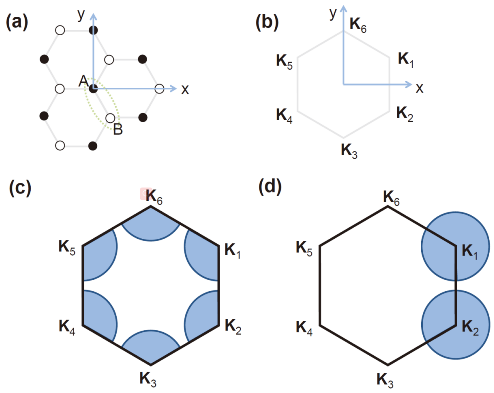
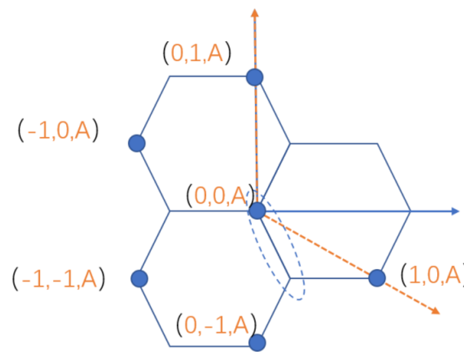
石墨烯哈密顿量的时间反演

如图所示，石墨烯的六角晶格由两种子格构成，分别用A，B来表示，且每一个单胞包含两个碳原子（每一个子格–原子–有一个p_z轨道） 石墨烯紧束缚模型的哈密顿量为：





$$H=-t\sum_i\left[|i_x,i_y,A\rangle\langle i_x,i_y,B|+|i_x,i_y,A\rangle\langle i_x,i_y+1,B|+|i_x,i_y,A\rangle\langle i_x-1,i_y,B|\right]$$

$$+|i_x,i_y,B\rangle\langle i_x,i_y,A|+|i_x,i_y+1,B\rangle\langle i_x,i_y,A|+|i_x-1,i_y,B\rangle\langle i_x,i_y,B|$$

$$H=-t\sum_{<\mathbf{i},\mathbf{j}>}|i_x,i_y,A\rangle\langle j_x,j_y,B|-t\sum_{<\mathbf{i},\mathbf{j}>}|j_x,j_y,B\rangle\langle i_x,i_y,A|$$

$|i_x,i_y,\lambda\rangle(\lambda=A,B)$表示单胞为$i$的$\lambda$子格的$p_z$轨道，如图所示的为坐标原点，在原点的单胞，AB两个子格坐标相对原点的位移分别为$\tau_A=0$，$\tau_B=\left(a/2,\frac{-\sqrt{3}a}{2}\right)$.$a$是碳碳键长。按照单胞的位置$R_i$来表示每个子格的位置为：$R_{i,\lambda}=R_i+\tau_\lambda$.

通过傅里叶变换，将实空间的基矢$|i_x,i_y,\lambda\rangle$变换到动量空间的基矢$|\mathbf{k},\lambda\rangle$

$$|\mathbf{k},\lambda\rangle\equiv\frac{1}{\sqrt{N}}\sum_i e^{i\mathbf{k}\cdot\mathbf{R}_i}|i_x,i_y,\lambda\rangle$$

$$|i_x,i_y,\lambda\rangle=\frac{1}{\sqrt{N}}\sum_k e^{-i\mathbf{k}\cdot\mathbf{R}_i}|\mathbf{k},\lambda\rangle$$

$$\begin{aligned}
H=&-t\textstyle\sum_i\left[|i_x,i_y,A\rangle\langle i_x,i_y,B|+|i_x,i_y,A\rangle\langle i_x,i_y+1,B|+|i_x,i_y,A\rangle\langle i_x-1,i_y,B|\right.\\
&\left.+|i_x,i_y,B\rangle\langle i_x,i_y,A|+|i_x,i_y+1,B\rangle\langle i_x,i_y,A|+|i_x-1,i_y,B\rangle\langle i_x,i_y,B|\right]\\
&=-t\tfrac{1}{N}\textstyle\sum_i\sum_{k'}\sum_k\Big[e^{i\mathbf{k}'\cdot\mathbf{R}_{i_x,i_y}}e^{-i\mathbf{k}\cdot\mathbf{R}_{i_x,i_y}}|\mathbf{k},A\rangle\langle\mathbf{k}',B|+e^{i\mathbf{k}'\cdot\mathbf{R}_{i_x,i_y+1}}e^{-i\mathbf{k}\cdot\mathbf{R}_{i_x,i_y}}|\mathbf{k},A\rangle\langle\mathbf{k}',B|+e^{i\mathbf{k}'\cdot\mathbf{R}_{i_x-1,i_y}}e^{-i\mathbf{k}\cdot\mathbf{R}_{i_x,i_y}}|\mathbf{k},A\rangle\langle\mathbf{k}',B|\\
&+e^{i\mathbf{k}'\cdot\mathbf{R}_{i_x,i_y}}e^{-i\mathbf{k}\cdot\mathbf{R}_{i_x,i_y}}|\mathbf{k},B\rangle\langle\mathbf{k}',A|+e^{i\mathbf{k}'\cdot\mathbf{R}_{i_x,i_y}}e^{-i\mathbf{k}\cdot\mathbf{R}_{i_x,i_y+1}}|\mathbf{k},B\rangle\langle\mathbf{k}',A|+e^{i\mathbf{k}'\cdot\mathbf{R}_{i_x,i_y}}e^{-i\mathbf{k}\cdot\mathbf{R}_{i_x-1,i_y}}|\mathbf{k},B\rangle\langle\mathbf{k}',A|\Big]\\
&=-t\textstyle\sum_k\frac{1}{N}\sum_i\sum_{k'}\Big[e^{-i\left(\mathbf{k}-\mathbf{k}'\right)\cdot\mathbf{R}_{i_x,i_y}}|\mathbf{k},A\rangle\langle\mathbf{k}',B|+e^{-i\left(\mathbf{k}-\mathbf{k}'\right)\cdot\mathbf{R}_{i_x,i_y}}e^{i\mathbf{k}\cdot\mathbf{d}_1}|\mathbf{k},A\rangle\langle\mathbf{k}',B|+e^{-i\left(\mathbf{k}-\mathbf{k}'\right)\cdot\mathbf{R}_{i_x,i_y}}e^{i\mathbf{k}\cdot\mathbf{d}_{-1}}|\mathbf{k},A\rangle\langle\mathbf{k}',B|\\
&-t\textstyle\sum_k\frac{1}{N}\sum_i\sum_{k'}\Big[e^{-i\left(\mathbf{k}-\mathbf{k}'\right)\cdot\mathbf{R}_{i_x,i_y}}|\mathbf{k},B\rangle\langle\mathbf{k}',A|+e^{-i\left(\mathbf{k}-\mathbf{k}'\right)\cdot\mathbf{R}_{i_x,i_y}}e^{-i\mathbf{k}\cdot\mathbf{d}_1}|\mathbf{k},B\rangle\langle\mathbf{k}',A|+e^{-i\left(\mathbf{k}-\mathbf{k}'\right)\cdot\mathbf{R}_{i_x,i_y}}e^{-i\mathbf{k}\cdot\mathbf{d}_{-1}}|\mathbf{k},B\rangle\langle\mathbf{k}',A|\\
&=-t\sum_{k\in FBZ}\left(1+e^{-i\mathbf{k}\cdot\mathbf{d}_1}+e^{-i\mathbf{k}\cdot\mathbf{d}_{-1}}\right)|\mathbf{k},A\rangle\langle\mathbf{k},B|-t\sum_{k\in FBZ}\left(1+e^{-i\mathbf{k}\cdot\mathbf{d}_1}+e^{-i\mathbf{k}\cdot\mathbf{d}_{-1}}\right)|\mathbf{k},B\rangle\langle\mathbf{k},A|\\
&=\sum_{k\in FBZ}f\left(\mathbf{k}\right)|\mathbf{k},A\rangle\langle\mathbf{k},B|+h.c.
\end{aligned}$$

这里$\mathbf{d}_1$,的定义为(0,1,A)到(0,0,A)的位移$\left(0,\sqrt{3}\right)$，$\mathbf{d}_{-1}$的定义为(-1,0,A)到(0,0,A)的位移$\left(-\frac{3}{2},\frac{\sqrt{3}}{2}\right)$.
此外，由δ函数的定义：

$$\frac{1}{N}\sum_i e^{-i\left(\mathbf{k}-\mathbf{k}'\right)\cdot\mathbf{R}_{i_x,i_y}}=\delta_{k,k'}$$

定义函数$f\left(\mathbf{k}\right)=-t\left(1+e^{-i\mathbf{k}\cdot\mathbf{d}_1}+e^{-i\mathbf{k}\cdot\mathbf{d}_{-1}}\right)$
该函数满足$f^*\left(\mathbf{k}\right)=f\left(-\mathbf{k}\right)=-t\left(1+e^{i\mathbf{k}\cdot\mathbf{d}_1}+e^{i\mathbf{k}\cdot\mathbf{d}_{-1}}\right)$

定义一个时间反演算符θ,我们有

$$\begin{aligned}\theta|i,\lambda\rangle&=|i,\lambda\rangle\Rightarrow\\\theta|\mathbf{k},\lambda\rangle&=|-\mathbf{k},\lambda\rangle\end{aligned}$$

使用$\theta|a\rangle\langle b|\theta^{-1}=|\theta a\rangle\langle\theta b|$

$$\begin{aligned}\theta H\theta^{-1}&=\theta\left(\sum_{k\in FBZ}f\left(\mathbf{k}\right)|\mathbf{k},A\rangle\langle\mathbf{k},B|+h.c.\right)\theta^{-1}\\&=\sum_{k\in FBZ}\left(\theta f\left(\mathbf{k}\right)\theta^{-1}\theta|\mathbf{k},A\rangle\langle\mathbf{k},B|\theta^{-1}\right)+h.c.\\&=\sum_{k\in FBZ}\left(f^*\left(\mathbf{k}\right)|\theta\mathbf{k},A\rangle\langle\theta\mathbf{k},B|\right)+h.c.\\&=\sum_{k\in FBZ}f^*\left(\mathbf{k}\right)|-\mathbf{k},A\rangle\langle-\mathbf{k},B|+h.c.\\&=\sum_{k\in FBZ}f^*\left(-\mathbf{k}\right)|\mathbf{k},A\rangle\langle\mathbf{k},B|+h.c.\\&=\sum_{k\in FBZ}f\left(\mathbf{k}\right)|\mathbf{k},A\rangle\langle\mathbf{k},B|+h.c.\end{aligned}$$

其中$\theta f\left(\mathbf{k}\right)\theta^{-1}=f^*\left(\mathbf{k}\right)$.
最后一步做了变量替换。
因此，$f^*\left(\mathbf{k}\right)=f\left(-\mathbf{k}\right)$的性质确保了石墨烯哈密顿量的时间反演不变性。
将哈密顿量对角化得到其导带和价带。

$$\begin{aligned}E_\pm&=\pm|f\left(\mathbf{k}\right)|\\&=\pm t\sqrt{3+2\cos\left(\sqrt{3}k_ya\right)+4\cos\frac{3k_xa}{2}\cos\frac{\sqrt{3k_y a}}{2}}\end{aligned}$$

导带和价带在六个狄拉克点处相交。并且$\mathbf{K}_4\equiv-\mathbf{K}_1,\mathbf{K}_5\equiv-\mathbf{K}_2,\mathbf{K}_6=-\mathbf{K}_3$.
此外$\mathbf{K}_1,\mathbf{K}_3,\mathbf{K}_5$相差一个倒格矢，所以他们是等价的。
即

$$|\mathbf{K}_1,\lambda\rangle=|\mathbf{K}_3,\lambda\rangle=|\mathbf{K}_5,\lambda\rangle$$

同理可得

$$|\mathbf{K}_2,\lambda\rangle=|\mathbf{K}_4,\lambda\rangle=|\mathbf{K}_6,\lambda\rangle$$

在连续模型下，将对第一布里渊区的求和限制在了狄拉克点附近。（图1c的阴影部分）

$$|\mathbf{k},\lambda\rangle = |\mathbf{k}+\mathbf{G},\lambda\rangle$$

其中$\mathbf{G}$是倒格矢，因此，对于在图1c的求和等价于图1d中阴影部分的求和

$$H = H_1 + H_2$$

$$\begin{aligned} H_m &= \sum_{\mathbf{k}\approx\mathbf{K}_m} f\left(\mathbf{k}\right)|\mathbf{k},A\rangle\langle\mathbf{k},B| + h.c. \\ &= \sum_{\mathbf{q}\approx\mathbf{0}} f_m\left(\mathbf{q}\right)|\mathbf{K}_m+\mathbf{q},A\rangle\langle\mathbf{K}_m+\mathbf{q},B| + h.c. \end{aligned}$$

是第m个谷的哈密顿量，且$\mathbf{q}=\mathbf{k}-\mathbf{K}_m$，此外$f_m\left(\mathbf{q}\right) = f\left(\mathbf{K}_m+\mathbf{q}\right)$.有性质$f^*\left(-\mathbf{k}\right) = f\left(\mathbf{k}\right)$,导致了$f_1^*\left(-\mathbf{q}\right) = f_2\left(\mathbf{q}\right)$.因为$-\mathbf{K}_1\left(\mathbf{K}_4\right)$与$\mathbf{K}_2$相差一个倒格矢。所以时间反演操作，将$\mathbf{K}_1$谷的$\mathbf{q}$态转变为了$\mathbf{K}_2$谷的$-\mathbf{q}$态

$$\begin{aligned} f_1^*\left(-\mathbf{q}\right) &= \theta f_1\left(-\mathbf{q}\right)\theta^{-1} = \theta f\left(\mathbf{K}_1-\mathbf{q}\right)\theta^{-1} = f\left(-\mathbf{K}_1+\mathbf{q}\right) \\ &= f\left(\mathbf{K}_2+\mathbf{G}+\mathbf{q}\right) = f\left(\mathbf{K}_2+\mathbf{q}\right) = f_2\left(\mathbf{q}\right) \end{aligned}$$

$$\theta|\mathbf{K}_1+\mathbf{q},\lambda\rangle = |-\mathbf{K}_1-\mathbf{q},\lambda\rangle = |\mathbf{K}_2-\mathbf{q},\lambda\rangle$$

所以时间反演将H_1变为了H_2，反之亦然。

$$\begin{aligned} \theta H_1\theta^{-1} &= \theta\left[\sum_{\mathbf{q}\approx\mathbf{0}} f_1\left(\mathbf{q}\right)|\mathbf{K}_1+\mathbf{q},A\rangle\langle\mathbf{K}_1+\mathbf{q},B| + h.c.\right]\theta^{-1} \\ &= \sum_{\mathbf{q}\approx\mathbf{0}} \theta f_1\left(\mathbf{q}\right)\theta^{-1}\theta|\mathbf{K}_1+\mathbf{q},A\rangle\langle\mathbf{K}_1+\mathbf{q},B|\theta^{-1} + h.c. \\ &= \sum_{\mathbf{q}\approx\mathbf{0}} f_1^*\left(\mathbf{q}\right)|-\mathbf{K}_1-\mathbf{q},A\rangle\langle-\mathbf{K}_1-\mathbf{q},B| + h.c. \\ &= \sum_{\mathbf{q}\approx\mathbf{0}} f_1^*\left(\mathbf{q}\right)|\mathbf{K}_2-\mathbf{q},A\rangle\langle\mathbf{K}_2-\mathbf{q},B| + h.c. \\ &= \sum_{\mathbf{q}\approx\mathbf{0}} f_1^*\left(-\mathbf{q}\right)|\mathbf{K}_2+\mathbf{q},A\rangle\langle\mathbf{K}_2+\mathbf{q},B| + h.c. \\ &= \sum_{\mathbf{q}\approx\mathbf{0}} f_2\left(\mathbf{q}\right)|\mathbf{K}_2+\mathbf{q},A\rangle\langle\mathbf{K}_2+\mathbf{q},B| + h.c. \end{aligned}$$

最后也做了符号变换$\mathbf{q}\to-\mathbf{q}$。

$$H_2 = \sum_{\mathbf{q}\approx\mathbf{0}} f_2\left(\mathbf{q}\right)|\mathbf{K}_2+\mathbf{q},A\rangle\langle\mathbf{K}_2+\mathbf{q},B| + h.c.$$

所以总的哈密顿量$H = H_1 + H_2$也是时间反演下不变的。即$\theta H\theta^{-1} = H$.

在有效质量近似下，把$|\mathbf{K}_m+\mathbf{q},A\rangle$分解为$|\mathbf{q}\rangle|\mathbf{K}_m,A\rangle$作为慢变平面波$|\mathbf{q}\rangle$和快速振荡带边Bloch态$|\mathbf{K}_m,A\rangle$的乘积，于是哈密顿量

$$\begin{aligned} \langle\mathbf{r}|\mathbf{K}_m+\mathbf{q},A\rangle &= \psi_{A,\mathbf{K}_m+\mathbf{q}}\left(\mathbf{r}\right) = e^{i(\mathbf{K}_m+\mathbf{q})\cdot\mathbf{r}}u_{A,\mathbf{K}_m+\mathbf{q}}\left(\mathbf{r}\right) \\ \langle\mathbf{r}|\mathbf{q}\rangle\langle\mathbf{r}|\mathbf{K}_m,A\rangle &= \psi_{A,\mathbf{K}_m}\left(\mathbf{r}\right)e^{i\mathbf{q}\mathbf{r}} = e^{i\mathbf{K}_m\cdot\mathbf{r}}e^{i\mathbf{q}\mathbf{r}}u_{A,\mathbf{K}_m}\left(\mathbf{r}\right) \end{aligned}$$

对比观察发现$\psi_{A,\mathbf{K}_m+\mathbf{q}}(\mathbf{r}) \approx \psi_{A,\mathbf{K}_m}(\mathbf{r})\, e^{i\mathbf{q}\mathbf{r}}$

两个函数仅仅在周期函数$u_{A,\mathbf{K}_m+\mathbf{q}}(\mathbf{r})$晶格动量相差一个非常小的$\mathbf{q}$。

$$\begin{aligned} H_m &= \sum_{\mathbf{q}\approx\mathbf{0}} f_m(\mathbf{q})\, |\mathbf{K}_m+\mathbf{q}, A\rangle\langle \mathbf{K}_m+\mathbf{q}, B| + h.c. \\ &= |\mathbf{K}_m, A\rangle \left(\sum_{\mathbf{q}\approx\mathbf{0}} f_m(\mathbf{q})\, |\mathbf{q}\rangle\langle\mathbf{q}|\right) \langle \mathbf{K}_m, B| + h.c. \\ &= |\mathbf{K}_m, A\rangle f_m(\hat{\mathbf{p}})\, \langle \mathbf{K}_m, B| + h.c. \end{aligned}$$

这里$\hat{\mathbf{p}} \equiv \sum_{\mathbf{q}\approx 0} \mathbf{q}|\mathbf{q}\rangle\langle\mathbf{q}|$是动量算符，但是被限制在了很小的动量中，因为有$\theta|\mathbf{K}_m+\mathbf{q},\lambda\rangle = |-\mathbf{K}_m-\mathbf{q},\lambda\rangle$

$$\theta|\mathbf{K}_1+\mathbf{q},\lambda\rangle = |-\mathbf{K}_1-\mathbf{q},\lambda\rangle$$
$$\theta\left(|\mathbf{q}\rangle|\mathbf{K}_m, A\rangle\right) = |-\mathbf{q}\rangle|-\mathbf{K}_m, A\rangle$$

$$\theta|\mathbf{q}\rangle = |-\mathbf{q}\rangle$$
$$\theta|\mathbf{K}_1, A\rangle = |-\mathbf{K}_1, A\rangle = |-\mathbf{K}_2, A\rangle$$

因此

$$\begin{aligned} \theta\hat{\mathbf{p}}\theta^{-1} &= \sum_{\mathbf{q}} \mathbf{q}|-\mathbf{q}\rangle\langle-\mathbf{q}| \\ &= -\sum_{\mathbf{q}} \mathbf{q}|\mathbf{q}\rangle\langle\mathbf{q}| \\ &= -\hat{\mathbf{p}} \end{aligned}$$

$$\theta f_1(\hat{\mathbf{p}})\,\theta^{-1} = f_1^*(-\hat{\mathbf{p}})$$

$$\begin{aligned} f_1^*(-\hat{\mathbf{p}}) &= f^*(\mathbf{K}_1-\hat{\mathbf{p}}) = f(-\mathbf{K}_1+\hat{\mathbf{p}}) \\ &= f(\mathbf{K}_2+\mathbf{G}+\hat{\mathbf{p}}) \\ &= f(\mathbf{K}_2+\hat{\mathbf{p}}) \\ &= f_2(\hat{\mathbf{p}}) \end{aligned}$$

利用$\theta f_1(\hat{\mathbf{p}})\,\theta^{-1} = f_1^*(-\hat{\mathbf{p}}) = f_2(\hat{\mathbf{p}})$,检验$\theta H_1\theta^{-1} = H_2$

$$\begin{aligned} H_1 &= |\mathbf{K}_1, A\rangle f_1(\hat{\mathbf{p}})\, \langle\mathbf{K}_1, B| + h.c \\ \theta H_1\theta^{-1} &= \theta\left(|\mathbf{K}_1, A\rangle f_1(\hat{\mathbf{p}})\, \langle\mathbf{K}_1, B| + h.c\right)\theta^{-1} \\ &= \left(|-\mathbf{K}_1, A\rangle\theta f_1(\hat{\mathbf{p}})\,\theta^{-1}\langle-\mathbf{K}_1, B| + h.c\right) \\ &= \left(|\mathbf{K}_2, A\rangle f_2(\hat{\mathbf{p}})\, \langle\mathbf{K}_2, B| + h.c\right) \\ &= H_2 \end{aligned}$$

明确写出$f_1(\mathbf{k})$

$$\begin{aligned}
f_1(\mathbf{k}) &= -t\left(e^{i\mathbf{k}\cdot\mathbf{d}_1} + e^{i\mathbf{k}\cdot\mathbf{d}_2} + e^{i\mathbf{k}\cdot\mathbf{d}_3}\right) \\
&= -t\left(e^{i(\mathbf{K}_1+\mathbf{q})\cdot\mathbf{d}_1} + e^{i(\mathbf{K}_1+\mathbf{q})\cdot\mathbf{d}_2} + e^{i(\mathbf{K}_1+\mathbf{q})\cdot\mathbf{d}_3}\right)
\end{aligned}$$

坐标信息为：

$\mathbf{K}_1 = \left(\frac{2\pi}{3a}, \frac{2\pi}{3\sqrt{3}a}\right); \mathbf{K}_2 = \left(\frac{2\pi}{3a}, -\frac{2\pi}{3\sqrt{3}a}\right)$

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

$$\begin{aligned}
f_1(\mathbf{k}) &= -t\left(e^{i(\mathbf{K}_1+\mathbf{q})\cdot\mathbf{d}_1} + e^{i(\mathbf{K}_1+\mathbf{q})\cdot\mathbf{d}_2} + e^{i(\mathbf{K}_1+\mathbf{q})\cdot\mathbf{d}_3}\right) \\
&= -t\left(e^{i\mathbf{q}\cdot\mathbf{d}_1} + e^{i2\pi/3}e^{i\mathbf{q}\cdot\mathbf{d}_2} + e^{-i2\pi/3}e^{i\mathbf{q}\cdot\mathbf{d}_3}\right) \\
&\approx -t\left(1 + e^{i2\pi/3} + e^{-i2\pi/3}\right) - it\mathbf{q}\cdot\left(\mathbf{d}_1 + e^{i2\pi/3}\mathbf{d}_2 + e^{-i2\pi/3}\mathbf{d}_3\right) \\
&= -it\mathbf{q}\cdot\left(\mathbf{d}_1 + e^{i2\pi/3}\mathbf{d}_2 + e^{-i2\pi/3}\mathbf{d}_3\right) \\
&= -it\mathbf{q}\cdot\left(e^{i2\pi/3}\mathbf{d}_2 + e^{-i2\pi/3}\mathbf{d}_3, \right) \\
&= -it\mathbf{q}\cdot\left(\left(\frac{i\sqrt{3}}{2} + \frac{1}{2}\right)\frac{3}{2}a, \left(\frac{\sqrt{3}}{2}i - \frac{1}{2}\right)\sqrt{3}a + \left(-\frac{i\sqrt{3}}{2} - \frac{1}{2}\right)\frac{\sqrt{3}}{2}a\right) \\
&= -iat\mathbf{q}\cdot\left(\left(\frac{i\sqrt{3}}{2} + \frac{1}{2}\right)\frac{3}{2}, \frac{3}{2}\left(\frac{1}{2}i - \frac{\sqrt{3}}{2}\right)\right) \\
&= \frac{3}{2}at\mathbf{q}\cdot\left(\left(\frac{\sqrt{3}}{2} - i\frac{1}{2}\right), i\left(\frac{\sqrt{3}}{2} - i\frac{1}{2}\right)\right) \\
&= \frac{3}{2}at\left(q_x + iq_y\right)\left(\frac{\sqrt{3}}{2} - i\frac{1}{2}\right) \\
f_1(\mathbf{k}) &= \frac{3}{2}at\left(q_x + iq_y\right)e^{-i\frac{\pi}{6}}
\end{aligned}$$

对于

$$\begin{aligned}
f_2(\mathbf{k}) &= -t\left(e^{i(\mathbf{K}_2+\mathbf{q})\cdot\mathbf{d}_1} + e^{i(\mathbf{K}_2+\mathbf{q})\cdot\mathbf{d}_2} + e^{i(\mathbf{K}_2+\mathbf{q})\cdot\mathbf{d}_3}\right) \\
&= -t\left(e^{i\mathbf{q}\cdot\mathbf{d}_1} + e^{-i2\pi/3}e^{i\mathbf{q}\cdot\mathbf{d}_2} + e^{i2\pi/3}e^{i\mathbf{q}\cdot\mathbf{d}_3}\right) \\
&\approx -t\left(1 + e^{-i2\pi/3} + e^{i2\pi/3}\right) - it\mathbf{q}\cdot\left(\mathbf{d}_1 + e^{-i2\pi/3}\mathbf{d}_2 + e^{i2\pi/3}\mathbf{d}_3\right) \\
&= -it\mathbf{q}\cdot\left(\mathbf{d}_1 + e^{-i2\pi/3}\mathbf{d}_2 + e^{i2\pi/3}\mathbf{d}_3\right) \\
&= -it\mathbf{q}\cdot\left(e^{-i2\pi/3}\mathbf{d}_2 + e^{i2\pi/3}\mathbf{d}_3, \right) \\
&= -it\mathbf{q}\cdot\left(\left(\frac{i\sqrt{3}}{2} - \frac{1}{2}\right)\frac{-3}{2}a, \left(-\frac{\sqrt{3}}{2}i - \frac{1}{2}\right)\sqrt{3}a + \left(\frac{i\sqrt{3}}{2} - \frac{1}{2}\right)\frac{\sqrt{3}}{2}a\right) \\
&= -iat\mathbf{q}\cdot\left(\left(-\frac{i\sqrt{3}}{2} + \frac{1}{2}\right)\frac{3}{2}, \frac{3}{2}\left(-\frac{1}{2}i - \frac{\sqrt{3}}{2}\right)\right) \\
&= \frac{3}{2}at\mathbf{q}\cdot\left(\left(-\frac{\sqrt{3}}{2} - i\frac{1}{2}\right), i\left(\frac{\sqrt{3}}{2} + i\frac{1}{2}\right)\right) \\
&= \frac{3}{2}at\left(-q_x + iq_y\right)\left(\frac{\sqrt{3}}{2} + i\frac{1}{2}\right) \\
f_2(\mathbf{k}) &= \frac{3}{2}at\left(-q_x + iq_y\right)e^{i\frac{\pi}{6}}
\end{aligned}$$

也就是有

$$\begin{aligned}f_1(\mathbf{k}) &= \frac{3}{2}at\left(q_x+iq_y\right)e^{-i\frac{\pi}{6}}\\ &= v_F\left(q_x+iq_y\right)e^{-i\frac{\pi}{6}}\\ f_2(\mathbf{k}) &= \frac{3}{2}at\left(-q_x+iq_y\right)e^{i\frac{\pi}{6}}\\ &= v_F\left(-q_x+iq_y\right)e^{i\frac{\pi}{6}}\end{aligned}$$

因此，谷$\mathbf{K}_1$和$\mathbf{K}_2$的哈密顿量为：

$$\begin{aligned}H_1 &= e^{-i\frac{\pi}{6}}|\mathbf{K}_1,A\rangle v_F\left(\hat{p}_x+i\hat{p}_y\right)\langle\mathbf{K}_1,B|+h.c\\ H_2 &= e^{i\frac{\pi}{6}}|\mathbf{K}_2,A\rangle v_F\left(-\hat{p}_x+i\hat{p}_y\right)\langle\mathbf{K}_2,B|+h.c\\ &= \theta H_1\theta^{-1}\end{aligned}$$

对于$\mathbf{K}_1$谷，定义$e^{-i\frac{\pi}{6}}|\mathbf{K}_1,A\rangle\equiv|\uparrow_1\rangle$ 作为自旋朝上态，$|\mathbf{K}_1,B\rangle$作为自旋朝下态$|\downarrow_1\rangle$，然后哈密顿量改写为：

$$H_1 = |\uparrow_1\rangle v_F\left(\hat{p}_x+i\hat{p}_y\right)\langle\downarrow_1|+h.c$$

同理，对于$\mathbf{K}_2$谷，定义$e^{i\frac{\pi}{6}}|\mathbf{K}_2,A\rangle\equiv|\uparrow_2\rangle$ 作为自旋朝上态，$|\mathbf{K}_2,B\rangle$作为自旋朝下态$|\downarrow_2\rangle$，然后哈密顿量改写为：

$$H_2 = |\uparrow_2\rangle v_F\left(-\hat{p}_x+i\hat{p}_y\right)\langle\downarrow_2|+h.c=\theta H_1\theta^{-1}$$

为了恢复传统的形式，定义

$$\begin{aligned}\sigma_x &\equiv \left[|\uparrow\rangle,|\downarrow\rangle\right]\begin{bmatrix}0&1\\1&0\end{bmatrix}\begin{bmatrix}\langle\uparrow|\\ \langle\downarrow|\end{bmatrix}\\ &= |\uparrow\rangle\langle\downarrow|+|\downarrow\rangle\langle\uparrow|\\ \sigma_y &\equiv \left[|\uparrow\rangle,|\downarrow\rangle\right]\begin{bmatrix}0&-i\\i&0\end{bmatrix}\begin{bmatrix}\langle\uparrow|\\ \langle\downarrow|\end{bmatrix}\\ &= -i|\uparrow\rangle\langle\downarrow|+i|\downarrow\rangle\langle\uparrow|\\ \sigma_z &\equiv \left[|\uparrow\rangle,|\downarrow\rangle\right]\begin{bmatrix}1&0\\0&-1\end{bmatrix}\begin{bmatrix}\langle\uparrow|\\ \langle\downarrow|\end{bmatrix}\\ &= |\uparrow\rangle\langle\uparrow|-|\downarrow\rangle\langle\downarrow|\end{aligned}$$

$$\begin{aligned}H_1 &= v_F\left(\hat{p}_x+i\hat{p}_y\right)|\uparrow_1\rangle\langle\downarrow_1|+v_F\left(\hat{p}_x-i\hat{p}_y\right)|\downarrow_1\rangle\langle\uparrow_1|\\ &= v_F\left(\hat{p}_x\sigma_x^{(1)}-\hat{p}_y\sigma_y^{(1)}\right)\end{aligned}$$

$$\begin{aligned}H_2 &= v_F\left(-\hat{p}_x+i\hat{p}_y\right)|\uparrow_2\rangle\langle\downarrow_2|+v_F\left(-\hat{p}_x-i\hat{p}_y\right)|\downarrow_2\rangle\langle\uparrow_2|\\ &= v_F\left(-\hat{p}_x\sigma_x^{(2)}-\hat{p}_y\sigma_y^{(2)}\right)\end{aligned}$$

再使用$\theta|\uparrow_1\rangle = |\uparrow_2\rangle$,以及$\theta|\downarrow_1\rangle = |\downarrow_2\rangle$，有：

$$\theta\sigma_x^{(1)}\theta^{-1} = \sigma_x^{(2)}$$
$$\theta\sigma_y^{(1)}\theta^{-1} = -\sigma_y^{(2)}$$
$$\theta\sigma_z^{(1)}\theta^{-1} = \sigma_z^{(2)}$$

因此，时间反演将哈密顿量H_1变为了H_2。