动能项

$$H_t = -t\sum_{\langle ij\rangle}\left(\vec{c}_i^{\,\dagger}\vec{c}_j + H.c.\right) = -t\sum_{\langle ij\rangle\sigma}\left(c_{i\sigma}^\dagger c_{j\sigma} + H.c.\right)$$ 常见的石墨烯 hopping 项

$$\vec{c}_i^{\,\dagger}\vec{c}_j = \left(c_{i\uparrow}^\dagger, c_{i\downarrow}^\dagger\right)\begin{pmatrix} c_{j\uparrow} \\ c_{j\downarrow}\end{pmatrix} = c_{i\uparrow}^\dagger c_{j\uparrow} + c_{i\downarrow}^\dagger c_{j\downarrow}$$

相互作用项

① $H_\lambda = -\lambda\sum_{\hexagon}\left(\sum_{\langle\langle ij\rangle\rangle\in\hexagon} i\,\nu_{ij}\,\vec{c}_i^{\,\dagger}\vec{\sigma}\vec{c}_j + H.c.\right)^2 = -\lambda\sum_{\hexagon} O^2$, $\vec{\sigma} = (\sigma_x, \sigma_y, \sigma_z)$, $\vec{c}_j = \begin{pmatrix} c_{j\uparrow} \\ c_{j\downarrow}\end{pmatrix}$

② $$e^{-\Delta\tau H_\lambda} = \prod_{\hexagon} e^{\Delta\tau\lambda O^2} \xlongequal{\text{HS变换}} \prod_{\hexagon}\sum_{l_{\hexagon}=\pm1,\pm2}\gamma(l_{\hexagon})\,e^{\sqrt{\Delta\tau\lambda}\,\eta(l_{\hexagon})\,O}$$

③ $$O = \sum_{\langle\langle ij\rangle\rangle\in\hexagon} i\,\nu_{ij}\,\vec{c}_i^{\,\dagger}\vec{\sigma}\vec{c}_j + H.c.$$

$$= \sum_{\langle\langle ij\rangle\rangle\in\hexagon} i\,\nu_{ij}\left(S_{ij}^x\vec{x} + S_{ij}^y\vec{y} + S_{ij}^z\vec{z}\right) + H.c.$$

$$= \sum_{\sigma=x,y,z}\ \sum_{\langle\langle ij\rangle\rangle\in\hexagon} i\,\nu_{ij}\,S_{ij}^\sigma + H.c.$$

$$S_{ij}^x \equiv \vec{c}_i^{\,\dagger}\sigma^x\vec{c}_j = \left(c_{i\uparrow}^\dagger\ c_{i\downarrow}^\dagger\right)\begin{pmatrix} & 1 \\ 1 & \end{pmatrix}\begin{pmatrix} c_{j\uparrow} \\ c_{j\downarrow}\end{pmatrix} = c_{i\uparrow}^\dagger c_{j\downarrow} + c_{i\downarrow}^\dagger c_{j\uparrow}$$

$$S_{ij}^y \equiv \vec{c}_i^{\,\dagger}\sigma^y\vec{c}_j = \left(c_{i\uparrow}^\dagger\ c_{i\downarrow}^\dagger\right)\begin{pmatrix} & -i \\ i & \end{pmatrix}\begin{pmatrix} c_{j\uparrow} \\ c_{j\downarrow}\end{pmatrix} = -i\,c_{i\uparrow}^\dagger c_{j\downarrow} + i\,c_{i\downarrow}^\dagger c_{j\uparrow}$$

$$S_{ij}^z \equiv \vec{c}_i^{\,\dagger}\sigma^z\vec{c}_j = \left(c_{i\uparrow}^\dagger\ c_{i\downarrow}^\dagger\right)\begin{pmatrix} 1 & \\ & -1\end{pmatrix}\begin{pmatrix} c_{j\uparrow} \\ c_{j\downarrow}\end{pmatrix} = c_{i\uparrow}^\dagger c_{j\uparrow} - c_{i\downarrow}^\dagger c_{j\downarrow}$$

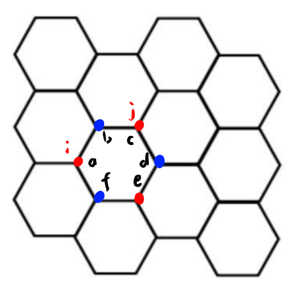
$$\left\{\begin{aligned} S_{ij}^{x\dagger} &= c_{j\uparrow}^\dagger c_{i\downarrow} + c_{j\downarrow}^\dagger c_{i\uparrow} = S_{ji}^x \\ S_{ij}^{y\dagger} &= -i\,c_{j\uparrow}^\dagger c_{i\downarrow} + i\,c_{j\downarrow}^\dagger c_{i\uparrow} = S_{ji}^y \\ S_{ij}^{z\dagger} &= c_{j\uparrow}^\dagger c_{i\uparrow} - c_{j\downarrow}^\dagger c_{i\downarrow} = S_{ji}^z \end{aligned}\right. \Rightarrow\ S_{ij}^{\sigma\dagger} = S_{ji}^\sigma$$

$\left(i\,\nu_{ij}S_{ij}^\sigma\right)^\dagger = -i\,\nu_{ij}S_{ij}^{\sigma\dagger} = -i\,\nu_{ij}S_{ji}^\sigma$, $\sum_{\langle\langle ij\rangle\rangle} i\,\nu_{ij}S_{ij}^\sigma = i\left(-S_{ij}^\sigma + S_{ji}^\sigma\right)$ (成多个负号)

$$\Rightarrow\left(\sum_{\langle\langle ij\rangle\rangle} i\,\nu_{ij}S_{ij}\right)^\dagger = i\left(S_{ij}^{\sigma\dagger} - S_{ji}^{\sigma\dagger}\right) = i\left(-S_{ij}^\sigma + S_{ji}^\sigma\right) = \sum_{\langle\langle ij\rangle\rangle} i\,\nu_{ij}S_{ij}$$

所以这一项同 $\sum_{\langle ij\rangle\sigma} c_{i\sigma}^\dagger c_{j\sigma}$ 一样，本身已经是厄米的了，$+H.c.$ 相当于2倍

在程序中我们不考虑 H.c.（动能项和相互作用项都是）



④ 定义 $m_{ij} = 1\sim6$，来表征一个元胞 $\hexagon$ 内的次近邻对

$m_{ij}=1$ 表示 ac 对，$\nu_1 S_1^\sigma = -S_{ac}^\sigma + S_{ca}^\sigma$

后面依次是 ae，ce，bd，bf，df

$$O=\sum_{\sigma=x,y,z}\sum_{m_{ij}=1\sim6} i\left(S_{ij}^{\sigma}-S_{ji}^{\sigma}\right)$$

这里±号取决于垂直晶格平面的 $\vec{e}_z$ 方向的选取，由于辅助场是正负对称的，选哪个方向都一样

$$e^{-\delta\tau H_\lambda}=\prod_{\square}\sum_{l_\square=\pm1,\pm2}\gamma(l_\square)\,e^{\sqrt{\delta\tau\lambda}\,\eta(l_\square)\,O}=\prod_{\square}\sum_{l_\square=\pm1,\pm2}\gamma(l_\square)\prod_{\sigma=xyz}\prod_{m_{ij}=1\sim6}e^{\sqrt{\delta\tau\lambda}\,\eta(l_\square)\,i(S_{ij}^{\sigma}-S_{ji}^{\sigma})}$$

这里格点耦合和自旋耦合依然存在，没法用H的那个trick化简，只能作4阶幺正变换

⑤ $\sigma=x$, $i(S_{ij}^x-S_{ji}^x)=i\left(c_{i\uparrow}^\dagger c_{j\downarrow}+c_{i\downarrow}^\dagger c_{j\uparrow}-c_{j\uparrow}^\dagger c_{i\downarrow}-c_{j\downarrow}^\dagger c_{i\uparrow}\right)$

矩阵表示为

$$\begin{pmatrix}c_{i\uparrow}^\dagger & c_{i\downarrow}^\dagger & c_{j\uparrow}^\dagger & c_{j\downarrow}^\dagger\end{pmatrix}\begin{pmatrix}0&0&&i\\0&0&i&\\&-i&0&0\\-i&&0&0\end{pmatrix}\begin{pmatrix}c_{i\uparrow}\\c_{i\downarrow}\\c_{j\uparrow}\\c_{j\downarrow}\end{pmatrix}$$

通过分块的方式 $\left(\boxed{\;}\right)$，发现只要考察 $\begin{pmatrix}&i\\-i&\end{pmatrix}$ 的幺正变换就行

$$i\begin{pmatrix}1&i\\1&-i\end{pmatrix}\begin{pmatrix}&1\\-1&\end{pmatrix}\begin{pmatrix}1&1\\-i&i\end{pmatrix}=i\begin{pmatrix}-i&1\\i&1\end{pmatrix}\begin{pmatrix}1&1\\-i&i\end{pmatrix}=\begin{pmatrix}2&\\&-2\end{pmatrix}$$

因此

$$U=\frac{1}{\sqrt2}\begin{pmatrix}1&&&1\\&1&1&\\&-i&i&\\-i&&&i\end{pmatrix}\qquad U^\dagger=\frac{1}{\sqrt2}\begin{pmatrix}1&&&i\\&1&i&\\&1&-i&\\1&&&-i\end{pmatrix}\qquad u^{x\dagger}\equiv\begin{pmatrix}1&i\\1&-i\end{pmatrix}$$

验证：

$$UU^\dagger=\frac12\begin{pmatrix}2&&&\\&2&&\\&&2&\\&&&2\end{pmatrix}=I=U^\dagger U$$

$b=U^\dagger c$, $c=Ub$, $U^\dagger\begin{pmatrix}&&&i\\&&i&\\&-i&&\\-i&&&\end{pmatrix}U=\begin{pmatrix}1&&&\\&1&&\\&&-1&\\&&&-1\end{pmatrix}$

$\sigma=y$, $i(S_{ij}^y-S_{ji}^y)=i\left(-i\,c_{i\uparrow}^\dagger c_{j\downarrow}+i\,c_{i\downarrow}^\dagger c_{j\uparrow}+i\,c_{j\uparrow}^\dagger c_{i\downarrow}-i\,c_{j\downarrow}^\dagger c_{i\uparrow}\right)$

矩阵表示为

$$\begin{array}{c|cccc} & i\uparrow & i\downarrow & j\uparrow & j\downarrow\\ \hline i\uparrow &&&&1\\ i\downarrow &&&-1&\\ j\uparrow &&-1&&\\ j\downarrow &1&&&\end{array}$$

分块后考察 $\begin{pmatrix}&1\\1&\end{pmatrix}$，$\begin{pmatrix}1&1\\1&-1\end{pmatrix}\begin{pmatrix}&1\\1&\end{pmatrix}\begin{pmatrix}1&1\\1&-1\end{pmatrix}=\begin{pmatrix}1&1\\-1&1\end{pmatrix}\begin{pmatrix}1&1\\1&-1\end{pmatrix}=\begin{pmatrix}2&\\&-2\end{pmatrix}$

因此

$$U=U^\dagger=\frac{1}{\sqrt2}\begin{pmatrix}1&&&1\\&1&1&\\&1&-1&\\1&&&-1\end{pmatrix},\qquad U^\dagger U=UU^\dagger=I\qquad u^y\equiv\begin{pmatrix}1&1\\1&-1\end{pmatrix}$$

$b=U^\dagger c$, $c=Ub$, $U^\dagger\begin{pmatrix}&&&1\\&&-1&\\&-1&&\\1&&&\end{pmatrix}U=\begin{pmatrix}1&&&\\&-1&&\\&&1&\\&&&-1\end{pmatrix}$

$\sigma = z$, $i(S^z_{ij} - S^z_{ji}) = i(c^\dagger_{i\uparrow}c_{j\uparrow} - c^\dagger_{i\downarrow}c_{j\downarrow} - c^\dagger_{j\uparrow}c_{i\uparrow} + c^\dagger_{j\downarrow}c_{i\downarrow})$

矩阵表示为
$$\begin{array}{c} \\ i\uparrow \\ i\downarrow \\ j\uparrow \\ j\downarrow \end{array}\begin{array}{c} \begin{array}{cccc} i\uparrow & i\downarrow & j\uparrow & j\downarrow \end{array} \\ \begin{pmatrix} & & i & 0 \\ & & 0 & -i \\ -i & 0 & & \\ 0 & i & & \end{pmatrix}\end{array}$$

分块后：

$$\begin{cases} \begin{pmatrix} \sigma & \\ & \sigma \end{pmatrix}\begin{pmatrix} & \beta \\ -\beta & \end{pmatrix} = \begin{pmatrix} & \sigma\beta \\ -\sigma\beta & \end{pmatrix} \\ \begin{pmatrix} & \beta \\ -\beta & \end{pmatrix}\begin{pmatrix} \sigma & \\ & \sigma \end{pmatrix} = \begin{pmatrix} & \beta\sigma \\ -\beta\sigma & \end{pmatrix} \end{cases} + \underbrace{\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}}_{u^{y\dagger}}\begin{pmatrix} 1 & \\ & -1 \end{pmatrix}\underbrace{\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}}_{u^{y}} = \begin{pmatrix} & 1 \\ 1 & \end{pmatrix}$$

$$\begin{pmatrix} 1 & 1 & & \\ 1 & -1 & & \\ & & 1 & 1 \\ & & 1 & -1 \end{pmatrix}\begin{pmatrix} & & 1 & 0 \\ & & 0 & -1 \\ -1 & 0 & & \\ 0 & 1 & & \end{pmatrix}\begin{pmatrix} 1 & 1 & & \\ 1 & -1 & & \\ & & 1 & 1 \\ & & 1 & -1 \end{pmatrix} = \begin{pmatrix} & & 1 & -1 \\ & & 1 & 1 \\ -1 & 1 & & \\ -1 & -1 & & \end{pmatrix}\begin{pmatrix} 1 & 1 & & \\ 1 & -1 & & \\ & & 1 & 1 \\ & & 1 & -1 \end{pmatrix}$$

$$= \begin{pmatrix} & & & 2 \\ & & 2 & \\ & -2 & & \\ -2 & & & \end{pmatrix}, \qquad U_1 = U_1^\dagger = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 & & \\ 1 & -1 & & \\ & & 1 & 1 \\ & & 1 & -1 \end{pmatrix}$$

又由 $u^{x\dagger}\begin{pmatrix} & 1 \\ -1 & \end{pmatrix}u^x = \begin{pmatrix} 1 & \\ & -1 \end{pmatrix} \Rightarrow U_2^\dagger = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & & & i \\ & 1 & i & \\ & 1 & -i & \\ 1 & & & -i \end{pmatrix}$

$$U^\dagger = U_2^\dagger U_1^\dagger = \frac{1}{2}\begin{pmatrix} 1 & & & i \\ & 1 & i & \\ & 1 & -i & \\ 1 & & & -i \end{pmatrix}\begin{pmatrix} 1 & 1 & & \\ 1 & -1 & & \\ & & 1 & 1 \\ & & 1 & -1 \end{pmatrix} = \frac{1}{2}\begin{pmatrix} 1 & 1 & i & -i \\ 1 & -1 & i & i \\ 1 & -1 & -i & -i \\ 1 & 1 & -i & i \end{pmatrix}$$

$$U = \frac{1}{2}\begin{pmatrix} 1 & 1 & 1 & 1 \\ 1 & -1 & -1 & 1 \\ -i & -i & i & i \\ i & -i & i & -i \end{pmatrix}, \quad U^\dagger U = \frac{1}{4}\begin{pmatrix} 4 & 0 & 0 & 0 \\ 0 & 4 & 0 & 0 \\ 0 & 0 & 4 & 0 \\ 0 & 0 & 0 & 4 \end{pmatrix} = \mathbb{I}$$

验证：

$$\frac{1}{4}\begin{pmatrix} 1 & 1 & i & -i \\ 1 & -1 & i & i \\ 1 & -1 & -i & -i \\ 1 & 1 & -i & i \end{pmatrix}\begin{pmatrix} 0 & 0 & i & 0 \\ 0 & 0 & 0 & -i \\ -i & 0 & 0 & 0 \\ 0 & i & 0 & 0 \end{pmatrix}\begin{pmatrix} 1 & 1 & 1 & 1 \\ 1 & -1 & -1 & 1 \\ -i & -i & i & i \\ i & -i & i & -i \end{pmatrix} = \frac{1}{4}\begin{pmatrix} 1 & 1 & i & -i \\ 1 & -1 & i & i \\ -1 & 1 & i & i \\ -1 & -1 & i & -i \end{pmatrix}\begin{pmatrix} 1 & 1 & 1 & 1 \\ 1 & -1 & -1 & 1 \\ -i & -i & i & i \\ i & -i & i & -i \end{pmatrix}$$

$$= \frac{1}{4}\begin{pmatrix} 4 & & & \\ & 4 & & \\ & & -4 & \\ & & & -4 \end{pmatrix} = \begin{pmatrix} 1 & & & \\ & 1 & & \\ & & -1 & \\ & & & -1 \end{pmatrix}$$

$\therefore$ $b = U^\dagger c$, $c = U b$, $U^\dagger\begin{pmatrix} & & i & 0 \\ & & 0 & -i \\ -i & 0 & & \\ 0 & i & & \end{pmatrix}U = \begin{pmatrix} 1 & & & \\ & 1 & & \\ & & -1 & \\ & & & -1 \end{pmatrix}$

参考SMG模型的写法

(2311.09970)

$$H=-t\sum_{\langle ij\rangle\sigma\alpha}(c^\dagger_{i\sigma\alpha}c_{j\sigma\alpha}+\text{h.c.})+J\sum_i \vec{S}_{i,1}\cdot\vec{S}_{i,2}$$

① $$\vec{S}_{i1}\cdot\vec{S}_{i2} = (S^x_{i1}\vec{x}+S^y_{i1}\vec{y}+S^z_{i1}\vec{z})\cdot(S^x_{i2}\vec{x}+S^y_{i2}\vec{y}+S^z_{i2}\vec{z})$$
$$= S^x_{i1}S^x_{i2}+S^y_{i1}S^y_{i2}+S^z_{i1}S^z_{i2}$$
$$=\frac{1}{4}\left[\left(S^{x\,2}_{i1}+2S^x_{i1}S^x_{i2}+S^{x\,2}_{i2}\right)-\left(S^{x\,2}_{i1}-2S^x_{i1}S^x_{i2}+S^{x\,2}_{i2}\right)+\cdots\cdots\right]$$
$$=\frac{1}{4}\left[(S^x_{i1}+S^x_{i2})^2-(S^x_{i1}-S^x_{i2})^2+\cdots\right]$$

6个完全平方项

对每个完全平方项分别作HS变换

② $$e^{-\Delta\tau H_I}=e^{-\Delta\tau J\sum_i \vec{S}_{i1}\cdot\vec{S}_{i2}}$$
$$=\exp\left\{-\frac{\Delta\tau J}{4}\sum_i\left[(S^x_{i1}+S^x_{i2})^2-\cdots+\cdots\right]\right\}$$
$$=\exp\left[-\frac{\Delta\tau J}{4}\sum_i(S^x_{i1}+S^x_{i2})^2\right]\exp\left[\frac{\Delta\tau J}{4}\sum_i(S^x_{i1}-S^x_{i2})^2\right]\cdots\cdots$$
$$=\prod_{\sigma_1=x,y,z}\exp\left[-\frac{\Delta\tau J}{4}\sum_i(S^{\sigma_1}_{i1}+S^{\sigma_1}_{i2})^2\right]\prod_{\sigma_2=x,y,z}\exp\left[\frac{\Delta\tau J}{4}\sum_i(S^{\sigma_2}_{i1}-S^{\sigma_2}_{i2})^2\right]$$
$$\overset{\text{HS变换}}{=\!=}\prod_i\prod_{\sigma_1=x,y,z}\sum_{l_1^{\sigma_1}=\pm1,\pm2}\gamma(l_1^{\sigma_1})\exp\Big[\underbrace{\sqrt{-\Delta\tau J/4}}_{\to i\sqrt{\Delta\tau J/4}}\,\eta(l_1^{\sigma_1})(S^{\sigma_1}_{i1}+S^{\sigma_1}_{i2})\Big]$$
$$\times\prod_i\prod_{\sigma_2=x,y,z}\sum_{l_1^{\sigma_2}=\pm1,\pm2}\gamma(l_2^{\sigma_2})\exp\left[\sqrt{\Delta\tau J/4}\,\eta(l_2^{\sigma_2})(S^{\sigma_2}_{i1}-S^{\sigma_2}_{i2})\right]$$

③ $$S^x=(c_\uparrow^\dagger\ c_\downarrow^\dagger)\begin{pmatrix}&1\\1&\end{pmatrix}\begin{pmatrix}c_\uparrow\\c_\downarrow\end{pmatrix}=(c_\downarrow^\dagger\ c_\uparrow^\dagger)\begin{pmatrix}c_\uparrow\\c_\downarrow\end{pmatrix}=c_\downarrow^\dagger c_\uparrow+\text{h.c.}$$

幺正变换用 $U=U^\dagger=\frac{1}{\sqrt2}\begin{pmatrix}1&1\\1&-1\end{pmatrix}$ $\Rightarrow b_1^\dagger b_1-b_2^\dagger b_2$

这里Pauli σ^y 也可视作算符 S^y 在粒子数表象下的矩阵表示

$$S^y=(c_\uparrow^\dagger\ c_\downarrow^\dagger)\begin{pmatrix}&-i\\i&\end{pmatrix}\begin{pmatrix}c_\uparrow\\c_\downarrow\end{pmatrix}=(ic_\downarrow^\dagger\ \ -ic_\uparrow^\dagger)\begin{pmatrix}c_\uparrow\\c_\downarrow\end{pmatrix}=ic_\downarrow^\dagger c_\uparrow-ic_\uparrow^\dagger c_\downarrow$$

$$\Rightarrow \begin{array}{c|cc} & \uparrow & \downarrow\\ \hline \uparrow & & -i\\ \downarrow & i & \end{array}$$
$$\begin{pmatrix}1&i\\1&-i\end{pmatrix}\begin{pmatrix}&-i\\i&\end{pmatrix}\begin{pmatrix}1&1\\-i&i\end{pmatrix}=\begin{pmatrix}-1&-i\\1&-i\end{pmatrix}\begin{pmatrix}1&1\\-i&i\end{pmatrix}=\begin{pmatrix}-2&\\&2\end{pmatrix}$$

程序中：$\begin{cases}b_1=\frac{1}{\sqrt2}(c_\uparrow+ic_\downarrow)\\ b_2=\frac{1}{\sqrt2}(c_\uparrow-ic_\downarrow)\end{cases}\Rightarrow\begin{cases}c_\uparrow=\frac{1}{\sqrt2}(b_1+b_2)\\ c_\downarrow=\frac{-i}{\sqrt2}(b_1-b_2)=\frac{i}{\sqrt2}(b_2-b_1)\end{cases}$

$$ic_\downarrow^\dagger c_\uparrow-ic_\uparrow^\dagger c_\downarrow$$
$$=i\cdot\frac{i}{\sqrt2}(b_1^\dagger-b_2^\dagger)\cdot\frac{1}{\sqrt2}(b_1+b_2)-i\cdot\frac{1}{\sqrt2}(b_1^\dagger+b_2^\dagger)\cdot\frac{-i}{\sqrt2}(b_1-b_2)$$
$$=-\frac12(b_1^\dagger b_1-b_2^\dagger b_1+b_1^\dagger b_2-b_2^\dagger b_2)-\frac12(b_1^\dagger b_1+b_2^\dagger b_1-b_1^\dagger b_2-b_2^\dagger b_2)$$
$$=-b_1^\dagger b_1+b_2^\dagger b_2$$

幺正变换用 $U=\frac{1}{\sqrt2}\begin{pmatrix}1&1\\-i&i\end{pmatrix}$

$U^\dagger=\frac{1}{\sqrt2}\begin{pmatrix}1&i\\1&-i\end{pmatrix}$

$$S^z=c_\uparrow^\dagger c_\uparrow-c_\downarrow^\dagger c_\downarrow$$

注意到这里 S^y 幺正变换后相对于 S^x 和 S^z 多了个负号，由于x、y、z辅助场是独立的，且辅助场又是正负对称的，所以 S^y 的负号可以给辅助场，最终不影响结果。

e.g. $+\sqrt{2(3-\sqrt6)}\longrightarrow-\sqrt{2(3-\sqrt6)}$ 辅助场由 $+1\to-1$ 抽样的关于y的辅助场与真实的辅助场差一负号

$$\hat h_1^\sigma = i\sqrt{\Delta\tau J/4}\,\eta(a)(S^\sigma_{i1}+S^\sigma_{i2})$$
$$\hat h_2^\sigma = \sqrt{\Delta\tau J/4}\,\eta(a)(S^\sigma_{i1}-S^\sigma_{i2})$$

$\gamma(\pm1)=1+\sqrt6/3,\quad \gamma(\pm2)=1-\sqrt6/3$

$\eta(\pm1)=\pm\sqrt{2\left(3-\sqrt6\right)},\quad \eta(\pm2)=\pm\sqrt{2\left(3+\sqrt6\right)}.$

④ HS变换后层间耦合被decouple，又由于无层间跃迁，这时候可以写成独立的两层

$$H=-t\sum_{\langle ij\rangle\sigma}\left(c^\dagger_{i\sigma1}c_{j\sigma1}+h.c.\right)-t\sum_{\langle ij\rangle\sigma}\left(c^\dagger_{i\sigma2}c_{j\sigma2}+h.c.\right)+\sum_i\Big[i\phi_1\left(S^x_{i1}+S^x_{i2}\right)+\phi_2\left(S^x_{i1}-S^x_{i2}\right)$$
$$+i\phi_3\left(S^y_{i1}+S^y_{i2}\right)+\phi_4\left(S^y_{i1}-S^y_{i2}\right)+i\phi_5\left(S^z_{i1}+S^z_{i2}\right)+\phi_6\left(S^z_{i1}-S^z_{i2}\right)\Big]$$

构造变换 $\vec{c}_{i2}\longrightarrow\tilde{\vec{c}}_{i2}=-i\sigma^y\vec{c}_{i2}=-i\begin{pmatrix} & -i\\ i & \end{pmatrix}\vec{c}_{i2}=\begin{pmatrix} & -1\\ 1 & \end{pmatrix}\begin{pmatrix}c_{i\uparrow2}\\ c_{i\downarrow2}\end{pmatrix}=\begin{pmatrix}-c_{i\downarrow2}\\ c_{i\uparrow2}\end{pmatrix}$

即 $\tilde{c}_{i\sigma2}=(-1)^{\sigma}c_{i\bar{\sigma}2}$ $\bar\sigma$ 相反的自旋

$(-1)^\sigma$：自旋分量

易得 $\tilde{S}^x_{i2}=-S^x_{i2}$，$\tilde{S}^z_{i2}=-S^z_{i2}$，$\tilde{S}^y_{i2}=i\tilde{c}^\dagger_\downarrow\tilde{c}_\uparrow-i\tilde{c}^\dagger_\uparrow\tilde{c}_\downarrow=-ic^\dagger_\uparrow c_\downarrow+ic^\dagger_\downarrow c_\uparrow=S^y_{i2}$，

$$H=-t\sum_{\langle ij\rangle\sigma}\left(c^\dagger_{i\sigma1}c_{j\sigma1}+h.c.\right)-t\sum_{\langle ij\rangle\sigma}\left(c^\dagger_{i\sigma2}c_{j\sigma2}+h.c.\right)+\sum_i\Big[i\phi_1\left(S^x_{i1}-\tilde{S}^x_{i2}\right)+\phi_2\left(S^x_{i1}+\tilde{S}^x_{i2}\right)$$
$$+i\phi_3\left(S^y_{i1}+\tilde{S}^y_{i2}\right)+\phi_4\left(S^y_{i1}-\tilde{S}^y_{i2}\right)+i\phi_5\left(S^z_{i1}-\tilde{S}^z_{i2}\right)+\phi_6\left(S^z_{i1}+\tilde{S}^z_{i2}\right)\Big]$$
$$=-t\sum_{\langle ij\rangle\sigma}\left(c^\dagger_{i\sigma1}c_{j\sigma1}+h.c.\right)+\sum_i\Big[\underline{(\phi_2+i\phi_1)S^x_{i1}+(\phi_4+i\phi_3)S^y_{i1}+(\phi_6+i\phi_5)S^z_{i1}}\Big]$$
$$-t\sum_{\langle ij\rangle\sigma}\left(c^\dagger_{i\sigma2}c_{j\sigma2}+h.c.\right)+\sum_i\Big[(\phi_2-i\phi_1)\tilde{S}^x_{i2}+(-\phi_4+i\phi_3)\tilde{S}^y_{i2}+(\phi_6-i\phi_5)\tilde{S}^z_{i2}\Big]$$
$$=H_1+\tilde{H}_2$$

H_1 非厄米！！
怎么能用非厄米去演化？

处理相互作用只要连乘这6项
在观测量中用 H_1 表示 $\tilde{H}_2$，从而表示 H_2

因为两层独立，我们可以将其看作是2个不同的系统，其中算符是相同的，故可以忽视算符的指标。这样的话，第一个系统的哈密顿量和第二个系统的哈密顿量是复共轭的。但是写成厄米共轭也没错，因为每部分算符都是厄米的。

若考虑 $\tilde{H}_2=H_1^\dagger$，得到 $\langle O\rangle_2^*=\langle\psi_T|e^{-\tau\tilde{H}_2}\,O\,e^{-\tau\tilde{H}_2}|\psi_T\rangle^*$
$=\langle\psi_T|e^{-\tau H_1^\dagger}\,O^\dagger\,e^{-\tau H_1^\dagger}|\psi_T\rangle$
$=\langle\psi_T|e^{-\tau H_1}\,O^\dagger\,e^{-\tau H_1}|\psi_T\rangle$
$=\langle O^\dagger\rangle$

内积的性质：
复共轭转置
算符期望值的复共轭等于
该算符厄米共轭的期望值

就应该是 $\langle\tilde{c}^\dagger_{i\sigma2}\tilde{c}_{j\sigma'2}\rangle=\langle c^\dagger_{j\sigma'1}c_{i\sigma1}\rangle^*$

若考虑 $H=\begin{pmatrix}H_1 & \\ & \tilde{H}_2\end{pmatrix}=\begin{pmatrix}H_1 & \\ & H_1^*\end{pmatrix}\Rightarrow P=\begin{pmatrix}P_1 & \\ & \tilde{P}_2\end{pmatrix}=\begin{pmatrix}P_1 & \\ & P_1^*\end{pmatrix}$

$B^>=\begin{pmatrix}B_1^> & \\ & \tilde{B}_2^>\end{pmatrix}=\begin{pmatrix}B_1^> & \\ & B_1^{>*}\end{pmatrix}$

$G=\begin{pmatrix}G_1 & \\ & \tilde{G}_2\end{pmatrix}=1-B^>(B^<B^>)^{-1}B^<$
$=\begin{pmatrix}1-B_1^>(B_1^<B_1^>)^{-1}B_1^< & \\ & 1-\tilde{B}_2^>(\tilde{B}_2^<\tilde{B}_2^>)^{-1}\tilde{B}_2^<\end{pmatrix}=\begin{pmatrix}1-B_1^>(B_1^<B_1^>)^{-1}B_1^< & \\ & (1-B_1^>(B_1^<B_1^>)^{-1}B_1^<)^*\end{pmatrix}$

$\Rightarrow\tilde{G}_2=G_1^*$

$\Rightarrow\langle\tilde{c}^\dagger_{i\sigma2}\tilde{c}_{j\sigma'2}\rangle=\langle c^\dagger_{i\sigma1}c_{j\sigma'1}\rangle^*$

即 $\langle c^\dagger_{i\sigma2}c_{j\sigma'2}\rangle=(-1)^{\sigma+\sigma'}\langle\tilde{c}^\dagger_{i\bar\sigma2}\tilde{c}_{j\bar\sigma'2}\rangle=(-1)^{\sigma+\sigma'}\langle c^\dagger_{i\bar\sigma1}c_{j\bar\sigma'1}\rangle^*$

这一方法并不要求H具有某种对称性，而只是一种 trick，只要某自由度能 decouple 掉，又无涉及该自由度的跃迁，就能构造。

该方法是通用的，比如 honeycomb Hubbard model，HS变换之后，↑↓耦合能decouple，又无↑↓间跃迁：$H = -t\sum_{\langle ij\rangle\sigma}(C_{i\sigma}^\dagger C_{j\sigma} + h.c.) + \sum_i i\varphi(n_{i\uparrow} + n_{i\downarrow})$

作规范变换 $C_{i\downarrow} \to \tilde{C}_{i\downarrow} = (-)^i C_{i\downarrow}^\dagger = \begin{cases} C_{i\downarrow}^\dagger & A\ sub \\ -C_{i\downarrow}^\dagger & B\ sub \end{cases}$

$$\tilde{C}_{i\downarrow}^\dagger = (-)^i C_{i\downarrow}$$

$$H = -t\sum_{\langle ij\rangle} C_{i\uparrow}^\dagger C_{j\uparrow} - t\sum_{\langle ij\rangle}(-)^{i+j}\tilde{C}_{i\downarrow}\tilde{C}_{j\downarrow}^\dagger + \sum_i i\varphi(C_{i\uparrow}^\dagger C_{i\uparrow} + \tilde{C}_{i\downarrow}\tilde{C}_{i\downarrow}^\dagger)$$

$$= -t\sum_{\langle ij\rangle} C_{i\uparrow}^\dagger C_{j\uparrow} - t\sum_{\langle ij\rangle}\tilde{C}_{i\downarrow}^\dagger\tilde{C}_{j\downarrow} + \sum_i i\varphi(C_{i\uparrow}^\dagger C_{i\uparrow} - \tilde{C}_{i\downarrow}^\dagger\tilde{C}_{i\downarrow}) + const$$

$$= \left(-t\sum_{\langle ij\rangle} C_{i\uparrow}^\dagger C_{j\uparrow} + \sum_i i\varphi C_{i\uparrow}^\dagger C_{i\uparrow}\right) + \left(-t\sum_{\langle ij\rangle}\underset{(+h.c.\text{略})}{\tilde{C}_{i\downarrow}^\dagger\tilde{C}_{j\downarrow}} - \sum_i i\varphi\tilde{C}_{i\downarrow}^\dagger\tilde{C}_{i\downarrow}\right) + const$$

$$= H_\uparrow + \tilde{H}_\downarrow \qquad \because H_\uparrow^\dagger = \tilde{H}_\downarrow$$

$$\therefore \langle\tilde{C}_{i\downarrow}^\dagger\tilde{C}_{j\downarrow}\rangle = \langle C_{i\uparrow}^\dagger C_{j\uparrow}\rangle^*$$

即 $\langle C_{i\downarrow}C_{j\downarrow}^\dagger\rangle = \begin{cases} \langle\tilde{C}_{i\downarrow}^\dagger\tilde{C}_{j\downarrow}\rangle = \langle C_{i\uparrow}^\dagger C_{j\uparrow}\rangle^* & ij\ same\ sub \\ -\langle\tilde{C}_{i\downarrow}^\dagger\tilde{C}_{j\downarrow}\rangle = -\langle C_{i\uparrow}^\dagger C_{j\uparrow}\rangle^* & ij\ diff\ sub \end{cases}$

启示：① 告诉了我们如何处理 $\vec{\sigma}$ 这个矢量：各方向分量放到连乘里面。对每个格点 i，乘 2×3=6 个不同项，幺正变换后乘1个项再幺正变换回去，不同方向的不同由幺正变换的不同体现

② 告诉了我们如何处理吸引相互作用 $\begin{cases} \sqrt{\delta\tau J/4}, & J>0,\ 类比于吸引 \\ i\sqrt{\delta\tau J/4}, & J>0,\ 类比于排斥 \end{cases}$

③ 告诉了我们如何处理相互作用非对角项：幺正变换到对角项

④ 告诉了我们如何在没有层间跃迁的情况下利用对称性把双层自由度在程序中写为单层自由度

For DSM - QSH - SC Model

Gross-Neveu

DQCP

Subroutine :

- ✓ SLI
- ✓ SetH / SetHproj
- ✓ Sproj
- ✓ StHop
- ✓ mmthr / mmthl / mmthrm1 / mmthlm1
- ✓ Salph
- ✓ mmuur / mmuul / mmuurm1 / mmuulm1
- ✓ inconfc / outconfc
- blockc / block_obs
- SunF
- preq

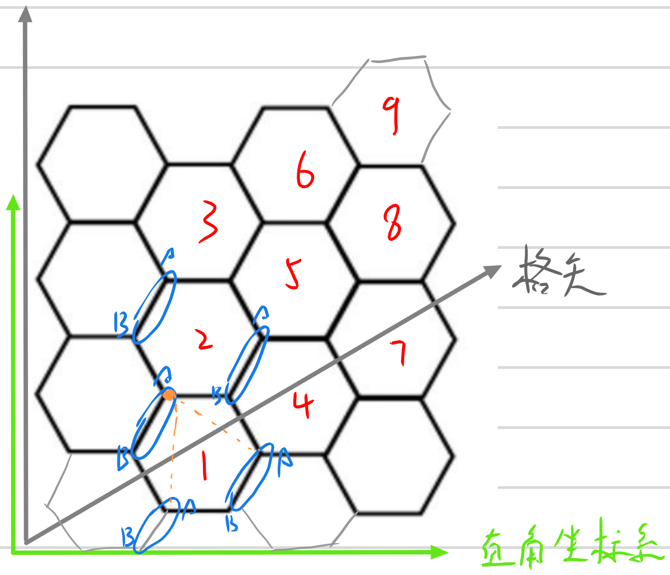
upgradeJ
obser

相较SMG没有改动的是：

calcgr
ortho
npbc
nranf
dyn
obsert
propr
proprm1
prtau

time-dependent measurement

SLI



将⬡与元胞一一对应

Set H （包含 Set Hproj） 程序与 $-t\sum_{\langle ij\rangle\sigma} c_{i\sigma}^{\dagger} c_{j\sigma}$ 一致

Salph / mmuur / mmuul / mmuurml / mmuulml 改成4阶

Inconfc NsigL-K（元胞序号，虚时位置）= ±1

UpgradeJ 和SM公式 改成4阶