with the following term:

$$H_{\text{so}} \to 3\sqrt{3}\lambda_{\text{so}} \begin{pmatrix} \sigma_z s^z & 0 \\ 0 & -\sigma_z s^z \end{pmatrix} = 3\sqrt{3}\lambda_{\text{so}} \tau_z \otimes \sigma_z \otimes s^z$$

the last term in this model is the nearest neighbor Rashba term

$$H_R = i\lambda_R \sum_{<i,j>} c^\dagger_i (s \times \hat{d}_{ij})_z c_j$$

where $\hat{d_{ij}}$ is the nearest bond from i to j. we can write done this term more concrete as

$$\begin{aligned} H_R = i\lambda_R \sum_{(m,n)} & (c^\dagger_{(m,n),A}(s \times -\hat{\delta}_1)_z c_{(m,n)-\delta_1,B} + c^\dagger_{(m,n),A}(s \times -\hat{\delta}_2)_z c_{(m,n)-\delta_2,B} + c^\dagger_{(m,n),A}(s \times -\hat{\delta}_3)_z c_{(m,n)-\delta_3,B}) \\ + i\lambda_R \sum_{(m,n)} & (c^\dagger_{(m,n),B}(s \times \hat{\delta}_1)_z c_{(m,n)+\delta_1,A} + c^\dagger_{(m,n),B}(s \times \hat{\delta}_2)_z c_{(m,n)+\delta_2,A} + c^\dagger_{(m,n),B}(s \times \hat{\delta}_3)_z c_{(m,n)+\delta_3,A}) \end{aligned}$$

if we make Fourier transform to this term, it read as

$$\begin{aligned} H_R = i\lambda_R \sum_k & (c^\dagger_{k,A} e^{-ik\cdot\delta_1}(-s \times \hat{\delta}_1)_z c_{k,B} + c^\dagger_{k,A} e^{-ik\cdot\delta_2}(-s \times \hat{\delta}_2)_z c_{k,B} + c^\dagger_{k,A} e^{-ik\cdot\delta_3}(-s \times \hat{\delta}_3)_z c_{k,B}) \\ + i\lambda_R \sum_k & (c^\dagger_{k,B} e^{ik\cdot\delta_1}(s \times \hat{\delta}_1)_z c_{k,A} + c^\dagger_{k,B} e^{ik\cdot\delta_2}(s \times \hat{\delta}_2)_z c_{k,A} + c^\dagger_{k,B} e^{ik\cdot\delta_3}(s \times \hat{\delta}_3)_z c_{k,A}) \end{aligned}$$

since we have $(s \times \hat{\delta}_1)_z = -\frac{\sqrt{3}}{2}s^x - \frac{1}{2}s^y$, $(s \times \hat{\delta}_2)_z = \frac{\sqrt{3}}{2}s^x - \frac{1}{2}s^y$ and $(s \times \hat{\delta}_3)_z = s^y$, so we have

$$\begin{aligned} H_R = i\lambda_R \sum_k & (c^\dagger_{k,A}\{s^x(\frac{\sqrt{3}}{2}e^{-ik\cdot\delta_1} - \frac{\sqrt{3}}{2}e^{-ik\cdot\delta_2}) + s^y(\frac{1}{2}e^{-ik\cdot\delta_1} + \frac{1}{2}e^{-ik\cdot\delta_2} - e^{-ik\cdot\delta_3})\} c_{k,B} \\ + i\lambda_R \sum_k & (c^\dagger_{k,B}\{s^x(-\frac{\sqrt{3}}{2}e^{ik\cdot\delta_1} + \frac{\sqrt{3}}{2}e^{ik\cdot\delta_2}) + s^y(-\frac{1}{2}e^{ik\cdot\delta_1} - \frac{1}{2}e^{ik\cdot\delta_2} + e^{ik\cdot\delta_3})\} c_{k,A} \end{aligned}$$

since we know that

$$\begin{aligned} \frac{\sqrt{3}}{2}e^{-ik\cdot\delta_1} - \frac{\sqrt{3}}{2}e^{-ik\cdot\delta_2} &= \frac{\sqrt{3}}{2}e^{-i\frac{1}{2}ak_x + i\frac{\sqrt{3}}{2}ak_y} - \frac{\sqrt{3}}{2}e^{-i\frac{1}{2}ak_x - i\frac{\sqrt{3}}{2}ak_y} \\ &= i\sqrt{3}\sin(\frac{\sqrt{3}}{2}ak_y)e^{-i\frac{1}{2}ak_x} \\ &= \sqrt{3}\sin(\frac{\sqrt{3}}{2}ak_y)\sin(\frac{1}{2}ak_x) + i\sqrt{3}\sin(\frac{\sqrt{3}}{2}ak_y)\cos(\frac{1}{2}ak_x) \\ &:= (-i)z^x_k \end{aligned}$$

$$\frac{1}{2}e^{-ik\cdot\delta_1} + \frac{1}{2}e^{-ik\cdot\delta_2} - e^{-ik\cdot\delta_3} = \frac{1}{2}e^{-i\frac{1}{2}ak_x + i\frac{\sqrt{3}}{2}ak_y} + \frac{1}{2}e^{-i\frac{1}{2}ak_x - i\frac{\sqrt{3}}{2}ak_y} - e^{iak_x}$$

$$
\begin{aligned}
&= \cos(\frac{\sqrt{3}}{2}ak_y)e^{-i\frac{1}{2}ak_x} - e^{iak_x} \\
&= (\cos(\frac{\sqrt{3}}{2}ak_y)\cos(\frac{1}{2}ak_x) - \cos(ak_x)) - i(\cos(\frac{\sqrt{3}}{2}ak_y)\sin(\frac{1}{2}ak_x) + \sin(ak_x)) \\
&:= (-i)z_k^y
\end{aligned}
$$

then the nearest neighbor Rashba term can be written as

$$
\begin{aligned}
H_R = \lambda_R \sum_k (c_{k,A}^\dagger \{s^x z_k^x + s^y z_k^y\} c_{k,B} \\
\lambda_R \sum_k (c_{k,B}^\dagger \{s^x z_k^{x,*} + s^y z_k^{y,*}\} c_{k,A}
\end{aligned}
$$

in order to write down the low energy effective hamiltonian, we need to calculate some values at K and K' points, we have

$$
\frac{\sqrt{3}}{2}e^{-iK\cdot\delta_1} - \frac{\sqrt{3}}{2}e^{-iK\cdot\delta_2} = \frac{\sqrt{3}}{2}e^{-i\frac{2\pi}{3}} - \frac{\sqrt{3}}{2}e^{-i0} = -\frac{3}{4}\sqrt{3} - \frac{3}{4}i = -iz_K^x \to z_K^x = \frac{3}{2}e^{-i\frac{\pi}{3}}
$$

$$
\frac{1}{2}e^{-iK\cdot\delta_1} + \frac{1}{2}e^{-iK\cdot\delta_2} - e^{-iK\cdot\delta_3} = \frac{1}{2}e^{-i\frac{2\pi}{3}} + \frac{1}{2} - e^{i\frac{2\pi}{3}} = -\frac{3}{4}\sqrt{3}i + \frac{3}{4} = -iz_K^y \to z_K^y = i\frac{3}{2}e^{-i\frac{\pi}{3}} = iz_K^x
$$

$$
\frac{\sqrt{3}}{2}e^{-iK'\cdot\delta_1} - \frac{\sqrt{3}}{2}e^{-iK'\cdot\delta_2} = \frac{\sqrt{3}}{2}e^{-i0} - \frac{\sqrt{3}}{2}e^{-i\frac{2\pi}{3}} = \frac{3}{4}\sqrt{3} + \frac{3}{4}i = -iz_{K'}^x \to z_{K'}^x = -\frac{3}{2}e^{-i\frac{\pi}{3}} = -z_K^x
$$

$$
\frac{1}{2}e^{-iK'\cdot\delta_1} + \frac{1}{2}e^{-iK'\cdot\delta_2} - e^{-iK'\cdot\delta_3} = \frac{1}{2}e^{-i0} + \frac{1}{2}e^{-i\frac{2\pi}{3}} - e^{i\frac{2\pi}{3}} = -\frac{3}{4}\sqrt{3}i + \frac{3}{4} = -iz_{K'}^y \to z_{K'}^y = i\frac{3}{2}e^{-i\frac{\pi}{3}} = iz_K^x = z_K^y
$$

so in the low energy effective hamiltonian, this term contribution with the following metrics

$$
\begin{aligned}
H_R = \lambda_R \begin{pmatrix} 0 & z_K^x s^x + z_K^y s^y & 0 & 0 \\ z_K^{x,*} s^x + z_K^{y,*} s^y & 0 & 0 & 0 \\ 0 & 0 & 0 & z_{K'}^x s^x + z_{K'}^y s^y \\ 0 & 0 & z_{K'}^{x,*} s^x + z_{K'}^{y,*} s^y & 0 \end{pmatrix} \\
\lambda_R \begin{pmatrix} 0 & z_K^x s^x + i z_K^x s^y & 0 & 0 \\ z_K^{x,*} s^x - i z_K^{x,*} s^y & 0 & 0 & 0 \\ 0 & 0 & 0 & -z_K^x s^x + i z_K^x s^y \\ 0 & 0 & -z_K^{x,*} s^x - i z_K^{x,*} s^y & 0 \end{pmatrix} \\
= \lambda_R(\tau_z(\mathrm{Re}[z_K^x]\sigma_x - \mathrm{Im}[z_K^x]\sigma_y)s^x + (-\mathrm{Im}[z_K^x]\sigma_x - \mathrm{Re}[z_K^x]\sigma_y)s^y)
\end{aligned}
$$

this is not consistent with the original paper of C.L.Kane and I don't know why. Finally, we have the full hamiltonian inn real space:

$$
\begin{aligned}
H &= H_\nu + H_t + H_{\mathrm{so}} + H_R \\
&= \sum_{i\in A} \lambda_\nu c_i^\dagger c_i + \sum_{i\in B} -\lambda_\nu c_i^\dagger c_i + t \sum_{<i,j>,\sigma} c_{i,\sigma}^\dagger c_{j,\sigma} + \sum_{<<i,j>>} i\lambda_{\mathrm{so}} v_{i,j} c_i^\dagger s^z c_j + i\lambda_R \sum_{<i,j>} c_i^\dagger (s \times \hat{d}_{ij})_z c_j
\end{aligned}
$$

and in the Fourier space read as

$$
\begin{aligned}
H_k = &\sum_k \lambda_\nu c_{k,A}^\dagger c_{k,A} - \sum_k \lambda_\nu c_{k,B}^\dagger c_{k,B} \\
&+ t(\sum_{i=1}^3 e^{-ik\cdot\delta_i}) c_{k,A}^\dagger c_{k,B} + t(\sum_{i=1}^3 e^{ik\cdot\delta_i}) c_{B,A}^\dagger c_{k,A}
\end{aligned}
$$

$$+\lambda_{\rm so}\sum_k -g(k)c^\dagger_{k,B}s^z c_{k,B}+g(k)c^\dagger_{k,A}s^z c_{k,A}$$
$$+\lambda_R\sum_k c^\dagger_{k,A}\{s^x z^x_k+s^y z^y_k\}c_{k,B}+\lambda_R\sum_k c^\dagger_{k,B}\{s^x z^{x,*}_k+s^y z^{y,*}_k\}c_{k,A}$$

or write in the basis $(c_{k,A},c_{k,B})$ as metrics:

$$H_k=\lambda_\nu\sigma_z+t\sum_{i=1}^3\cos(k\cdot\delta_i)\sigma_x+t\sum_{k=1}^3\sin(k\cdot\delta_i)\sigma_y+\lambda_{\rm so}g(k)\sigma_z s^z$$
$$+\lambda_R({\rm Re}[z^x_k]\sigma_x-{\rm Im}[z^x_k]\sigma_y)s^x+\lambda_R({\rm Re}[z^y_k]\sigma_x-{\rm Im}[z^y_k]\sigma_y)s^y \tag{9}$$

and the lower energy effective hamiltonian can be written as

$$\begin{aligned}H&=I\otimes\sigma_z+v_F(\tau_z\otimes\sigma_z+I\otimes\sigma_y)+3\sqrt{3}\lambda_{\rm so}\tau_z\otimes\sigma_z\otimes s^z\\&+\lambda_R(\tau_z({\rm Re}[z^x_K]\sigma_x-{\rm Im}[z^x_K]\sigma_y)s^x+(-{\rm Im}[z^x_K]\sigma_x-{\rm Re}[z^x_K]\sigma_y)s^y)\\&=I\otimes\sigma_z+v_F(\tau_z\otimes\sigma_z+I\otimes\sigma_y)+3\sqrt{3}\lambda_{\rm so}\tau_z\otimes\sigma_z\otimes s^z\\&+\frac{3}{4}\lambda_R(\tau_z\otimes(\sigma_x+\sqrt{3}\sigma_y)\otimes s^x+(\sqrt{3}\sigma_x-\sigma_y)\otimes s^y)\end{aligned}$$

if we define the time reversal operator as $T=I\otimes(is^y)K$, then $T^{-1}=I\otimes(-is^y)K$, when we consider a specific points in the Brillouin Zone, the 4X4 metrics can be expand by the sixteen Dirac Metrics $\sigma_i\otimes s^j$, we example the behavior of these metrics under Time Reversal

$$\begin{aligned}TI\otimes IT^{-1}&=(I\otimes(is^y)K)I\otimes I(I\otimes(-is^y)K)=I\otimes(s^yIs^y)=I\otimes I\ \text{ even}\\TI\otimes s^xT^{-1}&=(I\otimes(is^y)K)I\otimes s^x(I\otimes(-is^y)K)=I\otimes(s^ys^xs^y)=-I\otimes s^x\ \text{ odd}\\TI\otimes s^yT^{-1}&=(I\otimes(is^y)K)I\otimes s^y(I\otimes(-is^y)K)=I\otimes(-s^ys^ys^y)=-I\otimes s^y\ \text{ odd}\\TI\otimes s^zT^{-1}&=(I\otimes(is^y)K)I\otimes s^z(I\otimes(-is^y)K)=I\otimes(s^ys^zs^y)=-I\otimes s^z\ \text{ odd}\\T\sigma_x\otimes IT^{-1}&=(I\otimes(is^y)K)\sigma_x\otimes I(I\otimes(-is^y)K)=\sigma_x\otimes(s^yIs^y)=\sigma_x\otimes I\ \text{ even}\\T\sigma_x\otimes s^xT^{-1}&=(I\otimes(is^y)K)\sigma_x\otimes s^x(I\otimes(-is^y)K)=\sigma_x\otimes(s^ys^xs^y)=-\sigma_x\otimes s^x\ \text{ odd}\\T\sigma_x\otimes s^yT^{-1}&=(I\otimes(is^y)K)\sigma_x\otimes s^y(I\otimes(-is^y)K)=\sigma_x\otimes(-s^ys^ys^y)=-\sigma_x\otimes s^y\ \text{ odd}\\T\sigma_x\otimes s^zT^{-1}&=(I\otimes(is^y)K)\sigma_x\otimes s^z(I\otimes(-is^y)K)=\sigma_x\otimes(s^ys^zs^y)=-\sigma_x\otimes s^z\ \text{ odd}\\T\sigma_y\otimes IT^{-1}&=(I\otimes(is^y)K)\sigma_y\otimes I(I\otimes(-is^y)K)=-\sigma_y\otimes(s^yIs^y)=-\sigma_y\otimes I\ \text{ odd}\\T\sigma_y\otimes s^xT^{-1}&=(I\otimes(is^y)K)\sigma_y\otimes s^x(I\otimes(-is^y)K)=-\sigma_y\otimes(s^ys^xs^y)=\sigma_y\otimes s^x\ \text{ even}\\T\sigma_y\otimes s^yT^{-1}&=(I\otimes(is^y)K)\sigma_y\otimes s^y(I\otimes(-is^y)K)=-\sigma_y\otimes(-s^ys^ys^y)=\sigma_y\otimes s^y\ \text{ even}\\T\sigma_y\otimes s^zT^{-1}&=(I\otimes(is^y)K)\sigma_y\otimes s^z(I\otimes(-is^y)K)=-\sigma_y\otimes(s^ys^zs^y)=\sigma_y\otimes s^z\ \text{ even}\\T\sigma_z\otimes IT^{-1}&=(I\otimes(is^y)K)\sigma_z\otimes I(I\otimes(-is^y)K)=\sigma_z\otimes(s^yIs^y)=\sigma_x\otimes I\ \text{ even}\\T\sigma_z\otimes s^xT^{-1}&=(I\otimes(is^y)K)\sigma_z\otimes s^x(I\otimes(-is^y)K)=\sigma_z\otimes(s^ys^xs^y)=-\sigma_z\otimes s^x\ \text{ odd}\\T\sigma_z\otimes s^yT^{-1}&=(I\otimes(is^y)K)\sigma_z\otimes s^y(I\otimes(-is^y)K)=\sigma_z\otimes(-s^ys^ys^y)=-\sigma_z\otimes s^y\ \text{ odd}\\T\sigma_z\otimes s^zT^{-1}&=(I\otimes(is^y)K)\sigma_z\otimes s^z(I\otimes(-is^y)K)=\sigma_z\otimes(s^ys^zs^y)=-\sigma_z\otimes s^z\ \text{ odd}\end{aligned}$$

so besides the $I\otimes I$ there are only five are even under time reversal T

$$\Gamma^1=\sigma_x\otimes I$$

$$\Gamma^2 = \sigma_z \otimes I$$
$$\Gamma^3 = \sigma_y \otimes s^x$$
$$\Gamma^4 = \sigma_y \otimes s^y$$
$$\Gamma^5 = \sigma_y \otimes s^z$$

since others are odd, which can be written as $\Gamma^{a,b} := \frac{[\Gamma^a, \Gamma^b]}{2i}$.namely

$$\Gamma^{1,2} = -\sigma_y \otimes I \quad \Gamma^{1,3} = \sigma_z \otimes s^x \quad \Gamma^{1,4} = \sigma_z \otimes s^y \quad \Gamma^{1,5} = \sigma_z \otimes s^z$$
$$\Gamma^{2,3} = -\sigma_x \otimes s^x \quad \Gamma^{2,4} = -\sigma_x \otimes s^y \quad \Gamma^{2,5} = -\sigma_x \otimes s^z$$
$$\Gamma^{3,4} = I \otimes s^z \quad \Gamma^{3,5} = -I \otimes s^y$$
$$\Gamma^{4,5} = I \otimes s^x$$

then the equation (9) can be written in these basis as

$$H_k = \lambda_\nu \Gamma^2 + (t\sum_{i=1}^{3}\cos(k\cdot\delta_i))\Gamma^1 + (t\sum_{i=1}^{3}\sin(k\cdot\delta_i))(-\Gamma^{1,2}) + \lambda_{\mathrm{so}} g(k)\Gamma^{1,5}$$
$$+ \lambda_R \mathrm{Re}[z_k^x](-\Gamma^{2,3}) - \lambda_R \mathrm{Im}[z_k^x]\Gamma^3 + \lambda_R \mathrm{Re}[z_k^y](-\Gamma^{2,4}) - \lambda_R \mathrm{Im}[z_k^y]\Gamma^4$$

where we have define

$$g(k) = 2\sum_{i=1}^{3}\sin(k\cdot a_i)$$

and

$$\sum_{i=1}^{3} e^{-ik\cdot\delta_i}(-s\times\delta_i)_z = -i(z_k^x s^x + z_k^y s^y)$$

ℜ.2 The boundary Modes

in oder to work out the boundary modes, we should take periodic boundary condition in one dimension and open boundary condition in other dimension, which means that we can only make Fourier transform in one dimension of the lattice sites.Suppose that we choose periodic boundary condition along the a_2 direction, in this case we can write down that:

$$c_{m,k} = \frac{1}{\sqrt{N_2}}\sum_{n=1}^{N_2} e^{-ik\cdot r_{m,n}} c_{(m,n)}$$
$$c_{m,n} = \frac{1}{\sqrt{N_2}}\sum_{k} e^{ik\cdot r_{m,n}} c_{m,k}$$

in this case the onsite term in the model becomes:

$$\begin{aligned}\sum_{(m,n)} c_{m,n}^\dagger c_{m,n} &= \sum_{(m,n)}\frac{1}{N_2}\sum_{k,k'} e^{-ik\cdot r_{m,n}} e^{-ik'\cdot r_{m,n}} c_{m,k}^\dagger c_{m,k'} \\ &= \sum_m\sum_{k,k'} c_{m,k}^\dagger c_{m,k'}\delta_{k,k'} \\ &= \sum_k\sum_m c_{m,k}^\dagger c_{m,k}\end{aligned}$$

considering there are two kinds of atoms in each unite cell, we have the onsite term in k block read as

$$\lambda_\nu\sum_m c_{m,k,A}^\dagger c_{m,k,A} - \lambda_\nu\sum_m c_{m,k,B}^\dagger c_{m,k,B}$$

with the same reason, the nearest coupling term becomes

$$\begin{aligned}
t_1 \sum_{<(m,n),(m',n')>} c^\dagger_{(m,n),A} c_{(m',n'),B} &= t_1 \sum_{<(m,n),(m',n')>} \frac{1}{N_2} \sum_{k,k'} e^{-ik\cdot r_{m,n}} e^{ik'\cdot r_{m',n'}} c^\dagger_{m,k,A} c_{m',k',B} \\
&= t_1 \sum_{(m,n)} \frac{1}{N_2} \sum_{k,k'} e^{-ik\cdot r_{m,n}} e^{ik'\cdot r_{m,n}} (\sum_i e^{ik'\cdot\delta_{i,2}} c^\dagger_{m,k,A} c_{(m+\delta_{i,1}),k',B}) \\
&= t_1 \sum_m \sum_{k,k'} \delta_{k,k'} (\sum_i e^{ik'\cdot\delta_{i,2}} c^\dagger_{m,k} c_{m+\delta_{i,1},k'}) \\
&= t_1 \sum_k \sum_m (\sum_i e^{ik\cdot\delta_{i,2}} c^\dagger_{m,k} c_{m+\delta_{i,1},k})
\end{aligned}$$

the k block is just

$$\begin{aligned}
& t_1 \sum_m (\sum_i e^{ik\cdot\delta_{i,2}} c^\dagger_{m,k} c_{m+\delta_{i,1},k}) + h.c \\
&= t_1 \sum_m (e^{-ik\cdot\delta_{3,2}} c^\dagger_{m,k,A} c_{m,B,k} + e^{-ik\cdot\delta_{1,2}} c^\dagger_{m,k,A} c_{m-1,B,k} + e^{-ik\cdot\delta_{2,2}} c^\dagger_{m,k,A} c_{m,B,k}) \\
&+ t_1 \sum_m (e^{ik\cdot\delta_{1,2}} c^\dagger_{m,k,B} c_{m+1,A,k} + e^{ik\cdot\delta_{2,2}} c^\dagger_{m,k,B} c_{m,A,k} + e^{ik\cdot\delta_{3,2}} c^\dagger_{m,k,B} c_{m,A,k})
\end{aligned}$$

then we consider the next nearest SO term, as for this term, at first we consider the general term with the following form:

$$\begin{aligned}
\sum_{(m,n)} c^\dagger_{(m,n)} c_{(m,n)+(r,s)} &= \sum_{(m,n)} \sum_{k,k'} \frac{1}{N_2} e^{-ik\cdot r_{(m,n),2}} e^{ik'\cdot r_{(m,n)+(r,s),2}} c^\dagger_{m,k} c_{m+r,k'} \\
&= \sum_{(m,n)} \sum_{k,k'} \frac{1}{N_2} e^{-ik\cdot r_{(m,n),2}} e^{ik'\cdot r_{(m,n),2}} e^{ik'\cdot sa_2} c^\dagger_{m,k} c_{m+r,k'} \\
&= \sum_m \sum_{k,k'} \delta_{k,k'} e^{ik\cdot sa_2} c^\dagger_{m,k} c_{m+r,k'} \\
&= \sum_m \sum_k e^{ik\cdot sa_2} c^\dagger_{m,k} c_{m+r,k}
\end{aligned}$$

and the corresponding diagonal k block is

$$\sum_m e^{ik\cdot sa_2} c^\dagger_{m,k} c_{m+r,k}$$

so if we let a_1 and a_2 be the primitive lattice vectors of graphene as Figure 14 shows, we can write down the term of H_{so} as:

$$\begin{aligned}
H_{\text{so}} = i\lambda_{\text{so}} \sum_m & (c^\dagger_{m,k,A} s^z c_{m+1,k,A} e^{ik\cdot 0} - c^\dagger_{m,k,A} s^z c_{m,k,A} e^{ik\cdot a_2} + c^\dagger_{m,k,A} s^z c_{m-1,k,A} e^{ik\cdot a_2} \\
& - c^\dagger_{m,k,A} s^z c_{m-1,k,A} e^{ik\cdot 0} + c^\dagger_{m,k,A} s^z c_{m,k,A} e^{ik\cdot -a_2} - c^\dagger_{m,k,A} s^z c_{m+1,k,A} e^{ik\cdot -a_2}) \\
& + i\lambda_{\text{so}} \sum_m (-c^\dagger_{m,k,B} s^z c_{m+1,k,B} e^{ik\cdot 0} + c^\dagger_{m,k,A} s^z c_{m,k,B} e^{ik\cdot a_2} - c^\dagger_{m,k,B} s^z c_{m-1,k,B} e^{ik\cdot a_2} \\
& + c^\dagger_{m,k,B} s^z c_{m-1,k,B} e^{ik\cdot 0} - c^\dagger_{m,k,B} s^z c_{m,k,B} e^{ik\cdot -a_2} + c^\dagger_{m,k,B} s^z c_{m+1,k,B} e^{ik\cdot -a_2})
\end{aligned}$$

if $m \pm 1$ exceed the region of the lattice number in a_1 direction, that term should vanish in the above equation. this is the way we choose open boundary condition to calculate the boundary modes.

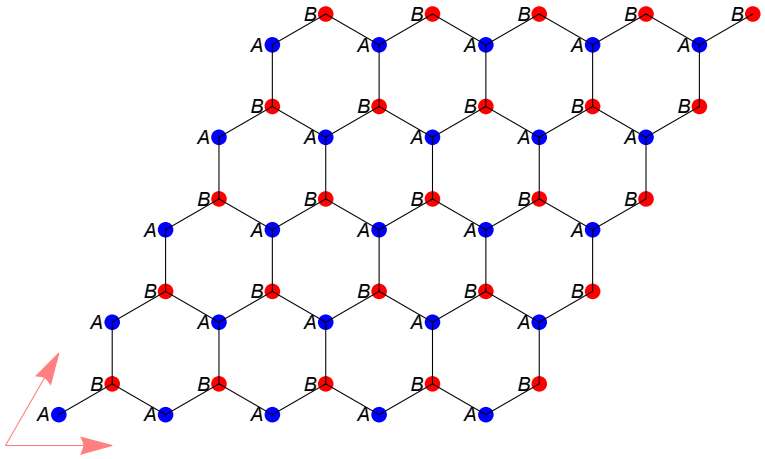

Figure 14: the open boundary of graphene

at last, we will consider the nearest neighbor Rashba term

$$H_R = i\lambda_R \sum_{<i,j>} c_i^\dagger (s \times \hat{d}_{ij})_z c_j$$

in our notation of Fourier Transform along the a_2 direction, this can be written as

$$H_R = i\lambda_R \sum_k \sum_m (c^\dagger_{m,k,A} e^{-ik\cdot\delta_{3,2}} (-s \times \hat{\delta}_3)_z c_{m,k,B} + c^\dagger_{m,k,A} e^{-ik\cdot\delta_{1,2}} (-s \times \hat{\delta}_1)_z c_{m-1,k,B} + c^\dagger_{m,k,A} e^{-ik\cdot\delta_{2,2}} (-s \times \hat{\delta}_2)_z c_{m,k,B})$$
$$+ i\lambda_R \sum_k \sum (c^\dagger_{m,k,B} e^{ik\cdot\delta_1} (s \times \hat{\delta}_1)_z c_{m+1,k,A} + c^\dagger_{m,k,B} e^{ik\cdot\delta_2} (s \times \hat{\delta}_2)_z c_{m,k,A} + c^\dagger_{m,k,B} e^{ik\cdot\delta_3} (s \times \hat{\delta}_3)_z c_{m,k,A})$$

sililarly, if $m \pm 1$ exceed the region of the lattice number in a_1 direction, which means that term should vanish in the above equation. so if we use the basis

$$\gamma_k = (\cdots, c_{m-1,k,A}, c_{m-1,k,B}, c_{m,k,A}, c_{m,k,B}, c_{m+1,k,A}, c_{m+1,k,B}, \cdots)^T$$

then the hamiltonian in the k diagonal block should be $\gamma_k^\dagger H_k \gamma_k$ and M_k is a 4NX4N metrics with N the number of unite cells along a_1 direction.

the onsite staggered potential terms will contribute to H_k a term with the following metrics

$$H_{\nu,k} = \lambda_\nu I_N \otimes \sigma_z$$

and the nearest hopping term will contribute to H_k a term with the following metrics multiply a general parameter t_1:

$$I_N \otimes \begin{pmatrix} 0 & e^{-ik\cdot\delta_{2,2}} + e^{-ik\cdot\delta_{3,2}} \\ e^{ik\cdot\delta_{2,2}} + e^{ik\cdot\delta_{3,2}} & 0 \end{pmatrix} + I_{N,1} \otimes \begin{pmatrix} 0 & 0 \\ e^{ik\delta_{1,2}} & 0 \end{pmatrix} + I_{N,-1} \otimes \begin{pmatrix} 0 & e^{-ik\delta_{1,2}} \\ 0 & 0 \end{pmatrix}$$

and the next nearest SO hopping term contribute to H_k a term with the following metrics multiply a general parameter λ_{so}

$$iI_N \otimes \begin{pmatrix} -e^{ika_2} + e^{-ika_2} & 0 \\ 0 & e^{ika_2} - e^{-ika_2} \end{pmatrix} \otimes s^z$$
$$+ iI_{N,1} \otimes \begin{pmatrix} 1 - e^{-ik\cdot a_2} & 0 \\ 0 & -1 + e^{-ik\cdot a_2} \end{pmatrix} \otimes s^z$$

$$+ iI_{N,-1} \otimes \begin{pmatrix} e^{ik\cdot a_2} - 1 & 0 \\ 0 & -e^{ik\cdot a_2} + 1 \end{pmatrix} \otimes s^z$$

Finally the nearest neighbor Rashba term will contribute to H_k a term with the following metrics multiply a general parameterλ_R:

$$\begin{aligned}
&iI_N \otimes \begin{pmatrix} 0 & e^{-ik\delta_{3,2}}(-s\times\delta_3)_z + e^{-ik\delta_{2,2}}(-s\times\delta_2)_z \\ e^{ik\delta_{3,2}}(s\times\delta_3)_z + e^{ik\delta_{2,2}}(s\times\delta_2)_z & 0 \end{pmatrix} \\
&+ iI_{N,1} \otimes \begin{pmatrix} 0 & 0 \\ e^{ik\cdot\delta_{1,2}}(s\times\delta_1)_z & \end{pmatrix} + iI_{N,-1} \otimes \begin{pmatrix} 0 & e^{-ik\cdot\delta_{1,2}}(-s\times\delta_1)_z \\ 0 & 0 \end{pmatrix} \\
&= iI_N \otimes \begin{pmatrix} 0 & -e^{-ik\delta_{3,2}} \\ e^{ik\delta_{3,2}} & 0 \end{pmatrix} (s\times\delta_3)_z + iI_N \otimes \begin{pmatrix} 0 & -e^{-ik\delta_{2,2}} \\ e^{ik\delta_{2,2}} & 0 \end{pmatrix} (s\times\delta_2)_z \\
&+ iI_{N,1} \otimes \begin{pmatrix} 0 & 0 \\ e^{ik\cdot\delta_{1,2}} & \end{pmatrix} (s\times\delta_1)_z + iI_{N,-1} \otimes \begin{pmatrix} 0 & -e^{-ik\cdot\delta_{1,2}} \\ 0 & 0 \end{pmatrix} (s\times\delta_1)_z
\end{aligned}$$

since we know $\delta_1 = \frac{1}{3}(2a_1 - a_2) = \frac{a}{2}(1, -\sqrt{3})$,$\delta_2 = \frac{1}{3}(2a_2 - a_1) = \frac{a}{2}(1, \sqrt{3})$,$\delta_3 = -\frac{1}{3}(a_1 + a_2) = \frac{a}{2}(-2, 0)$ and $|a_1| = |a_2| = \sqrt{3}a$,so we have (we set $a = \frac{1}{\sqrt{3}}$ so that $|a_1| = |a_2| = 1$ in the following context)

$$\begin{aligned}
e^{ik\cdot\delta_{1,2}} &= e^{ik(-\frac{1}{3}|a_2|)} = e^{-ik\frac{\sqrt{3}}{3}a} = e^{-ik\frac{1}{3}} \\
e^{ik\cdot\delta_{2,2}} &= e^{ik(\frac{2}{3}|a_2|)} = e^{ik\frac{2\sqrt{3}}{3}a} = e^{ik\frac{2}{3}} \\
e^{ik\cdot\delta_{3,2}} &= e^{ik(-\frac{1}{3}|a_2|)} = e^{-ik\frac{\sqrt{3}}{3}a} = e^{-ik\frac{1}{3}} \\
e^{ika_2} &= e^{ik\sqrt{3}a} = e^{ik}
\end{aligned}$$

and the values for $(s\times\delta_i)_z$

$$\begin{aligned}
(s\times\hat{\delta}_1)_z &= -\frac{\sqrt{3}}{2}s^x - \frac{1}{2}s^y \\
(s\times\hat{\delta}_2)_z &= \frac{\sqrt{3}}{2}s^x - \frac{1}{2}s^y \\
(s\times\hat{\delta}_3)_z &= s^y
\end{aligned}$$

so finally the nearest neighbor Rashba term can be written as

$$\begin{aligned}
&= iI_N \otimes \begin{pmatrix} 0 & -e^{-ik\delta_{3,2}} \\ e^{ik\delta_{3,2}} & 0 \end{pmatrix} s^y + iI_N \otimes \begin{pmatrix} 0 & -e^{-ik\delta_{2,2}} \\ e^{ik\delta_{2,2}} & 0 \end{pmatrix} (\frac{\sqrt{3}}{2}s^x - \frac{1}{2}s^y) \\
&+ iI_{N,1} \otimes \begin{pmatrix} 0 & 0 \\ e^{ik\cdot\delta_{1,2}} & 0 \end{pmatrix} (-\frac{\sqrt{3}}{2}s^x - \frac{1}{2}s^y) + iI_{N,-1} \otimes \begin{pmatrix} 0 & -e^{-ik\cdot\delta_{1,2}} \\ 0 & 0 \end{pmatrix} (-\frac{\sqrt{3}}{2}s^x - \frac{1}{2}s^y) \\
&= \{\frac{\sqrt{3}}{2}iI_N \otimes \begin{pmatrix} 0 & -e^{-ik\delta_{2,2}} \\ e^{ik\delta_{2,2}} & 0 \end{pmatrix} - \frac{\sqrt{3}}{2}iI_{N,1} \otimes \begin{pmatrix} 0 & 0 \\ e^{ik\cdot\delta_{1,2}} & 0 \end{pmatrix} \\
&- \frac{\sqrt{3}}{2}iI_{N,-1} \otimes \begin{pmatrix} 0 & -e^{-ik\cdot\delta_{1,2}} \\ 0 & 0 \end{pmatrix}\} s^x \\
&+ \{iI_N \otimes \begin{pmatrix} 0 & -e^{-ik\delta_{3,2}} \\ e^{ik\delta_{3,2}} & 0 \end{pmatrix} - \frac{1}{2}iI_N \otimes \begin{pmatrix} 0 & -e^{-ik\delta_{2,2}} \\ e^{ik\delta_{2,2}} & 0 \end{pmatrix}
\end{aligned}$$

$$-\frac{1}{2}iI_{N,1}\otimes\begin{pmatrix}0&0\\e^{ik\cdot\delta_{1,2}}&0\end{pmatrix}-\frac{1}{2}iI_{N,-1}\otimes\begin{pmatrix}0&-e^{-ik\cdot\delta_{1,2}}\\0&0\end{pmatrix}\}s^y$$

in the end of the story, after collecting all the terms, the hamiltonian in diagonal k block with open boundary conditions in the a_1 direction consisting of the following terms

$$H=H_\nu+H_t+H_{\rm so}+H_R$$

wher H_ν is the following metrics multiply a global parameter multiplier λ_ν

$$I_N\otimes\sigma_z$$

wher H_t is the following metrics multiply a global parameter multiplier t_1

$$I_N\otimes\begin{pmatrix}0&e^{-ik\cdot\delta_{2,2}}+e^{-ik\cdot\delta_{3,2}}\\e^{ik\cdot\delta_{2,2}}+e^{ik\cdot\delta_{3,2}}&0\end{pmatrix}+I_{N,1}\otimes\begin{pmatrix}0&0\\e^{ik\delta_{1,2}}&0\end{pmatrix}+I_{N,-1}\otimes\begin{pmatrix}0&e^{-ik\delta_{1,2}}\\0&0\end{pmatrix}$$

wher $H_{\rm so}$ is the following metrics multiply a global parameter multiplier $\lambda_{\rm so}$

$$\begin{aligned}&iI_N\otimes\begin{pmatrix}-e^{ika_2}+e^{-ika_2}&0\\0&e^{ika_2}-e^{-ika_2}\end{pmatrix}\otimes s^z\\&+iI_{N,1}\otimes\begin{pmatrix}1-e^{-ik\cdot a_2}&0\\0&-1+e^{-ik\cdot a_2}\end{pmatrix}\otimes s^z\\&+iI_{N,-1}\otimes\begin{pmatrix}e^{ik\cdot a_2}-1&0\\0&-e^{ik\cdot a_2}+1\end{pmatrix}\otimes s^z\end{aligned}$$

wher H_R is the following metrics multiply a global parameter multiplier λ_R

$$\begin{aligned}&\{\frac{\sqrt{3}}{2}iI_N\otimes\begin{pmatrix}0&-e^{-ik\delta_{2,2}}\\e^{ik\delta_{2,2}}&0\end{pmatrix}-\frac{\sqrt{3}}{2}iI_{N,1}\otimes\begin{pmatrix}0&0\\e^{ik\cdot\delta_{1,2}}&0\end{pmatrix}\\&-\frac{\sqrt{3}}{2}iI_{N,-1}\otimes\begin{pmatrix}0&-e^{-ik\cdot\delta_{1,2}}\\0&0\end{pmatrix}\}s^x\\&+\{iI_N\otimes\begin{pmatrix}0&-e^{-ik\delta_{3,2}}\\e^{ik\delta_{3,2}}&0\end{pmatrix}-\frac{1}{2}iI_N\otimes\begin{pmatrix}0&-e^{-ik\delta_{2,2}}\\e^{ik\delta_{2,2}}&0\end{pmatrix}\\&-\frac{1}{2}iI_{N,1}\otimes\begin{pmatrix}0&0\\e^{ik\cdot\delta_{1,2}}&0\end{pmatrix}-\frac{1}{2}iI_{N,-1}\otimes\begin{pmatrix}0&-e^{-ik\cdot\delta_{1,2}}\\0&0\end{pmatrix}\}s^y\end{aligned}$$

§5 Kagome Lattice

another important lattice model constructed from the honeycomb lattice is the so called kagome lattice, which holds flat band, Dirac cone and Van Hove singularity, in this section, we will demonstrate these features.

the lattice configuration can be seen in Figure 15. it's quite similar to graphene but in each unite cell, there are three sites. Considering the nearest coupling, the hamiltonian in the kagome lattice can be written as

$$H=\sum_{<i,j>}t_{i,j}c_i^\dagger c_j$$

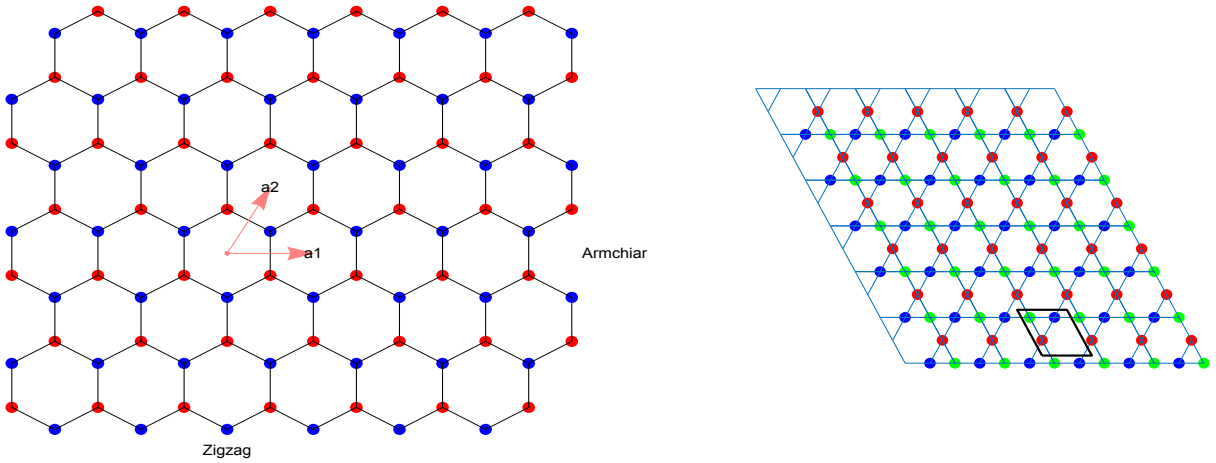

Figure 15: Left: the graphene lattice, which can be seen as translation of the regular hexagon along the reflection symmetry line passing the midpoint of each edge, in this kind of translation, the regular hexagon can fill up the whole plane thus the lattice sites in each unite cell is two, labeled aa A and B in literature. Right: the kagome lattice, it can be seen as translation of the regular hexagon along the reflection symmetry line passing the vertexes of the hexagon, in this kind of translation, the regular hexagon can not fill up the whole plane, there are regular triangles in the unfilled parts, so the unite cell must be larger than that in the graphene or equivalently, there are three sites in each unite cell which is larger than that in graphene.

in the following, we consider the fully symmetric case, that is $t_{i,j} = t$ for all the bonds, we can write down the Fourier transform of lattice model to the momentum space which is, in the spinor $\gamma_k = (c_{k,1}, c_{k,2}, c_{k,3})^T$, it read as

$$
\begin{aligned}
H(k) = &\begin{pmatrix} 0 & 1 & 1 \\ 1 & 0 & 1 \\ 1 & 1 & 0 \end{pmatrix} \\
&+ e^{-ik\cdot a_1}\begin{pmatrix} 0 & 0 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} + e^{ik\cdot a_1}\begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \\
&+ e^{-ik\cdot a_2}\begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} + e^{ik\cdot a_2}\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix} \\
&+ e^{-ik\cdot (a_2+a_1)}\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 0 & 0 \end{pmatrix} + e^{ik\cdot (a_2+a_1)}\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix} \\
= &\begin{pmatrix} 0 & 1+e^{ik\cdot a_1} & 1+e^{-ik\cdot a_2} \\ 1+e^{-ik\cdot a_1} & 0 & 1+e^{-ik\cdot (a_1+a_2)} \\ 1+e^{ik\cdot a_2} & 1+e^{ik\cdot (a_1+a_2)} & 0 \end{pmatrix}
\end{aligned}
$$

then we can derive the band of this hamiltonian

$$
\begin{aligned}
|H(k) - EI| = &-E(E^2 - (1+e^{ik\cdot (a_1+a_2)})(1+e^{-ik\cdot (a_1+a_2)})) \\
&- (1+e^{-ik\cdot a_1})(-E(1+e^{ik\cdot a_1}) - (1+e^{-ik\cdot a_2})(1+e^{ik\cdot (a_1+a_2)}))
\end{aligned}
$$

$$
\begin{aligned}
&+ (1+e^{ik\cdot a_2})((1+e^{ik\cdot a_1})(1+e^{-ik\cdot(a_1+a_2)}) + E(1+e^{-ik\cdot a_2})) \\
&= -E^3 + E(2+2\cos(k\cdot(a_1+a_2)) + 2 + 2\cos(k\cdot a_1) + 2 + 2\cos(k\cdot a_2)) \\
&+ \{(1+e^{ik\cdot a_2})(1+e^{ik\cdot a_1})(1+e^{-ik\cdot(a_1+a_2)}) + c.c\} \\
&= -E^3 + E(2+2\cos(k\cdot(a_1+a_2)) + 2 + 2\cos(k\cdot a_1) + 2 + 2\cos(k\cdot a_2)) \\
&+ \{1 + e^{ik\cdot a_1} + e^{ik\cdot a_2} + e^{ik\cdot(a_1+a_2)} + e^{-ik\cdot(a_1+a_2)} + e^{-ik\cdot a_1} + e^{-ik\cdot a_2} + 1 + c.c\} \\
&= -E^3 + E(2+2\cos(k\cdot(a_1+a_2)) + 2 + 2\cos(k\cdot a_1) + 2 + 2\cos(k\cdot a_2)) \\
&+ 4(1+\cos(k\cdot(a_1+a_2)) + \cos(k\cdot a_1) + \cos(k\cdot a_2)) \\
&= 0
\end{aligned}
$$

we can find that the solution to the above equation is

$$E_1(k) = -2$$

which is independent of k.

and then dividing the above equation with $(E+2)$ we have

$$
\begin{aligned}
&- E^2 + 2E + (2+2\cos(k\cdot(a_1+a_2)) + 2 + 2\cos(k\cdot a_1) + 2 + 2\cos(k\cdot a_2)) - 4 = 0 \\
&\rightarrow (E-1)^2 = 3 + 2\cos(k\cdot(a_1+a_2)) + 2\cos(k\cdot a_1) + 2\cos(k\cdot a_2)
\end{aligned}
$$

thus we have

$$E_{\pm}(k) = 1 \pm \sqrt{3 + 2\cos(k\cdot(a_1+a_2)) + 2\cos(k\cdot a_1) + 2\cos(k\cdot a_2)}$$

since the unite cell is the sam as that of graphene except the volume, so we can directly use the results from graphene and find that

$$2\cos(k\cdot(a_1+a_2)) + 2\cos(k\cdot a_1) + 2\cos(k\cdot a_2) = f(k) = 2\cos(\sqrt{3}ak_y) + 4\cos(\frac{3}{2}ak_x)\cos(\frac{\sqrt{3}}{2}ak_y)$$

in conclusion, we have the band structure of the kagome lattice

$$
\begin{aligned}
E_1(k) &= -2t \\
E_{\pm}(k) &= t(1 \pm \sqrt{3+f(k)})
\end{aligned}
$$

References

[1] F. D. M. Haldane, *Model for a quantum hall effect without landau levels: Condensed-matter realization of the parity anomaly*, Physical review letters **61**, 2015 (1988).