1 石墨烯的紧束缚模型

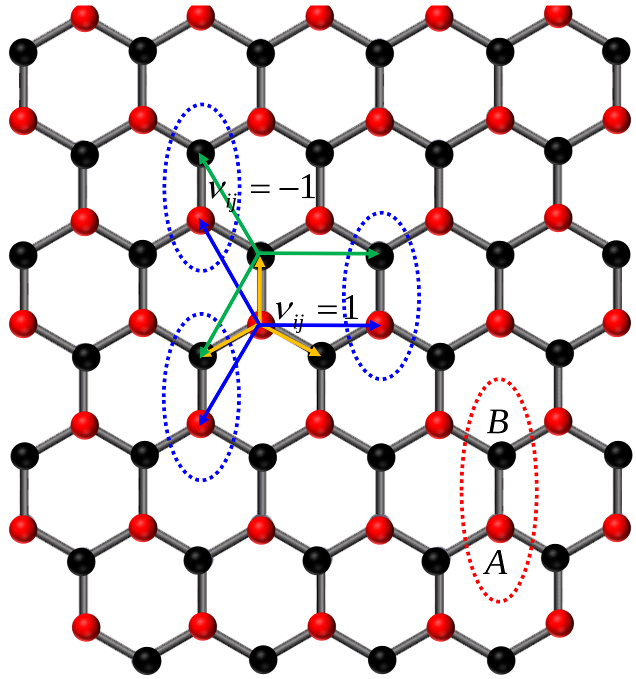

图 1: 石墨烯晶格示意图.

在六角石墨烯晶格中，选择一组原胞后，每个原子与其最近邻的原子之间相差的矢量分别为：

$$\mathbf{e}_0=(0,1);\mathbf{e}_1=(-\frac{\sqrt{3}}{2},-\frac{1}{2});\mathbf{e}_2=(\frac{\sqrt{3}}{2},-\frac{1}{2})$$

首先考虑电子的最近邻跃迁的哈密顿量H_1：

$$\begin{aligned}H_1&=t\sum_{\langle i,j\rangle}(a_i^\dagger b_j+b_j^\dagger a_i)\\&=t\sum_i(a_{\mathbf{r}_i}^\dagger b_{\mathbf{r}_i+\mathbf{e}_0}+a_{\mathbf{r}_i}^\dagger b_{\mathbf{r}_i+\mathbf{e}_1}+a_{\mathbf{r}_i}^\dagger b_{\mathbf{r}_i+\mathbf{e}_2}+b_{\mathbf{r}_i+\mathbf{e}_0}^\dagger a_{\mathbf{r}_i}+b_{\mathbf{r}_i+\mathbf{e}_1}^\dagger a_{\mathbf{r}_i}+b_{\mathbf{r}_i+\mathbf{e}_2}^\dagger a_{\mathbf{r}_i})\end{aligned}$$

利用Fourier变换关系：

$$\begin{aligned}a_i&=\frac{1}{\sqrt{N}}\sum_{\mathbf{k}}a_k e^{-i\mathbf{k}\cdot\mathbf{r}_i}\\b_i&=\frac{1}{\sqrt{N}}\sum_{\mathbf{k}}b_k e^{-i\mathbf{k}\cdot\mathbf{r}_i}\end{aligned}$$

于是位置的产生湮灭算符构造的哈密顿量写为：

$$\sum_i a_{\mathbf{r}_i}^\dagger b_{\mathbf{r}_i+\mathbf{e}_0}=\sum_{\mathbf{k}}a_{\mathbf{k}}^\dagger b_{\mathbf{k}}e^{-i\mathbf{k}\cdot\mathbf{e}_0};\sum_i a_{\mathbf{r}_i}^\dagger b_{\mathbf{r}_i+\mathbf{e}_1}=\sum_{\mathbf{k}}a_{\mathbf{k}}^\dagger b_{\mathbf{k}}e^{-i\mathbf{k}\cdot\mathbf{e}_1};\sum_i a_{\mathbf{r}_i}^\dagger b_{\mathbf{r}_i+\mathbf{e}_2}=\sum_{\mathbf{k}}a_{\mathbf{k}}^\dagger b_{\mathbf{k}}e^{-i\mathbf{k}\cdot\mathbf{e}_2}$$

$$\sum_i(b_{\mathbf{r}_i+\mathbf{e}_0}^\dagger a_{\mathbf{r}_i})=\sum_{\mathbf{k}}b_{\mathbf{k}}^\dagger a_{\mathbf{k}}e^{i\mathbf{k}\cdot\mathbf{e}_0};\sum_i(b_{\mathbf{r}_i+\mathbf{e}_1}^\dagger a_{\mathbf{r}_i})=\sum_{\mathbf{k}}b_{\mathbf{k}}^\dagger a_{\mathbf{k}}e^{i\mathbf{k}\cdot\mathbf{e}_1};\sum_i(b_{\mathbf{r}_i+\mathbf{e}_2}^\dagger a_{\mathbf{r}_i})=\sum_{\mathbf{k}}b_{\mathbf{k}}^\dagger a_{\mathbf{k}}e^{i\mathbf{k}\cdot\mathbf{e}_2}$$

于是得到哈密顿量为：

$$\begin{aligned}H_1 &= t\sum_i(a^\dagger_{\mathbf{r}_i}b_{\mathbf{r}_i+\mathbf{e}_0}+a^\dagger_{\mathbf{r}_i}b_{\mathbf{r}_i+\mathbf{e}_1}+a^\dagger_{\mathbf{r}_i}b_{\mathbf{r}_i+\mathbf{e}_2}+b^\dagger_{\mathbf{r}_i+\mathbf{e}_0}a_{\mathbf{r}_i}+b^\dagger_{\mathbf{r}_i+\mathbf{e}_1}a_{\mathbf{r}_i}+b^\dagger_{\mathbf{r}_i+\mathbf{e}_2}a_{\mathbf{r}_i})\\ &= t\sum_{\mathbf{k}}a^\dagger_{\mathbf{k}}b_{\mathbf{k}}e^{-i\mathbf{k}\cdot\mathbf{e}_0}+a^\dagger_{\mathbf{k}}b_{\mathbf{k}}e^{-i\mathbf{k}\cdot\mathbf{e}_1}+a^\dagger_{\mathbf{k}}b_{\mathbf{k}}e^{-i\mathbf{k}\cdot\mathbf{e}_2}+b^\dagger_{\mathbf{k}}a_{\mathbf{k}}e^{i\mathbf{k}\cdot\mathbf{e}_0}+b^\dagger_{\mathbf{k}}a_{\mathbf{k}}e^{i\mathbf{k}\cdot\mathbf{e}_1}+b^\dagger_{\mathbf{k}}a_{\mathbf{k}}e^{i\mathbf{k}\cdot\mathbf{e}_2}\\ &= t\sum_{\mathbf{k}}\begin{pmatrix}a^\dagger_{\mathbf{k}} & b^\dagger_{\mathbf{k}}\end{pmatrix}\begin{pmatrix}0 & e^{-i\mathbf{k}\cdot\mathbf{e}_0}+e^{-i\mathbf{k}\cdot\mathbf{e}_1}+e^{-i\mathbf{k}\cdot\mathbf{e}_2}\\ e^{i\mathbf{k}\cdot\mathbf{e}_0}+e^{i\mathbf{k}\cdot\mathbf{e}_1}+e^{i\mathbf{k}\cdot\mathbf{e}_2} & 0\end{pmatrix}\begin{pmatrix}a_{\mathbf{k}}\\ b_{\mathbf{k}}\end{pmatrix}\end{aligned}$$

哈密顿量在动量空间的矩阵核则写为：

$$\mathbf{H}(\mathbf{k})=\mathbf{H}_1(\mathbf{k})=\begin{pmatrix}0 & f(\mathbf{k})\\ f^*(\mathbf{k}) & 0\end{pmatrix}$$

其中$f(\mathbf{k})$为

$$f(\mathbf{k})=t\left(e^{-i\mathbf{k}\cdot\mathbf{e}_0}+e^{-i\mathbf{k}\cdot\mathbf{e}_1}+e^{-i\mathbf{k}\cdot\mathbf{e}_2}\right)$$
$$f^*(\mathbf{k})=t\left(e^{i\mathbf{k}\cdot\mathbf{e}_0}+e^{i\mathbf{k}\cdot\mathbf{e}_1}+e^{i\mathbf{k}\cdot\mathbf{e}_2}\right)$$

仅仅考虑最近邻的哈密顿量时，$\mathbf{H}(\mathbf{k})$得到的能谱色散关系为：

$$E(\mathbf{k})=\pm\sqrt{|f(\mathbf{k})|^2}=\pm|t|\sqrt{3+2\cos\sqrt{3}k_x+4\cos(\frac{\sqrt{3}k_x}{2})\cos(\frac{3\sqrt{3}k_y}{2})}$$

$$\mathbf{e}_0=(0,1);\mathbf{e}_1=(-\frac{\sqrt{3}}{2},-\frac{1}{2});\mathbf{e}_2=(\frac{\sqrt{3}}{2},-\frac{1}{2})$$

接下来再考虑次近邻相互作用的石墨烯的哈密顿量H_2：

$$H_2=t'\sum_{\langle\langle i,j\rangle\rangle}(a^\dagger_i a_j+b^\dagger_i b_j)+h.c.$$

注意，次近邻的只有三个矢量，而不是六个矢量，需要利用的次近邻的矢量有：

$$\mathbf{d}_1=(\sqrt{3},0);\mathbf{d}_2=(-\frac{\sqrt{3}}{2},-\frac{3}{2});\mathbf{d}_3=(-\frac{\sqrt{3}}{2},\frac{3}{2})$$

则傅里叶变换之后

$$\begin{aligned}t'\sum_{\langle\langle i,j\rangle\rangle}a^\dagger_i a_j+h.c. &= t'\sum_i(a^\dagger_{\mathbf{r}_i}a_{\mathbf{r}_i+\mathbf{d}_1}+a^\dagger_{\mathbf{r}_i}a_{\mathbf{r}_i+\mathbf{d}_2}+a^\dagger_{\mathbf{r}_i}a_{\mathbf{r}_i+\mathbf{d}_3})+h.c.\\ &= t'\sum_{\mathbf{k}}a^\dagger_{\mathbf{k}}a_{\mathbf{k}}(e^{-i\mathbf{k}\cdot\mathbf{d}_1}+e^{-i\mathbf{k}\cdot\mathbf{d}_2}+e^{-i\mathbf{k}\cdot\mathbf{d}_3}+e^{i\mathbf{k}\cdot\mathbf{d}_1}+e^{i\mathbf{k}\cdot\mathbf{d}_2}+e^{i\mathbf{k}\cdot\mathbf{d}_3})\\ &= 2t'\sum_{\mathbf{k}}a^\dagger_{\mathbf{k}}a_{\mathbf{k}}[\cos(\mathbf{k}\cdot\mathbf{d}_1)+\cos(\mathbf{k}\cdot\mathbf{d}_2)+\cos(\mathbf{k}\cdot\mathbf{d}_3)]\\ &= t'\sum_{\mathbf{k}}a^\dagger_{\mathbf{k}}a_{\mathbf{k}}[2\cos(\sqrt{3}k_x)+2\cos(\frac{\sqrt{3}}{2}k_x+\frac{3}{2}k_y)+2\cos(\frac{\sqrt{3}}{2}k_x-\frac{3}{2}k_y)]\\ &= t'\sum_{\mathbf{k}}a^\dagger_{\mathbf{k}}a_{\mathbf{k}}[2\cos(\sqrt{3}k_x)+4\cos(\frac{\sqrt{3}}{2}k_x)\cos(\frac{3}{2}k_y)]\end{aligned}$$

同理对于子格B

$$t' \sum_{\langle\langle i,j \rangle\rangle} b_i^\dagger b_j + h.c. = t' \sum_{\mathbf{k}} b_{\mathbf{k}}^\dagger b_{\mathbf{k}} [2\cos(\sqrt{3}k_x) + 4\cos(\frac{\sqrt{3}}{2}k_x)\cos(\frac{3}{2}k_y)]$$

因此，得到的哈密顿量为：

$$\begin{aligned} H_2 &= t' \sum_{\langle\langle i,j \rangle\rangle} (a_i^\dagger a_j + b_i^\dagger b_j) + h.c. \\ &= \sum_{\mathbf{k}} \begin{pmatrix} a_{\mathbf{k}}^\dagger & b_{\mathbf{k}}^\dagger \end{pmatrix} t' \begin{pmatrix} h(\mathbf{k}) & 0 \\ 0 & h(\mathbf{k}) \end{pmatrix} \begin{pmatrix} a_{\mathbf{k}} \\ b_{\mathbf{k}} \end{pmatrix} \end{aligned}$$

其中

$$h(\mathbf{k}) = t'(2\cos(\sqrt{3}k_x) + 4\cos(\frac{\sqrt{3}}{2}k_x)\cos(\frac{3}{2}k_y))$$

则次近邻贡献的矩阵核为

$$\mathbf{H}_2(\mathbf{k}) = \begin{pmatrix} h(\mathbf{k}) & 0 \\ 0 & h(\mathbf{k}) \end{pmatrix}$$

因此总的哈密顿量为：

$$\mathbf{H}(\mathbf{k}) = \mathbf{H}_1(\mathbf{k}) + \mathbf{H}_2(\mathbf{k}) = \begin{pmatrix} h(\mathbf{k}) & f(\mathbf{k}) \\ f^*(\mathbf{k}) & h(\mathbf{k}) \end{pmatrix}$$

当考虑了次近邻效应后的能谱则为

$$\begin{aligned} E(\mathbf{k}) &= \pm\sqrt{|f(\mathbf{k})|^2} + h(\mathbf{k}) \\ &= \pm|t|\sqrt{3 + h(\mathbf{k})} + h(\mathbf{k}) \end{aligned}$$

其中t为最近邻跃迁系数，t'为次近邻的跃迁。

2 Haldane模型

紧束缚哈密顿量

$$\begin{aligned} H &= M\sum_i (a_i^\dagger a_i - b_i^\dagger b_i) + t\sum_{\langle i,j \rangle}(a_i^\dagger b_j + b_j^\dagger a_i) + \sum_{\langle\langle i,j \rangle\rangle}[t' e^{i\nu_{ij}\phi}(a_i^\dagger a_j + b_i^\dagger b_j) + h.c]. \\ &= H_0 + H_1 + H_2 \end{aligned}$$

其中第一项是引入的交错势能项；第二项为最近邻跃迁项，第三项为带了磁通的次近邻跃迁项。
第一项是交错的在位势能，

$$H_0 = M\sum_i (a_i^\dagger a_i - b_i^\dagger b_i)$$

利用Fourier变换关系：

$$a_i = \frac{1}{\sqrt{N}} \sum_{\mathbf{k}} a_k e^{-i\mathbf{k}\cdot\mathbf{r}_i}$$
$$b_i = \frac{1}{\sqrt{N}} \sum_{\mathbf{k}} b_k e^{-i\mathbf{k}\cdot\mathbf{r}_i}$$

$$H_0 = M\sum_i (a_i^\dagger a_i - b_i^\dagger b_i) = M\sum_{\mathbf{k}} (a_{\mathbf{k}}^\dagger a_{\mathbf{k}} - b_{\mathbf{k}}^\dagger b_{\mathbf{k}})$$
$$= \sum_{\mathbf{k}} \begin{pmatrix} a_{\mathbf{k}}^\dagger & b_{\mathbf{k}}^\dagger \end{pmatrix} \begin{pmatrix} M & 0 \\ 0 & -M \end{pmatrix} \begin{pmatrix} a_{\mathbf{k}} \\ b_{\mathbf{k}} \end{pmatrix}$$

因此交错势能项矩阵的核为

$$\mathbf{H}_0 = \begin{pmatrix} M & 0 \\ 0 & -M \end{pmatrix}$$

最近邻跃迁项与石墨烯一致，即

$$\mathbf{H}_1(\mathbf{k}) = \begin{pmatrix} 0 & f(\mathbf{k}) \\ f^*(\mathbf{k}) & 0 \end{pmatrix}$$

与石墨烯不一致的是，Haldane模型引入了带磁通的次近邻跃迁项

$$\sum_{\langle\langle i,j\rangle\rangle} [t' e^{i\nu_{ij}\phi}(a_i^\dagger a_j + b_i^\dagger b_j) + h.c].$$

其中ν_{ij}表示手性

$$\nu_{ij} = \frac{2}{\sqrt{3}} (\mathbf{d}_{ij}^{(1)} \times \mathbf{d}_{ij}^{(2)}) \cdot \mathbf{e}_z$$

考虑两个次近邻的位置分别为i和j，因为是次近邻跃迁，即六角晶格中原胞间相同子格间的跃迁，记作α_j到α_i，因此这两个共同子格α必然有一个公共的最近邻的子格β，这里$\mathbf{d}_{ij}^{(1)}$表示从位置原胞为j地方子格α指向子格β的矢量，$\mathbf{d}_{ij}^{(2)}$表示从子格β指向原胞i中的α子格的矢量。

举例：对于A子格，当从位置$j(\sqrt{3},0)$跳回位置$i(0,0)$需要的中间格点为$(\frac{\sqrt{3}}{2},-\frac{1}{2})$，相应的中间矢量分别为：

$$\mathbf{d}_{ij}^{(1)} = (-\frac{\sqrt{3}}{2}, \frac{1}{2}); \mathbf{d}_{ij}^{(2)} = (-\frac{\sqrt{3}}{2}, -\frac{1}{2})$$

因此此时的手性为：

$$\nu_{ij} = \frac{2}{\sqrt{3}} \begin{pmatrix} \mathbf{e}_x & \mathbf{e}_y & \mathbf{e}_z \\ -\frac{\sqrt{3}}{2} & \frac{1}{2} & 0 \\ -\frac{\sqrt{3}}{2} & -\frac{1}{2} & 0 \end{pmatrix} \cdot \mathbf{e}_z = 1$$

从位置$j(\frac{\sqrt{3}}{2},\frac{3}{2})$跳回位置$i(0,0)$需要的中间点为$(0,1)$，相应的中间矢量分别为：

$$\mathbf{d}_{ij}^{(1)} = (0,-1); \mathbf{d}_{ij}^{(2)} = (\frac{\sqrt{3}}{2}, \frac{1}{2})$$

手性为：

$$\nu_{ij} = \frac{2}{\sqrt{3}} \begin{pmatrix} \mathbf{e}_x & \mathbf{e}_y & \mathbf{e}_z \\ 0 & -1 & 0 \\ \frac{\sqrt{3}}{2} & \frac{1}{2} & 0 \end{pmatrix} \cdot \mathbf{e}_z = 1$$

从位置$j(-\frac{\sqrt{3}}{2},-\frac{3}{2})$跳回位置$i(0,0)$需要的中间点为$(-\frac{\sqrt{3}}{2},-\frac{1}{2})$，相应的中间矢量分别为：

$$\mathbf{d}_{ij}^{(1)}=(\frac{\sqrt{3}}{2},\frac{1}{2});\mathbf{d}_{ij}^{(2)}=(0,1)$$

手性为：

$$\nu_{ij}=\frac{2}{\sqrt{3}}\begin{pmatrix}\mathbf{e}_x & \mathbf{e}_y & \mathbf{e}_z\\ \frac{\sqrt{3}}{2} & \frac{1}{2} & 0\\ 0 & 1 & 0\end{pmatrix}\cdot\mathbf{e}_z=1$$

对于B子格，从位置$j(\sqrt{3},1)$跳回位置$i(0,1)$需要的中间点为$(\frac{\sqrt{3}}{2},\frac{3}{2})$，相应的中间矢量分别为：

$$\mathbf{d}_{ij}^{(1)}=(-\frac{\sqrt{3}}{2},-\frac{1}{2});\mathbf{d}_{ij}^{(2)}=(-\frac{\sqrt{3}}{2},\frac{1}{2})$$

手性为：

$$\nu_{ij}=\frac{2}{\sqrt{3}}\begin{pmatrix}\mathbf{e}_x & \mathbf{e}_y & \mathbf{e}_z\\ -\frac{\sqrt{3}}{2} & -\frac{1}{2} & 0\\ -\frac{\sqrt{3}}{2} & \frac{1}{2} & 0\end{pmatrix}\cdot\mathbf{e}_z=-1$$

从位置$j(-\frac{\sqrt{3}}{2},\frac{5}{2})$跳回位置$i(0,1)$需要的中间点为$(-\frac{\sqrt{3}}{2},\frac{3}{2})$，相应的中间矢量分别为：

$$\mathbf{d}_{ij}^{(1)}=(\frac{\sqrt{3}}{2},-\frac{1}{2});\mathbf{d}_{ij}^{(2)}=(0,-1)$$

手性为：

$$\nu_{ij}=\frac{2}{\sqrt{3}}\begin{pmatrix}\mathbf{e}_x & \mathbf{e}_y & \mathbf{e}_z\\ \frac{\sqrt{3}}{2} & -\frac{1}{2} & 0\\ 0 & -1 & 0\end{pmatrix}\cdot\mathbf{e}_z=-1$$

从位置$j(-\frac{\sqrt{3}}{2},-\frac{1}{2})$跳回位置$i(0,1)$需要的中间点为$(0,0)$，相应的中间矢量分别为：

$$\mathbf{d}_{ij}^{(1)}=(0,1);\mathbf{d}_{ij}^{(2)}=(\frac{\sqrt{3}}{2},\frac{1}{2})$$

手性为：

$$\nu_{ij}=\frac{2}{\sqrt{3}}\begin{pmatrix}\mathbf{e}_x & \mathbf{e}_y & \mathbf{e}_z\\ 0 & 1 & 0\\ \frac{\sqrt{3}}{2} & \frac{1}{2} & 0\end{pmatrix}\cdot\mathbf{e}_z=-1$$

则傅里叶变换之后

$$
\begin{aligned}
H_2 &= t' \sum_{\langle\langle i,j\rangle\rangle} [e^{i\nu_{ij}\phi}(a_i^\dagger a_j + b_i^\dagger b_j) + h.c] \\
&= t' \sum_i [e^{i\phi}(a_{\mathbf{r}_i}^\dagger a_{\mathbf{r}_i+\mathbf{d}_1} + a_{\mathbf{r}_i}^\dagger a_{\mathbf{r}_i+\mathbf{d}_2} + a_{\mathbf{r}_i}^\dagger a_{\mathbf{r}_i+\mathbf{d}_3}) + e^{-i\phi}(b_{\mathbf{r}_i}^\dagger b_{\mathbf{r}_i+\mathbf{d}_1} + b_{\mathbf{r}_i}^\dagger b_{\mathbf{r}_i+\mathbf{d}_2} + b_{\mathbf{r}_i}^\dagger b_{\mathbf{r}_i+\mathbf{d}_3})] + h.c. \\
&= t' \sum_{\mathbf{k}} [a_{\mathbf{k}}^\dagger a_{\mathbf{k}} e^{i\phi}(e^{i\mathbf{k}\cdot\mathbf{d}_1} + e^{i\mathbf{k}\cdot\mathbf{d}_2} + e^{i\mathbf{k}\cdot\mathbf{d}_3}) + b_{\mathbf{k}}^\dagger b_{\mathbf{k}} e^{-i\phi}(e^{i\mathbf{k}\cdot\mathbf{d}_1} + e^{i\mathbf{k}\cdot\mathbf{d}_2} + e^{i\mathbf{k}\cdot\mathbf{d}_3})] + h.c. \\
&= 2t' \sum_{\mathbf{k}} a_{\mathbf{k}}^\dagger a_{\mathbf{k}} [\cos(\mathbf{k}\cdot\mathbf{d}_1 + \phi) + \cos(\mathbf{k}\cdot\mathbf{d}_2 + \phi) + \cos(\mathbf{k}\cdot\mathbf{d}_3 + \phi)] \\
&+ 2t' \sum_{\mathbf{k}} b_{\mathbf{k}}^\dagger b_{\mathbf{k}} [\cos(\mathbf{k}\cdot\mathbf{d}_1 - \phi) + \cos(\mathbf{k}\cdot\mathbf{d}_2 - \phi) + \cos(\mathbf{k}\cdot\mathbf{d}_3 - \phi)] \\
&= \sum_{\mathbf{k}} \begin{pmatrix} a_{\mathbf{k}}^\dagger & b_{\mathbf{k}}^\dagger \end{pmatrix} \begin{pmatrix} f_1(\mathbf{k}) & 0 \\ 0 & f_2(\mathbf{k}) \end{pmatrix} \begin{pmatrix} a_{\mathbf{k}} \\ b_{\mathbf{k}} \end{pmatrix}
\end{aligned}
$$

对于加了磁通之后的次近邻相互作用的哈密顿量的核为

$$\mathbf{H}_2 = \begin{pmatrix} h_1(\mathbf{k}) & 0 \\ 0 & h_2(\mathbf{k}) \end{pmatrix}$$

其中

$$
\begin{aligned}
h_1(\mathbf{k}) &= 2t'[\cos(\sqrt{3}k_x + \phi) + 2\cos(\frac{\sqrt{3}}{2}k_x - \phi)\cos(\frac{3}{2}k_y)] \\
h_2(\mathbf{k}) &= 2t'[\cos(\sqrt{3}k_x - \phi) + 2\cos(\frac{\sqrt{3}}{2}k_x + \phi)\cos(\frac{3}{2}k_y)]
\end{aligned}
$$

因此在k空间中Haldane模型的哈密顿量为：

$$
\begin{aligned}
\mathbf{H} &= \mathbf{H}_0 + \mathbf{H}_1 + \mathbf{H}_2 \\
&= \begin{pmatrix} h_1(\mathbf{k}) + M & f(\mathbf{k}) \\ f^*(\mathbf{k}) & h_2(\mathbf{k}) - M \end{pmatrix}
\end{aligned}
$$

2.1 石墨烯纳米带

最近邻跃迁

首先考虑zigzag情形，如图2所示：其中一个原胞有4个原子，最近邻跃迁构成的哈密顿量为

$$H = t\sum_i a_i^\dagger b_i + b_i^\dagger c_i + c_i^\dagger d_i + b_i^\dagger a_{i+1} + d_i^\dagger c_{i+1} + h.c.$$

每个原子与其最近邻的原子之间相差的矢量分别为：

$$
\begin{aligned}
&\mathbf{e}_0 = (0,0); \mathbf{e}_1 = (\frac{\sqrt{3}}{2}, -\frac{1}{2}); \mathbf{e}_2 = (\frac{\sqrt{3}}{2}, -\frac{3}{2}); \\
&\mathbf{e}_3 = (\sqrt{3}, 0); \mathbf{e}_4 = (\sqrt{3}, -2); \mathbf{e}_5 = (\frac{3\sqrt{3}}{2}, -\frac{3}{2});
\end{aligned}
$$

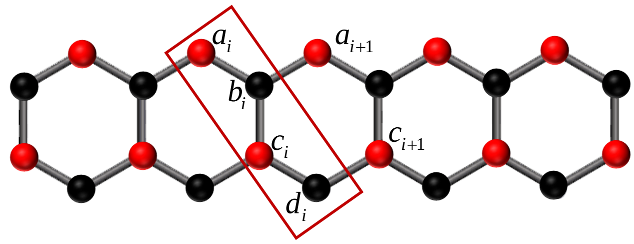

图 2: N=1时石墨烯纳米带示意图.

由于x方向具有周期性，取$k_y=0$。因此利用Fourier变换关系

$$a_i = \frac{1}{\sqrt{N}}\sum_{k_x} a_{k_x} e^{-ik_x r_x}$$

即转换为一维无线长的原子链条，其中每个位置有四个原子轨道：

$$\begin{aligned}
H &= t\sum_i a_i^\dagger b_i + b_i^\dagger c_i + c_i^\dagger d_i + b_i^\dagger a_{i+1} + d_i^\dagger c_{i+1} + h.c. \\
&= t\sum_i a^\dagger_{\mathbf{r}_i+\mathbf{e}_0} b_{\mathbf{r}_i+\mathbf{e}_1} + b^\dagger_{\mathbf{r}_i+\mathbf{e}_1} c_{\mathbf{r}_i+\mathbf{e}_2} + c^\dagger_{\mathbf{r}_i+\mathbf{e}_2} d_{\mathbf{r}_i+\mathbf{e}_4} + b^\dagger_{\mathbf{r}_i+\mathbf{e}_1} a_{\mathbf{r}_i+\mathbf{e}_3} + d^\dagger_{\mathbf{r}_i+\mathbf{e}_4} c_{\mathbf{r}_i+\mathbf{e}_5} + h.c. \\
&= t\sum_{k_x} 2\cos(\frac{\sqrt{3}}{2}k_x)(a^\dagger_{k_x} b_{k_x} + b^\dagger_{k_x} a_{k_x} + d^\dagger_{k_x} c_{k_x} + c^\dagger_{k_x} d_{k_x}) + b^\dagger_{k_x} c_{k_x} + c^\dagger_{k_x} b_{k_x} \\
&= t\begin{pmatrix} a^\dagger_{k_x} & b^\dagger_{k_x} & c^\dagger_{k_x} & d^\dagger_{k_x} \end{pmatrix}
\begin{pmatrix} 0 & 2\cos(\frac{\sqrt{3}}{2}k_x) & 0 & 0 \\ 2\cos(\frac{\sqrt{3}}{2}k_x) & 0 & 1 & 0 \\ 0 & 1 & 0 & 2\cos(\frac{\sqrt{3}}{2}k_x) \\ 0 & 0 & 2\cos(\frac{\sqrt{3}}{2}k_x) & 0 \end{pmatrix}
\begin{matrix} a_{k_x} \\ b_{k_x} \\ c_{k_x} \\ d_{k_x} \end{matrix}
\end{aligned}$$

$$\begin{aligned}
\sum_i a^\dagger_{\mathbf{r}_i+\mathbf{e}_0} b_{\mathbf{r}_i+\mathbf{e}_1} + h.c. &= \sum_{k_x} a^\dagger_{k_x} b_{k_x} e^{-i\frac{\sqrt{3}}{2}k_x} + b^\dagger_{k_x} a_{k_x} e^{i\frac{\sqrt{3}}{2}k_x} \\
\sum_i b^\dagger_{\mathbf{r}_i+\mathbf{e}_1} c_{\mathbf{r}_i+\mathbf{e}_2} + h.c. &= \sum_{k_x} b^\dagger_{k_x} c_{k_x} + c^\dagger_{k_x} b_{k_x} \\
\sum_i c^\dagger_{\mathbf{r}_i+\mathbf{e}_2} d_{\mathbf{r}_i+\mathbf{e}_4} + h.c. &= \sum_{k_x} c^\dagger_{k_x} d_{k_x} e^{-i\frac{\sqrt{3}}{2}k_x} + d^\dagger_{k_x} c_{k_x} e^{i\frac{\sqrt{3}}{2}k_x} \\
\sum_i b^\dagger_{\mathbf{r}_i+\mathbf{e}_1} a_{\mathbf{r}_i+\mathbf{e}_3} + h.c. &= \sum_{k_x} b^\dagger_{k_x} a_{k_x} e^{-i\frac{\sqrt{3}}{2}k_x} + a^\dagger_{k_x} b_{k_x} e^{i\frac{\sqrt{3}}{2}k_x} \\
\sum_i d^\dagger_{\mathbf{r}_i+\mathbf{e}_4} c_{\mathbf{r}_i+\mathbf{e}_5} + h.c. &= \sum_{k_x} d^\dagger_{k_x} c_{k_x} e^{-i\frac{\sqrt{3}}{2}k_x} + c^\dagger_{k_x} d_{k_x} e^{i\frac{\sqrt{3}}{2}k_x}
\end{aligned}$$

于是得到哈密顿量得核为

$$\mathbf{H}(k_x) = \begin{pmatrix} 0 & 2\cos(\frac{\sqrt{3}}{2}k_x) & 0 & 0 \\ 2\cos(\frac{\sqrt{3}}{2}k_x) & 0 & 1 & 0 \\ 0 & 1 & 0 & 2\cos(\frac{\sqrt{3}}{2}k_x) \\ 0 & 0 & 2\cos(\frac{\sqrt{3}}{2}k_x) & 0 \end{pmatrix}$$

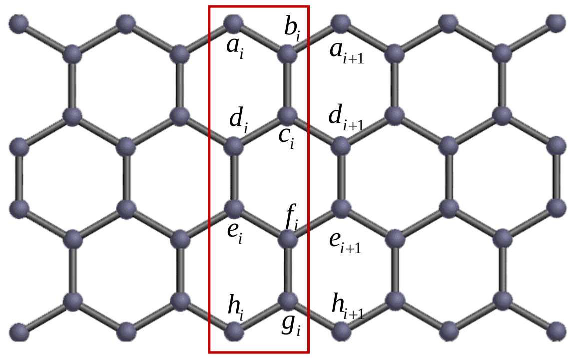

图 3: N=3时石墨烯纳米带示意图.

首先考虑zigzag情形，如图所示：

当$N=3$,

其中一个原胞有8个原子，最近邻跃迁构成的哈密顿量为

$$H_1 = t\sum_i a_i^\dagger b_i + b_i^\dagger c_i + c_i^\dagger d_i + d_i^\dagger e_i + e_i^\dagger f_i + f_i^\dagger g_i + g_i^\dagger h_i$$
$$+ b_i^\dagger a_{i+1} + c_i^\dagger d_{i+1} + f_i^\dagger e_{i+1} + g_i^\dagger h_{i+1} + h.c.$$

每个原子与其最近邻的原子之间相差的矢量分别为：

$$\mathbf{e}_a = (0,0); \mathbf{e}_b = (\frac{\sqrt{3}}{2}, -\frac{1}{2}); \mathbf{e}_c = (\frac{\sqrt{3}}{2}, -\frac{3}{2}); \mathbf{e}_d = (0,-2);$$
$$\mathbf{e}_e = (0,-3); \mathbf{e}_f = (\frac{\sqrt{3}}{2}, -\frac{7}{2}); \mathbf{e}_g = (\frac{\sqrt{3}}{2} - \frac{9}{2}); \mathbf{e}_h = (0,-5);$$
$$\mathbf{e}_{a_{i+1}} = (\sqrt{3},0); \mathbf{e}_{d_{i+1}} = (\sqrt{3},-2); \mathbf{e}_{e_{i+1}} = (\sqrt{3},-3); \mathbf{e}_{h_{i+1}} = (\sqrt{3},-5);$$

由于x方向具有周期性，取$k_y = 0$。因此利用Fourier变换关系

$$a_i = \frac{1}{\sqrt{N}}\sum_{k_x} a_{k_x} e^{-ik_x r_x}$$

即转换为一维无线长的原子链条，其中每个位置有8个原子轨道：

$$
\begin{aligned}
H_1 &= t\sum_i a_i^\dagger b_i + b_i^\dagger c_i + c_i^\dagger d_i + d_i^\dagger e_i + e_i^\dagger f_i + f_i^\dagger g_i + g_i^\dagger h_i \\
&+ b_i^\dagger a_{i+1} + c_i^\dagger d_{i+1} + f_i^\dagger e_{i+1} + g_i^\dagger h_{i+1} + h.c. \\
&= t\sum_{k_x} a_{k_x}^\dagger b_{k_x} e^{-i\frac{\sqrt{3}}{2}k_x} + b_{k_x}^\dagger c_{k_x} + c_{k_x}^\dagger d_{k_x} e^{i\frac{\sqrt{3}}{2}k_x} + d_{k_x}^\dagger e_{k_x} + e_{k_x}^\dagger f_{k_x} e^{-i\frac{\sqrt{3}}{2}k_x} + f_{k_x}^\dagger g_{k_x} + g_{k_x}^\dagger h_{k_x} e^{i\frac{\sqrt{3}}{2}k_x} \\
&+ b_{k_x}^\dagger a_{k_x} e^{-i\frac{\sqrt{3}}{2}k_x} + c_{k_x}^\dagger d_{k_x} e^{-i\frac{\sqrt{3}}{2}k_x} + f_{k_x}^\dagger e_{k_x} e^{-i\frac{\sqrt{3}}{2}k_x} + g_{k_x}^\dagger h_{k_x} e^{-i\frac{\sqrt{3}}{2}k_x} + h.c. \\
&= t\sum_{k_x} a_{k_x}^\dagger b_{k_x} e^{-i\frac{\sqrt{3}}{2}k_x} + c_{k_x}^\dagger d_{k_x} e^{i\frac{\sqrt{3}}{2}k_x} + e_{k_x}^\dagger f_{k_x} e^{-i\frac{\sqrt{3}}{2}k_x} + g_{k_x}^\dagger h_{k_x} e^{i\frac{\sqrt{3}}{2}k_x} + b_{k_x}^\dagger c_{k_x} + d_{k_x}^\dagger e_{k_x} + f_{k_x}^\dagger g_{k_x} \\
&+ b_{k_x}^\dagger a_{k_x} e^{-i\frac{\sqrt{3}}{2}k_x} + c_{k_x}^\dagger d_{k_x} e^{-i\frac{\sqrt{3}}{2}k_x} + f_{k_x}^\dagger e_{k_x} e^{-i\frac{\sqrt{3}}{2}k_x} + g_{k_x}^\dagger h_{k_x} e^{-i\frac{\sqrt{3}}{2}k_x} + h.c. \\
&= t\begin{pmatrix} a_{k_x} \\ b_{k_x} \\ c_{k_x} \\ d_{k_x} \\ e_{k_x} \\ f_{k_x} \\ g_{k_x} \\ h_{k_x} \end{pmatrix}^T
\begin{pmatrix}
0 & 2\cos(\frac{\sqrt{3}}{2}k_x) & 0 & 0 & 0 & 0 \\
2\cos(\frac{\sqrt{3}}{2}k_x) & 0 & 1 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 & 0 & 0 \\
0 & 0 & & \ddots & 0 & 0 \\
0 & 0 & 0 & 0 & 1 & 0 \\
0 & 0 & 0 & 1 & 0 & 2\cos(\frac{\sqrt{3}}{2}k_x) \\
0 & 0 & 0 & 0 & 2\cos(\frac{\sqrt{3}}{2}k_x) & 0
\end{pmatrix}
\begin{pmatrix} a_{k_x} \\ b_{k_x} \\ c_{k_x} \\ d_{k_x} \\ e_{k_x} \\ f_{k_x} \\ g_{k_x} \\ h_{k_x} \end{pmatrix}
\end{aligned}
$$

于是得到哈密顿量得核为

$$
\mathbf{H}_1(k_x) = t\begin{pmatrix}
0 & 2\cos(\frac{\sqrt{3}}{2}k_x) & 0 & 0 & 0 & 0 & 0 & 0 \\
2\cos(\frac{\sqrt{3}}{2}k_x) & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\
0 & 1 & 0 & 2\cos(\frac{\sqrt{3}}{2}k_x) & 0 & 0 & 0 & 0 \\
0 & 0 & 2\cos(\frac{\sqrt{3}}{2}k_x) & 0 & 1 & 0 & 0 & 0 \\
0 & 0 & 0 & 1 & 0 & 2\cos(\frac{\sqrt{3}}{2}k_x) & 0 & 0 \\
0 & 0 & 0 & 0 & 2\cos(\frac{\sqrt{3}}{2}k_x) & 0 & 1 & 0 \\
0 & 0 & 0 & 0 & 0 & 1 & 0 & 2\cos(\frac{\sqrt{3}}{2}k_x) \\
0 & 0 & 0 & 0 & 0 & 0 & 2\cos(\frac{\sqrt{3}}{2}k_x) & 0
\end{pmatrix}
$$

当$N=1$,

$$
\mathbf{H}_1(k_x) = t\begin{pmatrix}
0 & 2\cos(\frac{\sqrt{3}}{2}k_x) & 0 & 0 \\
2\cos(\frac{\sqrt{3}}{2}k_x) & 0 & 1 & 0 \\
0 & 1 & 0 & 2\cos(\frac{\sqrt{3}}{2}k_x) \\
0 & 0 & 2\cos(\frac{\sqrt{3}}{2}k_x) & 0
\end{pmatrix}
$$

当$N=2$,

$$\mathbf{H}_1(k_x)=t\begin{pmatrix} 0 & 2\cos(\frac{\sqrt{3}}{2}k_x) & 0 & 0 & 0 & 0 \\ 2\cos(\frac{\sqrt{3}}{2}k_x) & 0 & 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 2\cos(\frac{\sqrt{3}}{2}k_x) & 0 & 0 \\ 0 & 0 & 2\cos(\frac{\sqrt{3}}{2}k_x) & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 & 0 & 2\cos(\frac{\sqrt{3}}{2}k_x) \\ 0 & 0 & 0 & 0 & 2\cos(\frac{\sqrt{3}}{2}k_x) & 0 \end{pmatrix}$$

规律，临近主对角线附近的对角线上的值不为零。
当六角晶格的环有N层时：矩阵的维度为2N+2维度。

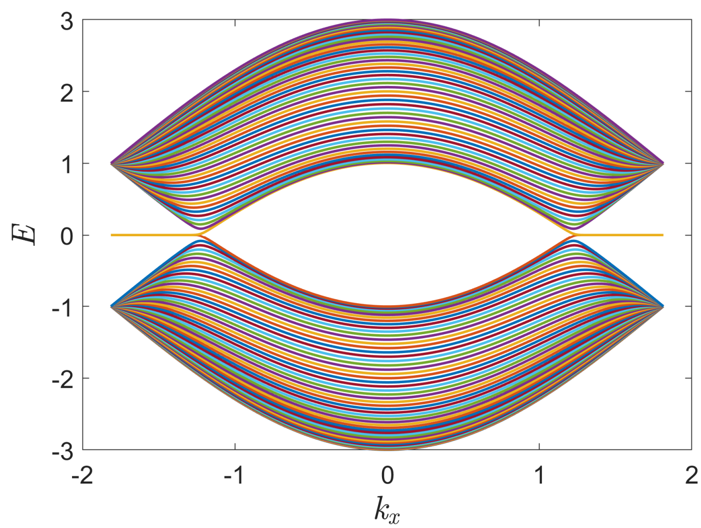

图 4: N=50，时纳米带色散关系.

3 次近邻相互作用

考虑次近邻的纳米带
当$N=1$时，一个原胞有4个原子，次近邻跃迁构成的哈密顿量为

$$\begin{aligned} H_2 = t'\sum_i a_i^\dagger c_i + b_i^\dagger d_i + a_i^\dagger a_{i+1} + b_i^\dagger b_{i+1} + c_i^\dagger c_{i+1} \\ + d_i^\dagger d_{i+1} + c_i^\dagger a_{i+1} + d_i^\dagger b_{i+1} + h.c. \end{aligned}$$

$$\mathbf{a}_i=(0,0);\mathbf{b}_i=(\frac{\sqrt{3}}{2},-\frac{1}{2});\mathbf{c}_i=(\frac{\sqrt{3}}{2},-\frac{3}{2});\mathbf{d}_i=(\sqrt{3},-2)$$

$$\mathbf{a}_{i+1}=(\sqrt{3},0);\mathbf{b}_{i+1}=(\frac{3\sqrt{3}}{2},-\frac{1}{2});\mathbf{c}_{i+1}=(\frac{3\sqrt{3}}{2},-\frac{3}{2});\mathbf{d}_{i+1}=(2\sqrt{3},-2)$$

$$\begin{aligned}
H_2 &= t'\sum_i a_i^\dagger c_i + b_i^\dagger d_i + a_i^\dagger a_{i+1} + b_i^\dagger b_{i+1} + c_i^\dagger c_{i+1} \\
&+ d_i^\dagger d_{i+1} + c_i^\dagger a_{i+1} + d_i^\dagger b_{i+1} + h.c. \\
&= t'\sum_{k_x} a_{k_x}^\dagger c_{k_x} e^{-i\frac{\sqrt{3}}{2}} + b_{k_x}^\dagger d_{k_x} e^{-i\frac{\sqrt{3}}{2}} + a_{k_x}^\dagger a_{k_x} e^{-i\sqrt{3}} + b_{k_x}^\dagger b_{k_x} e^{-i\sqrt{3}} + c_{k_x}^\dagger c_{k_x} e^{-i\sqrt{3}} \\
&+ d_{k_x}^\dagger d_{k_x} e^{-i\sqrt{3}} + c_{k_x}^\dagger a_{k_x} e^{-i\frac{\sqrt{3}}{2}} + d_{k_x}^\dagger b_{k_x} e^{-i\frac{\sqrt{3}}{2}} + h.c. \\
&= \\
&= \begin{pmatrix} a_{k_x}^\dagger & b_{k_x}^\dagger & c_{k_x}^\dagger & d_{k_x}^\dagger \end{pmatrix} \begin{pmatrix} 2t'\cos(\sqrt{3}k_x) & 0 & 2t'\cos(\frac{\sqrt{3}}{2}k_x) & 0 \\ 0 & 2t'\cos(\sqrt{3}k_x) & 0 & 2t'\cos(\frac{\sqrt{3}}{2}k_x) \\ 2t'\cos(\frac{\sqrt{3}}{2}k_x) & 0 & 2t'\cos(\sqrt{3}k_x) & 0 \\ 0 & 2t'\cos(\frac{\sqrt{3}}{2}k_x) & 0 & 2t'\cos(\sqrt{3}k_x) \end{pmatrix} \begin{matrix} a_{k_x} \\ b_{k_x} \\ c_{k_x} \\ d_{k_x} \end{matrix}
\end{aligned}$$

$$\mathbf{H}_2(k_x) = t' \begin{pmatrix} 2\cos(\sqrt{3}k_x) & 0 & 2\cos(\frac{\sqrt{3}}{2}k_x) & 0 \\ 0 & 2\cos(\sqrt{3}k_x) & 0 & 2\cos(\frac{\sqrt{3}}{2}k_x) \\ 2\cos(\frac{\sqrt{3}}{2}k_x) & 0 & 2\cos(\sqrt{3}k_x) & 0 \\ 0 & 2\cos(\frac{\sqrt{3}}{2}k_x) & 0 & 2\cos(\sqrt{3}k_x) \end{pmatrix}$$

总的哈密顿量为：

$$\mathbf{H} = \mathbf{H_1} + \mathbf{H}_2 = \begin{pmatrix} 2t'\cos(\sqrt{3}k_x) & 2t\cos(\frac{\sqrt{3}}{2}k_x) & 2t'\cos(\frac{\sqrt{3}}{2}k_x) & 0 \\ 2t\cos(\frac{\sqrt{3}}{2}k_x) & 2t'\cos(\sqrt{3}k_x) & t & 2t'\cos(\frac{\sqrt{3}}{2}k_x) \\ 2t'\cos(\frac{\sqrt{3}}{2}k_x) & t & 2t'\cos(\sqrt{3}k_x) & 2t\cos(\frac{\sqrt{3}}{2}k_x) \\ 0 & 2t'\cos(\frac{\sqrt{3}}{2}k_x) & 2t\cos(\frac{\sqrt{3}}{2}k_x) & 2t'\cos(\sqrt{3}k_x) \end{pmatrix}$$

与石墨烯不一致的是，Haldane模型引入了带磁通的次近邻跃迁项

$$\sum_{\langle\langle i,j\rangle\rangle} [t' e^{i\nu_{ij}\phi}(a_i^\dagger a_j + b_i^\dagger b_j) + h.c].$$

对于Haldane模型的纳米带，由于次近邻项的哈密顿加了磁通，因此哈密顿量为：

$$\begin{aligned}
H_2 = t'\sum_i & e^{-i\phi} a_i^\dagger c_i + e^{i\phi} b_i^\dagger d_i + e^{i\phi} a_i^\dagger a_{i+1} + e^{-i\phi} b_i^\dagger b_{i+1} + e^{i\phi} c_i^\dagger c_{i+1} \\
& + e^{-i\phi} d_i^\dagger d_{i+1} + e^{-i\phi} c_i^\dagger a_{i+1} + e^{i\phi} d_i^\dagger b_{i+1} + h.c.
\end{aligned}$$

需要判断手性，这里，如图2所示，顺时针跳动的手性$\nu_{ij} = 1$，逆时针跳动的手性为$\nu_{ij} = -1$，

举例：跳动为顺时针时，当从位置$j(\sqrt{3}, 0)$跳回位置$i(0, 0)$需要的中间格点为$(\frac{\sqrt{3}}{2}, -\frac{1}{2})$，相应的中间矢量分别为：

$$\mathbf{d}_{ij}^{(1)} = (-\frac{\sqrt{3}}{2}, \frac{1}{2}); \mathbf{d}_{ij}^{(2)} = (-\frac{\sqrt{3}}{2}, -\frac{1}{2})$$

此时的手性为：

$$\nu_{ij} = \frac{2}{\sqrt{3}} \begin{pmatrix} \mathbf{e}_x & \mathbf{e}_y & \mathbf{e}_z \\ -\frac{\sqrt{3}}{2} & \frac{1}{2} & 0 \\ -\frac{\sqrt{3}}{2} & -\frac{1}{2} & 0 \end{pmatrix} \cdot \mathbf{e}_z = 1$$

跳动为逆时针时，当从位置$j(\frac{\sqrt{3}}{2},-\frac{3}{2})$跳回位置$i(0,0)$需要的中间格点为$(\frac{\sqrt{3}}{2},-\frac{1}{2})$，相应的中间矢量分别为：

$$\mathbf{d}_{ij}^{(1)}=(-\frac{\sqrt{3}}{2},\frac{1}{2});\mathbf{d}_{ij}^{(2)}=(0,1)$$

此时的手性为：

$$\nu_{ij}=\frac{2}{\sqrt{3}}\begin{pmatrix}\mathbf{e}_x & \mathbf{e}_y & \mathbf{e}_z\\ -\frac{\sqrt{3}}{2} & \frac{1}{2} & 0\\ 0 & 1 & 0\end{pmatrix}\cdot\mathbf{e}_z=-1$$

因此只需要知道hopping的转动方向，即可知道手性。

$$\begin{aligned}H_2&=t'\sum_i e^{-i\phi}a_i^\dagger c_i+e^{i\phi}b_i^\dagger d_i+e^{i\phi}a_i^\dagger a_{i+1}+e^{-i\phi}b_i^\dagger b_{i+1}+e^{i\phi}c_i^\dagger c_{i+1}\\
&+e^{-i\phi}d_i^\dagger d_{i+1}+e^{-i\phi}c_i^\dagger a_{i+1}+e^{i\phi}d_i^\dagger b_{i+1}+h.c.\\
&=t'\sum_{k_x} a_{k_x}^\dagger c_{k_x}e^{-i\phi}e^{-i\frac{\sqrt{3}}{2}}+b_{k_x}^\dagger d_{k_x}e^{i\phi}e^{-i\frac{\sqrt{3}}{2}}+a_{k_x}^\dagger a_{k_x}e^{i\phi}e^{-i\sqrt{3}}+b_{k_x}^\dagger b_{k_x}e^{-i\phi}e^{-i\sqrt{3}}+c_{k_x}^\dagger c_{k_x}e^{i\phi}e^{-i\sqrt{3}}\\
&+d_{k_x}^\dagger d_{k_x}e^{-i\phi}e^{-i\sqrt{3}}+c_{k_x}^\dagger a_{k_x}e^{-i\phi}e^{-i\frac{\sqrt{3}}{2}}+d_{k_x}^\dagger b_{k_x}e^{i\phi}e^{-i\frac{\sqrt{3}}{2}}+h.c.\\
&=\begin{pmatrix}a_{k_x}\\ b_{k_x}\\ c_{k_x}\\ d_{k_x}\end{pmatrix}^T\begin{pmatrix}2t'\cos(\sqrt{3}k_x-\phi) & 0 & 2t'\cos(\frac{\sqrt{3}}{2}k_x+\phi) & 0\\ 0 & 2t'\cos(\sqrt{3}k_x+\phi) & 0 & 2t'\cos(\frac{\sqrt{3}}{2}k_x-\phi)\\ 2t'\cos(\frac{\sqrt{3}}{2}k_x+\phi) & 0 & 2t'\cos(\sqrt{3}k_x-\phi) & 0\\ 0 & 2t'\cos(\frac{\sqrt{3}}{2}k_x-\phi) & 0 & 2t'\cos(\sqrt{3}k_x+\phi)\end{pmatrix}\begin{pmatrix}a_{k_x}\\ b_{k_x}\\ c_{k_x}\\ d_{k_x}\end{pmatrix}\end{aligned}$$

于是得到Haldane模型中的次近邻得相互作用Hamiltonian为：

$$\mathbf{H}_2=\begin{pmatrix}2t'\cos(\sqrt{3}k_x-\phi) & 0 & 2t'\cos(\frac{\sqrt{3}}{2}k_x+\phi) & 0\\ 0 & 2t'\cos(\sqrt{3}k_x+\phi) & 0 & 2t'\cos(\frac{\sqrt{3}}{2}k_x-\phi)\\ 2t'\cos(\frac{\sqrt{3}}{2}k_x+\phi) & 0 & 2t'\cos(\sqrt{3}k_x-\phi) & 0\\ 0 & 2t'\cos(\frac{\sqrt{3}}{2}k_x-\phi) & 0 & 2t'\cos(\sqrt{3}k_x+\phi)\end{pmatrix}$$

以上讨论是对$N=1$进行的。

当$N=2$

$$\mathbf{H}_2=\begin{pmatrix}2t'\cos(\sqrt{3}k_x-\phi) & 0 & 2t'\cos(\frac{\sqrt{3}}{2}k_x+\phi) & 0 & & \\ 0 & 2t'\cos(\sqrt{3}k_x+\phi) & 0 & 2t'\cos(\frac{\sqrt{3}}{2}k_x-\phi) & & \\ 2t'\cos(\frac{\sqrt{3}}{2}k_x+\phi) & 0 & 2t'\cos(\sqrt{3}k_x-\phi) & 0 & 2t'\cos(\frac{\sqrt{3}}{2}k_x+\phi) & \\ 0 & 2t'\cos(\frac{\sqrt{3}}{2}k_x-\phi) & 0 & 2t'\cos(\sqrt{3}k_x+\phi) & & 2t'\cos(\frac{\sqrt{3}}{2}k_x-\phi)\\ & & 2t'\cos(\frac{\sqrt{3}}{2}k_x+\phi) & & 2t'\cos(\sqrt{3}k_x-\phi) & \\ & & & 2t'\cos(\frac{\sqrt{3}}{2}k_x-\phi) & & 2t'\cos(\sqrt{3}k_x+\phi)\end{pmatrix}$$

主对角线中$2t'\cos(\sqrt{3}k_x-\phi)$与$2t'\cos(\sqrt{3}k_x+\phi)$交替出现，
上第二条对角线$2t'\cos(\frac{\sqrt{3}}{2}k_x+\phi)$和$2t'\cos(\sqrt{3}k_x+\phi)$交替出现
下第二条对角线同上。

当$N=2$时总的哈密顿量

$$
\mathbf{H}_2 = \begin{pmatrix}
2t'\cos(\sqrt{3}k_x-\phi) & 2t\cos(\frac{\sqrt{3}}{2}k_x) & 2t'\cos(\frac{\sqrt{3}}{2}k_x+\phi) & 0 & 0 & 0 \\
2t\cos(\frac{\sqrt{3}}{2}k_x) & 2t'\cos(\sqrt{3}k_x+\phi) & t & 2t'\cos(\frac{\sqrt{3}}{2}k_x-\phi) & 0 & 0 \\
2t'\cos(\frac{\sqrt{3}}{2}k_x+\phi) & t & 2t'\cos(\sqrt{3}k_x-\phi) & 2t\cos(\frac{\sqrt{3}}{2}k_x) & 2t'\cos(\frac{\sqrt{3}}{2}k_x+\phi) & 0 \\
0 & 2t'\cos(\frac{\sqrt{3}}{2}k_x-\phi) & 2t\cos(\frac{\sqrt{3}}{2}k_x) & 2t'\cos(\sqrt{3}k_x+\phi) & t & 2t'\cos(\frac{\sqrt{3}}{2}k_x-\phi) \\
0 & 0 & 2t'\cos(\frac{\sqrt{3}}{2}k_x+\phi) & t & 2t'\cos(\sqrt{3}k_x-\phi) & 2t\cos(\frac{\sqrt{3}}{2}k_x) \\
0 & 0 & 0 & 2t'\cos(\frac{\sqrt{3}}{2}k_x-\phi) & 2t\cos(\frac{\sqrt{3}}{2}k_x) & 2t'\cos(\sqrt{3}k_x+\phi)
\end{pmatrix}
$$