1

$$|\sigma_1,\cdots,\sigma_N\rangle \mapsto ?$$

single spin vs. single two-modes fermion

$$|\sigma_i\rangle \mapsto f_{\sigma_i}^{\dagger}|0\rangle, \quad \sigma_i=\pm 1/2 \tag{1}$$

单占据子空间投影算符

$$\mathcal{P}_i \equiv \sum_{\sigma_i} f_{\sigma_i}^{\dagger}|0\rangle\langle 0| f_{\sigma_i} \tag{2}$$

首先想证明

$$\forall \sigma_i,\sigma_i^{\prime}, \quad f_{\sigma_i}^{\dagger}|0\rangle\langle 0| f_{\sigma_i^{\prime}}=\mathcal{P}_i f_{\sigma_i}^{\dagger} f_{\sigma_i^{\prime}} \mathcal{P}_i \tag{3}$$

首先恒等算符

$$\begin{aligned}
\mathcal{P}_i f_{\sigma_i}^{\dagger} f_{\sigma_i^{\prime}} \mathcal{P}_i & =\left(\sum_{\sigma_i^{\prime\prime}} f_{\sigma_i^{\prime\prime}}^{\dagger}|0\rangle\langle 0| f_{\sigma_i^{\prime\prime}}\right) f_{\sigma_i}^{\dagger} f_{\sigma_i^{\prime}}\left(\sum_{\sigma_i^{\prime\prime\prime}} f_{\sigma_i^{\prime\prime\prime}}^{\dagger}|0\rangle\langle 0| f_{\sigma_i^{\prime\prime\prime}}\right) \\
& =\sum_{\sigma_i^{\prime\prime} \sigma_i^{\prime\prime\prime}} f_{\sigma_i^{\prime\prime}}^{\dagger}|0\rangle\left\langle 0\left| f_{\sigma_i^{\prime\prime}} f_{\sigma_i}^{\dagger} f_{\sigma_i^{\prime}} f_{\sigma_i^{\prime\prime\prime}}^{\dagger}\right| 0\right\rangle\langle 0| f_{\sigma_i^{\prime\prime\prime}} \\
& =\sum_{\sigma_i^{\prime\prime} \sigma_i^{\prime\prime\prime}} f_{\sigma_i^{\prime\prime}}^{\dagger}|0\rangle\left\langle 0\left|\left(\delta_{\sigma_i, \sigma_i^{\prime\prime}}-f_{\sigma_i}^{\dagger} f_{\sigma_i^{\prime\prime}}\right) f_{\sigma_i^{\prime}} f_{\sigma_i^{\prime\prime\prime}}^{\dagger}\right| 0\right\rangle\langle 0| f_{\sigma_i^{\prime\prime\prime}} \\
& =\sum_{\sigma_i^{\prime\prime} \sigma_i^{\prime\prime\prime}} \delta_{\sigma_i, \sigma_i^{\prime\prime}} f_{\sigma_i^{\prime\prime}}^{\dagger}|0\rangle\left\langle 0\left| f_{\sigma_i^{\prime}} f_{\sigma_i^{\prime\prime\prime}}^{\dagger}\right| 0\right\rangle\langle 0| f_{\sigma_i^{\prime\prime\prime}} \\
& =\sum_{\sigma_i^{\prime\prime} \sigma_i^{\prime\prime\prime}} \delta_{\sigma_i, \sigma_i^{\prime\prime}} f_{\sigma_i^{\prime\prime}}^{\dagger}|0\rangle \delta_{\sigma_i^{\prime}, \sigma_i^{\prime\prime\prime}}\langle 0| f_{\sigma_i^{\prime\prime\prime}} \\
& =f_{\sigma_i}^{\dagger}|0\rangle\langle 0| f_{\sigma_i^{\prime}}
\end{aligned} \tag{4}$$

格点 i 上单自旋任意算符

$$\begin{aligned}
O_i & =\sum_{\sigma_i \sigma_i^{\prime}}\left\langle\sigma_i\left|O_i\right| \sigma_i^{\prime}\right\rangle\left|\sigma_i\right\rangle\left\langle\sigma_i^{\prime}\right| \mapsto \sum_{\sigma_i \sigma_i^{\prime}}\left\langle\sigma_i\left|O_i\right| \sigma_i^{\prime}\right\rangle f_{\sigma_i}^{\dagger}|0\rangle\langle 0| f_{\sigma_i^{\prime}} \\
& =\sum_{\sigma_i \sigma_i^{\prime}}\left\langle\sigma_i\left|O_i\right| \sigma_i^{\prime}\right\rangle \mathcal{P}_i f_{\sigma_i}^{\dagger} f_{\sigma_i^{\prime}} \mathcal{P}_i
\end{aligned} \tag{5}$$

考虑把这样一个映射分为两次映射:

$$\Gamma: \mathcal{H}_i^{\text{spin}} \rightarrow \mathcal{H}_i^1 \tag{6}$$

$$\Gamma_1: \mathcal{H}_i^{\text{spin}} \rightarrow \mathcal{H}_i^{\text{Fock}}, \quad \Gamma_2: \mathcal{H}_i^{\text{Fock}} \rightarrow \mathcal{H}_i^1 \tag{7}$$

$$\Gamma=\Gamma_2 \circ \Gamma_1 \tag{8}$$

想证明 算符

$$\Gamma\left(O_1 O_2\right)=\Gamma_2\left(\Gamma_1\left(O_1\right) \Gamma_1\left(O_1\right)\right) \tag{9}$$

多自旋与多2模式费米子单占据子空间一一对应

态矢的映射

$$|\sigma_1,\cdots,\sigma_N\rangle \mapsto f^\dagger_{1,\sigma_1}\cdots f^\dagger_{N,\sigma_N}|0\rangle \tag{10}$$

$$\langle\sigma_1,\cdots,\sigma_N| \mapsto \langle 0| f_{N,\sigma_N}\cdots f_{1,\sigma_1} \tag{11}$$

各格点单占据子空间投影算符

$$\mathcal{P}\equiv\sum_{\sigma_1,\cdots,\sigma_N} f^\dagger_{1,\sigma_1}\cdots f^\dagger_{N,\sigma_N}|0\rangle\langle 0| f_{N,\sigma_N}\cdots f_{1,\sigma_1} \tag{12}$$

投影算符与任意算符对易

$$\left[\mathcal{P},\tilde{O}\right]=0. \tag{13}$$

算符的映射

$$\begin{aligned} O &= \sum_{\sigma_1,\cdots,\sigma_N}\sum_{\sigma'_1,\cdots,\sigma'_N}\langle\sigma_1,\cdots,\sigma_N\,|\,O\,|\,\sigma'_1,\cdots,\sigma'_N\rangle\,|\sigma_1,\cdots,\sigma_N\rangle\langle\sigma_1,\cdots,\sigma_N| \\ &\mapsto \sum_{\sigma_1,\cdots,\sigma_N}\sum_{\sigma'_1,\cdots,\sigma'_N}\langle\sigma_1,\cdots,\sigma_N\,|\,O\,|\,\sigma'_1,\cdots,\sigma'_N\rangle\, f^\dagger_{1,\sigma_1}\cdots f^\dagger_{N,\sigma_N}|0\rangle\langle 0| f_{N,\sigma_N}\cdots f_{1,\sigma_1} \\ &\mapsto \mathcal{P}\left(\sum_{\sigma_1,\cdots,\sigma_N}\sum_{\sigma'_1,\cdots,\sigma'_N}\langle\sigma_1,\cdots,\sigma_N\,|\,O\,|\,\sigma'_1,\cdots,\sigma'_N\rangle\, f^\dagger_{1,\sigma_1}\cdots f^\dagger_{N,\sigma_N} f_{N,\sigma_N}\cdots f_{1,\sigma_1}\right)\mathcal{P} \end{aligned} \tag{14}$$

也就是说，算符的一一映射等价于先把算符映射到 Fock 空间中的相应算符，再投影到各格点单占据子空间。

映射保算符对态矢作用、保算符乘积

本征方程对应关系

设 H 是 N 自旋Hilbert空间上的算符，E 和 $|\psi\rangle$ 是某一组本征解；设 $\tilde{H}$ 是相应 N 两模式费米子Fock空间上的算符；设 H' 是相应 N 两模式费米子各格点单占据子空间上的算符，则

$$H|\psi\rangle = E|\psi\rangle, \tag{15}$$

两边同时做 tilde 映射

$$\tilde{H}\left|\tilde{\psi}\right\rangle = E\left|\tilde{\psi}\right\rangle, \tag{16}$$

利用投影算符与任意算符对易这一性质，以及 $\mathcal{P}^2=\mathcal{P}$，投影算符作用

$$\mathcal{P}\tilde{H}\left|\tilde{\psi}\right\rangle = E\mathcal{P}\left|\tilde{\psi}\right\rangle, \tag{17}$$

左边

$$\mathcal{P}\tilde{H}\left|\tilde{\psi}\right\rangle = \mathcal{P}^2\tilde{H}\left|\tilde{\psi}\right\rangle = \mathcal{P}\tilde{H}\mathcal{P}\left|\tilde{\psi}\right\rangle = \mathcal{P}\tilde{H}\mathcal{P}\mathcal{P}\left|\tilde{\psi}\right\rangle = H'|\psi'\rangle \tag{18}$$

右边

$$E\mathcal{P}\left|\tilde{\psi}\right\rangle = E|\psi'\rangle, \tag{19}$$

即

$$H'\left|\psi'\right\rangle = E\left|\psi'\right\rangle, \tag{20}$$

设 $\tilde{H}$ 的某一组本征解为 $E, \left|\tilde{\psi}\right\rangle$，下面证明 $E, \left|\psi'\right\rangle$ 也是 H' 的本征解。

$$\tilde{H}\left|\tilde{\psi}\right\rangle = E\left|\tilde{\psi}\right\rangle, \tag{21}$$

Abrikosov Pseudo-Fermion Representation

从自旋-1/2到 2-模式复费米子体系的映射：

$$\left|\uparrow\right\rangle \mapsto f_\uparrow^\dagger\left|0\right\rangle, \quad \left|\downarrow\right\rangle \mapsto f_\downarrow^\dagger\left|0\right\rangle. \tag{22}$$

$$\Gamma: \sigma^\alpha \mapsto \sum_{ab} f_a^\dagger \sigma_{ab}^\alpha f_b, \tag{23}$$

$$\begin{cases} \sigma^x \mapsto f_\uparrow^\dagger f_\downarrow + f_\downarrow^\dagger f_\uparrow, \\ \sigma^y \mapsto -\mathrm{i}\left(f_\uparrow^\dagger f_\downarrow - f_\downarrow^\dagger f_\uparrow\right), \\ \sigma^z \mapsto f_\uparrow^\dagger f_\uparrow - f_\downarrow^\dagger f_\downarrow, \\ f_\uparrow^\dagger f_\uparrow + f_\downarrow^\dagger f_\downarrow = 1. \end{cases} \tag{24}$$

指定第一种复费米子模式为 $f_\uparrow, f_\uparrow^\dagger$，第二种复费米子模式为 $f_\downarrow, f_\downarrow^\dagger$，则

在单占据子空间

$$\sum_a f_a^\dagger f_a = 1 \tag{25}$$

保持算符乘法和自旋-1/2李代数：

$$\Gamma\left(\sigma^\alpha\sigma^\beta\right) = \Gamma\left(\sigma^\alpha\right)\Gamma\left(\sigma^\beta\right), \tag{26}$$

$$\left[\sigma^\alpha, \sigma^\beta\right] = 2\mathrm{i}\varepsilon^{\alpha\beta\gamma}\sigma^\gamma, \quad \left[\Gamma\left(\sigma^\alpha\right), \Gamma\left(\sigma^\beta\right)\right] = 2\mathrm{i}\varepsilon^{\alpha\beta\gamma}\Gamma\left(\sigma^\gamma\right). \tag{27}$$

证明：

首先

$$\left[\sigma^\alpha, \sigma^\beta\right] = 2\mathrm{i}\varepsilon^{\alpha\beta\gamma}\sigma^\gamma, \quad \left\{\sigma^\alpha, \sigma^\beta\right\} = 2\delta^{\alpha\beta} I \tag{28}$$

$$\sigma^\alpha\sigma^\beta = \frac{1}{2}\left(\left[\sigma^\alpha, \sigma^\beta\right] + \left\{\sigma^\alpha, \sigma^\beta\right\}\right) = \delta^{\alpha\beta} I + \mathrm{i}\varepsilon^{\alpha\beta\gamma}\sigma^\gamma \tag{29}$$

Majorana Representation of Complex Fermion

设 $c, c^\dagger$ 分别是某种费米子模式的湮灭、产生算符，利用它们可构造出两个 Majorana 算符：

$$\gamma_1 \equiv c + c^\dagger, \quad \gamma_2 \equiv -\mathrm{i}\left(c - c^\dagger\right), \tag{30}$$

或者说复费米子算符可由 Majorana 算符表示：

$$c = \frac{1}{2}\left(\gamma_1 + \mathrm{i}\gamma_2\right), \quad c^\dagger = \frac{1}{2}\left(\gamma_1 - \mathrm{i}\gamma_2\right). \tag{31}$$

利用复费米子反对易关系

$$\left\{c, c^\dagger\right\} = 1, \quad \left\{c, c\right\} = \left\{c^\dagger, c^\dagger\right\} = 0, \tag{32}$$

可以得到 Majorana 算符反对易关系：

$$\{\gamma_1,\gamma_2\}=0,\quad \{\gamma_1,\gamma_1\}=2,\quad \{\gamma_2,\gamma_2\}=2, \tag{33}$$

或统一写为:

$$\{\gamma_i,\gamma_j\}=2\delta_{ij},\quad ij\in\{1,2\}\,. \tag{34}$$

$$\gamma_1^2=\gamma_2^2=1,\quad \gamma_1^\dagger=\gamma_1,\quad \gamma_2^\dagger=\gamma_2. \tag{35}$$

从 spin-1/2 到 2-模式复费米子再到 Majorana 费米子

$$\begin{cases}\sigma^x\mapsto f_\uparrow^\dagger f_\downarrow+f_\downarrow^\dagger f_\uparrow,\\ \sigma^y\mapsto -\mathrm{i}\left(f_\uparrow^\dagger f_\downarrow-f_\downarrow^\dagger f_\uparrow\right),\\ \sigma^z\mapsto f_\uparrow^\dagger f_\uparrow-f_\downarrow^\dagger f_\downarrow,\\ f_\uparrow^\dagger f_\uparrow+f_\downarrow^\dagger f_\downarrow=1.\end{cases} \tag{36}$$

用复费米子算符构造如下的 Majorana 算符:

$$\gamma_{\uparrow,1}=f_\uparrow+f_\uparrow^\dagger,\quad \gamma_{\uparrow,2}=-\mathrm{i}\left(f_\uparrow-f_\uparrow^\dagger\right), \tag{37}$$

$$\gamma_{\downarrow,1}=f_\downarrow+f_\downarrow^\dagger,\quad \gamma_{\downarrow,2}=-\mathrm{i}\left(f_\downarrow-f_\downarrow^\dagger\right). \tag{38}$$

可以反解出

$$f_\uparrow=\frac{1}{2}\left(\gamma_{\uparrow,1}+\mathrm{i}\gamma_{\uparrow,2}\right),\quad f_\uparrow^\dagger=\frac{1}{2}\left(\gamma_{\uparrow,1}-\mathrm{i}\gamma_{\uparrow,2}\right) \tag{39}$$

$$f_\downarrow=\frac{1}{2}\left(\gamma_{\downarrow,1}+\mathrm{i}\gamma_{\downarrow,2}\right),\quad f_\downarrow^\dagger=\frac{1}{2}\left(\gamma_{\downarrow,1}-\mathrm{i}\gamma_{\downarrow,2}\right) \tag{40}$$

则

$$\sigma^x\mapsto f_\uparrow^\dagger f_\downarrow+f_\downarrow^\dagger f_\uparrow=\mathrm{i}\gamma_{\uparrow,1}\gamma_{\downarrow,2}, \tag{41}$$

$$\sigma^y\mapsto -\mathrm{i}\left(f_\uparrow^\dagger f_\downarrow-f_\downarrow^\dagger f_\uparrow\right)=-\mathrm{i}\gamma_{\uparrow,1}\gamma_{\downarrow,1}, \tag{42}$$

$$\sigma^z\mapsto f_\uparrow^\dagger f_\uparrow-f_\downarrow^\dagger f_\downarrow=\mathrm{i}\gamma_{\uparrow,1}\gamma_{\uparrow,2}. \tag{43}$$

单占据条件 $f_\uparrow^\dagger f_\uparrow+f_\downarrow^\dagger f_\downarrow=1$ 化为:

$$\gamma_{\uparrow,1}\gamma_{\uparrow,2}\gamma_{\downarrow,1}\gamma_{\downarrow,2}=1 \tag{44}$$

若令:

$$\gamma_{\uparrow,1}=c,\quad \gamma_{\uparrow,2}=-b^z,\quad \gamma_{\downarrow,1}=b^y,\quad \gamma_{\downarrow,2}=-b^x, \tag{45}$$

则有

$$\sigma^x\mapsto \mathrm{i}b^xc, \tag{46}$$

$$\sigma^y\mapsto \mathrm{i}b^yc, \tag{47}$$

$$\sigma^z\mapsto \mathrm{i}b^zc \tag{48}$$

单占据条件化为

$$b^xb^yb^zc=1. \tag{49}$$

用 Majorana 算符表达 Kitaev Honeycomb 模型哈密顿量

Kitaev Honeycomb 哈密顿量:

$$H=K_x\sum_{\langle j,k\rangle_x}\sigma_j^x\sigma_k^x+K_y\sum_{\langle j,k\rangle_y}\sigma_j^y\sigma_k^y+K_z\sum_{\langle j,k\rangle_z}\sigma_j^z\sigma_k^z. \tag{50}$$

定义 α_{jk} 为最近邻 j,k 格点的 bond 类型，$\alpha_{ij}\in\{x,y,z\}$，则

$$H=\sum_{\langle j,k\rangle}K_{\alpha_{jk}}\sigma_j^{\alpha_{jk}}\sigma_k^{\alpha_{jk}}. \tag{51}$$

哈密顿量映射为：

$$\begin{aligned}H\mapsto\widetilde{H}&=\sum_{\langle j,k\rangle}K_{\alpha_{jk}}\left(\mathrm{i}b_j^{\alpha_{jk}}c_j\right)\left(\mathrm{i}b_k^{\alpha_{jk}}c_k\right)\\&=\mathrm{i}\sum_{\langle j,k\rangle}K_{\alpha_{jk}}\left(-\mathrm{i}b_j^{\alpha_{jk}}b_k^{\alpha_{jk}}\right)c_jc_k.\end{aligned} \tag{52}$$

为了方便数值计算，定义：

$$\hat{u}_{jk}\equiv\begin{cases}-\mathrm{i}b_j^{\alpha_{jk}}b_k^{\alpha_{jk}} & ,j\text{和}k\text{最近邻}\\0 & ,\text{其他情况}\end{cases} \tag{53}$$

则

$$\widetilde{H}=\mathrm{i}\sum_{\langle j,k\rangle}K_{\alpha_{jk}}\hat{u}_{jk}c_jc_k \tag{54}$$

考虑构型 $\{u_{jk}\}$，则

$$\widetilde{H}=\mathrm{i}\sum_{\langle j,k\rangle}K_{\alpha_{jk}}u_{jk}c_jc_k, \tag{55}$$

其中 u_{jk} 是 $\hat{u}_{jk}$ 的本征值。

把每个 unit cell 内两格点的 Majorana-c 算符组合成复费米子

首先 c_j 是 j 格点的 Majorana-c 算符。若区分 A,B 子格，用 $c_{\boldsymbol{r},\alpha}$ 表示 $\boldsymbol{r}$ unit cell 内 β 子格格点上的 Majorana-c 算符，则哈密顿量可改写为：

$$\begin{aligned}\widetilde{H}&=\mathrm{i}\sum_{\langle j,k\rangle}K_{\alpha_{jk}}u_{jk}c_jc_k\\&=\mathrm{i}\sum_{\boldsymbol{r}\in\mathrm{UC}}\left(K_xu_{\boldsymbol{r},A;\boldsymbol{r},B}c_{\boldsymbol{r},A}c_{\boldsymbol{r},B}+K_yu_{\boldsymbol{r},A;\boldsymbol{r}+\boldsymbol{a}_1,B}c_{\boldsymbol{r},A}c_{\boldsymbol{r}+\boldsymbol{a}_1,B}+K_zu_{\boldsymbol{r},A;\boldsymbol{r}+\boldsymbol{a}_2,B}c_{\boldsymbol{r},A}c_{\boldsymbol{r}+\boldsymbol{a}_2,B}\right)\\&=\mathrm{i}\sum_{\boldsymbol{r}\in\mathrm{UC}}\sum_{\boldsymbol{\delta}\in\{\boldsymbol{0},\boldsymbol{a}_1,\boldsymbol{a}_2\}}K_{\boldsymbol{\delta}}u_{\boldsymbol{r},A;\boldsymbol{r}+\boldsymbol{\delta},B}c_{\boldsymbol{r},A}c_{\boldsymbol{r}+\boldsymbol{\delta},B}.\end{aligned} \tag{56}$$

其中

$$\mathrm{UC}\equiv\{\boldsymbol{r}_1,\boldsymbol{r}_2,\cdots,\boldsymbol{r}_N\}, \tag{57}$$

$N=N_1N_2$ 为总 unit cell 数，$\boldsymbol{r}_i$ 为第 i 个元胞的位置矢量，

$$K_{\boldsymbol{\delta}}\equiv\begin{cases}K_x, & \boldsymbol{\delta}=\boldsymbol{0},\\K_y, & \boldsymbol{\delta}=\boldsymbol{a}_1,\\K_z, & \boldsymbol{\delta}=\boldsymbol{a}_2.\end{cases} \tag{58}$$

把 $\boldsymbol{r}$ unit cell 内的两个 Majorana-c 算符组合成复费米子算符：

$$a_{\boldsymbol{r}}\equiv\frac{1}{2}\left(c_{\boldsymbol{r},A}+\mathrm{i}c_{\boldsymbol{r},B}\right),\quad a_{\boldsymbol{r}}^\dagger\equiv\frac{1}{2}\left(c_{\boldsymbol{r},A}-\mathrm{i}c_{\boldsymbol{r},B}\right),\quad \boldsymbol{r}\in\mathrm{UC}, \tag{59}$$

可以反解出

$$c_{\boldsymbol{r},A}=a_{\boldsymbol{r}}+a_{\boldsymbol{r}}^{\dagger},\quad c_{\boldsymbol{r},B}=\frac{1}{\mathrm{i}}\left(a_{\boldsymbol{r}}-a_{\boldsymbol{r}}^{\dagger}\right), \tag{60}$$

则哈密顿量可表达为

$$\begin{aligned}
\widetilde{H}&=\mathrm{i}\sum_{\boldsymbol{r}\in\mathrm{UC}}\sum_{\boldsymbol{\delta}\in\{\boldsymbol{0},\boldsymbol{a}_1,\boldsymbol{a}_2\}}K_{\boldsymbol{\delta}}u_{\boldsymbol{r},A;\boldsymbol{r}+\boldsymbol{\delta},B}c_{\boldsymbol{r},A}c_{\boldsymbol{r}+\boldsymbol{\delta},B}\\
&=\mathrm{i}\sum_{\boldsymbol{r}}\sum_{\boldsymbol{\delta}}K_{\boldsymbol{\delta}}u_{\boldsymbol{r},A;\boldsymbol{r}+\boldsymbol{\delta},B}\left(a_{\boldsymbol{r}}+a_{\boldsymbol{r}}^{\dagger}\right)\cdot\frac{1}{\mathrm{i}}\left(a_{\boldsymbol{r}+\boldsymbol{\delta}}-a_{\boldsymbol{r}+\boldsymbol{\delta}}^{\dagger}\right)\\
&=\sum_{\boldsymbol{r}}\sum_{\boldsymbol{\delta}}K_{\boldsymbol{\delta}}u_{\boldsymbol{r},A;\boldsymbol{r}+\boldsymbol{\delta},B}\left(a_{\boldsymbol{r}}+a_{\boldsymbol{r}}^{\dagger}\right)\left(a_{\boldsymbol{r}+\boldsymbol{\delta}}-a_{\boldsymbol{r}+\boldsymbol{\delta}}^{\dagger}\right)\\
&=\sum_{\boldsymbol{\delta}}\sum_{\boldsymbol{r}}K_{\boldsymbol{\delta}}u_{\boldsymbol{r},A;\boldsymbol{r}+\boldsymbol{\delta},B}\left(a_{\boldsymbol{r}}+a_{\boldsymbol{r}}^{\dagger}\right)\left(a_{\boldsymbol{r}+\boldsymbol{\delta}}-a_{\boldsymbol{r}+\boldsymbol{\delta}}^{\dagger}\right)\\
&=\sum_{\boldsymbol{\delta}}\sum_{\boldsymbol{r}}\sum_{\boldsymbol{r}'\in\mathrm{UC}}\sum_{\boldsymbol{r}''\in\mathrm{UC}}\delta_{\boldsymbol{r}',\boldsymbol{r}}\delta_{\boldsymbol{r}'',\boldsymbol{r}+\boldsymbol{\delta}}K_{\boldsymbol{\delta}}u_{\boldsymbol{r},A;\boldsymbol{r}+\boldsymbol{\delta},B}\left(a_{\boldsymbol{r}'}+a_{\boldsymbol{r}'}^{\dagger}\right)\left(a_{\boldsymbol{r}''}-a_{\boldsymbol{r}''}^{\dagger}\right)\\
&=\sum_{\boldsymbol{\delta}}\sum_{\boldsymbol{r}'}\sum_{\boldsymbol{r}''}\sum_{\boldsymbol{r}}\delta_{\boldsymbol{r}',\boldsymbol{r}}\delta_{\boldsymbol{r}'',\boldsymbol{r}+\boldsymbol{\delta}}K_{\boldsymbol{\delta}}u_{\boldsymbol{r},A;\boldsymbol{r}+\boldsymbol{\delta},B}\left(a_{\boldsymbol{r}'}+a_{\boldsymbol{r}'}^{\dagger}\right)\left(a_{\boldsymbol{r}''}-a_{\boldsymbol{r}''}^{\dagger}\right)\\
&=\sum_{\boldsymbol{\delta}}\sum_{\boldsymbol{r}'}\sum_{\boldsymbol{r}''}\delta_{\boldsymbol{r}',\boldsymbol{r}''-\boldsymbol{\delta}}K_{\boldsymbol{\delta}}u_{\boldsymbol{r}',A;\boldsymbol{r}'',B}\left(a_{\boldsymbol{r}'}+a_{\boldsymbol{r}'}^{\dagger}\right)\left(a_{\boldsymbol{r}''}-a_{\boldsymbol{r}''}^{\dagger}\right)\\
&=\sum_{\boldsymbol{r}'}\sum_{\boldsymbol{r}''}\left(\sum_{\boldsymbol{\delta}}\delta_{\boldsymbol{r}',\boldsymbol{r}''-\boldsymbol{\delta}}K_{\boldsymbol{\delta}}u_{\boldsymbol{r}',A;\boldsymbol{r}'',B}\right)\left(a_{\boldsymbol{r}'}+a_{\boldsymbol{r}'}^{\dagger}\right)\left(a_{\boldsymbol{r}''}-a_{\boldsymbol{r}''}^{\dagger}\right)\\
&=\sum_{i=1}^{N}\sum_{j=1}^{N}\left(\sum_{\boldsymbol{\delta}}\delta_{\boldsymbol{r}_i,\boldsymbol{r}_j-\boldsymbol{\delta}}K_{\boldsymbol{\delta}}u_{\boldsymbol{r}_i,A;\boldsymbol{r}_j,B}\right)\left(a_i+a_i^{\dagger}\right)\left(a_j-a_j^{\dagger}\right)
\end{aligned}\tag{61}$$

令

$$t_{ij}=\sum_{\boldsymbol{\delta}\in\{\boldsymbol{0},\boldsymbol{a}_1,\boldsymbol{a}_2\}}\delta_{\boldsymbol{r}_i,\boldsymbol{r}_j-\boldsymbol{\delta}}K_{\boldsymbol{\delta}}u_{\boldsymbol{r}_i,A;\boldsymbol{r}_j,B}, \tag{62}$$

则

$$\begin{aligned}
\widetilde{H}&=\sum_{i=1}^{N}\sum_{j=1}^{N}\left(\sum_{\boldsymbol{\delta}}\delta_{\boldsymbol{r}_i,\boldsymbol{r}_j-\boldsymbol{\delta}}K_{\boldsymbol{\delta}}u_{\boldsymbol{r}_i,A;\boldsymbol{r}_j,B}\right)\left(a_i+a_i^{\dagger}\right)\left(a_j-a_j^{\dagger}\right)\\
&=\sum_{i=1}^{N}\sum_{j=1}^{N}t_{ij}\left(a_i+a_i^{\dagger}\right)\left(a_j-a_j^{\dagger}\right)\\
&=\sum_{i=1}^{N}\sum_{j=1}^{N}\left(t_{ij}a_ia_j-t_{ij}a_i^{\dagger}a_j^{\dagger}-t_{ij}a_ia_j^{\dagger}+t_{ij}a_i^{\dagger}a_j\right)
\end{aligned}\tag{63}$$

$$\begin{aligned}
\sum_{i=1}^{N}\sum_{j=1}^{N}(t_{ij})a_ia_j&=\frac{1}{2}\sum_{i=1}^{N}\sum_{j=1}^{N}(t_{ij})a_ia_j+\frac{1}{2}\sum_{i=1}^{N}\sum_{j=1}^{N}(t_{ij})a_ia_j\\
&=\frac{1}{2}\sum_{i=1}^{N}\sum_{j=1}^{N}-t_{ij}a_ja_i+\frac{1}{2}\sum_{i=1}^{N}\sum_{j=1}^{N}(t_{ij})a_ia_j\\
&=\frac{1}{2}\sum_{j=1}^{N}\sum_{i=1}^{N}-t_{ji}a_ia_j+\frac{1}{2}\sum_{i=1}^{N}\sum_{j=1}^{N}(t_{ij})a_ia_j\\
&=\frac{1}{2}\sum_{i=1}^{N}\sum_{j=1}^{N}\left(t_{ij}-t_{ji}\right)a_ia_j
\end{aligned}\tag{64}$$

$$
\begin{aligned}
\sum_{i=1}^{N}\sum_{j=1}^{N}-t_{ij}a_i^\dagger a_j^\dagger &= \frac{1}{2}\sum_{i=1}^{N}\sum_{j=1}^{N}-t_{ij}a_i^\dagger a_j^\dagger+\frac{1}{2}\sum_{i=1}^{N}\sum_{j=1}^{N}-t_{ij}a_i^\dagger a_j^\dagger \\
&= \frac{1}{2}\sum_{i=1}^{N}\sum_{j=1}^{N}t_{ij}a_j^\dagger a_i^\dagger+\frac{1}{2}\sum_{i=1}^{N}\sum_{j=1}^{N}-t_{ij}a_i^\dagger a_j^\dagger \\
&= \frac{1}{2}\sum_{j=1}^{N}\sum_{i=1}^{N}t_{ji}a_i^\dagger a_j^\dagger+\frac{1}{2}\sum_{i=1}^{N}\sum_{j=1}^{N}-t_{ij}a_i^\dagger a_j^\dagger \\
&= \frac{1}{2}\sum_{i=1}^{N}\sum_{j=1}^{N}-\left(t_{ij}-t_{ji}\right)a_i^\dagger a_j^\dagger
\end{aligned}
\tag{65}
$$

$$
\begin{aligned}
\sum_{i,j}\left(-t_{ij}a_ia_j^\dagger+t_{ij}a_i^\dagger a_j\right) &= \frac{1}{2}\sum_{i,j}\left(-t_{ij}a_ia_j^\dagger+t_{ij}a_i^\dagger a_j\right)+\frac{1}{2}\sum_{i,j}\left(-t_{ij}a_ia_j^\dagger+t_{ij}a_i^\dagger a_j\right) \\
&= \frac{1}{2}\sum_{i,j}\left[-t_{ij}\left(\delta_{ij}-a_j^\dagger a_i\right)+t_{ij}\left(\delta_{ij}-a_ja_i^\dagger\right)\right]+\frac{1}{2}\sum_{i,j}\left(-t_{ij}a_ia_j^\dagger+t_{ij}a_i^\dagger a_j\right) \\
&= \frac{1}{2}\sum_{i,j}\left(t_{ij}a_j^\dagger a_i-t_{ij}a_ja_i^\dagger\right)+\frac{1}{2}\sum_{i,j}\left(-t_{ij}a_ia_j^\dagger+t_{ij}a_i^\dagger a_j\right) \\
&= \frac{1}{2}\sum_{j,i}\left(t_{ji}a_i^\dagger a_j-t_{ji}a_ia_j^\dagger\right)+\frac{1}{2}\sum_{i,j}\left(-t_{ij}a_ia_j^\dagger+t_{ij}a_i^\dagger a_j\right) \\
&= \frac{1}{2}\sum_{i,j}\left(t_{ij}+t_{ji}\right)a_i^\dagger a_j+\frac{1}{2}\sum_{i,j}-\left(t_{ij}+t_{ji}\right)a_ia_j^\dagger
\end{aligned}
\tag{66}
$$

--- above revised

于是

$$
\begin{aligned}
\widetilde{H} &= \sum_{i=1}^{N}\sum_{j=1}^{N}\left(t_{ij}a_ia_j-t_{ij}a_i^\dagger a_j^\dagger-t_{ij}a_ia_j^\dagger+t_{ij}a_i^\dagger a_j\right) \\
&= \frac{1}{2}\sum_{i=1}^{N}\sum_{j=1}^{N}\left(t_{ij}-t_{ji}\right)a_ia_j+\frac{1}{2}\sum_{i=1}^{N}\sum_{j=1}^{N}-\left(t_{ij}-t_{ji}\right)a_i^\dagger a_j^\dagger+\frac{1}{2}\sum_{i,j}\left(t_{ij}+t_{ji}\right)a_i^\dagger a_j+\frac{1}{2}\sum_{i,j}-\left(t_{ij}+t_{ji}\right)a_ia_j^\dagger
\end{aligned}
\tag{67}
$$

设

$$
\begin{aligned}
\widetilde{H} &= \frac{1}{2}\mathbf{\Psi}^\dagger\mathbf{h}\mathbf{\Psi} \\
&= \frac{1}{2}\begin{bmatrix}a_1^\dagger & \cdots & a_N^\dagger & a_1 & \cdots & a_N\end{bmatrix}\mathbf{h}\begin{bmatrix}a_1\\ \vdots\\ a_N\\ a_1^\dagger\\ \vdots\\ a_N^\dagger\end{bmatrix} \\
&= \frac{1}{2}\begin{bmatrix}a_1^\dagger & \cdots & a_N^\dagger & a_1 & \cdots & a_N\end{bmatrix}\begin{bmatrix}\mathbf{h}_{11} & \mathbf{h}_{12}\\ \mathbf{h}_{21} & \mathbf{h}_{22}\end{bmatrix}\begin{bmatrix}a_1\\ \vdots\\ a_N\\ a_1^\dagger\\ \vdots\\ a_N^\dagger\end{bmatrix} \\
&= \frac{1}{2}\sum_{i,j}\left(\mathbf{h}_{11}\right)_{ij}a_i^\dagger a_j+\frac{1}{2}\sum_{i,j}\left(\mathbf{h}_{12}\right)_{ij}a_i^\dagger a_j^\dagger+\frac{1}{2}\sum_{i,j}\left(\mathbf{h}_{21}\right)_{ij}a_ia_j+\frac{1}{2}\sum_{i,j}\left(\mathbf{h}_{22}\right)_{ij}a_ia_j^\dagger
\end{aligned}
\tag{68}
$$

一种取法为

$$(\mathbf{h}_{11})_{ij}=t_{ij}+t_{ji} \tag{69}$$

$$(\mathbf{h}_{12})_{ij}=-\left(t_{ij}-t_{ji}\right) \tag{70}$$

$$(\mathbf{h}_{21})_{ij}=t_{ij}-t_{ji} \tag{71}$$

$$(\mathbf{h}_{22})_{ij}=-(t_{ij}+t_{ji}) \tag{72}$$

--- above revised

磁场微扰

如果考虑

$$H_{\text{eff}}^{(3)}=-\kappa\sum_{\langle j,k,l\rangle}\sigma_j^x\sigma_k^y\sigma_l^z=-\kappa\sum_{\boldsymbol{r}\in\text{UC}}\left(\text{around}A+\text{around}B\right), \tag{73}$$

$$\begin{aligned}\text{around}A&=\sigma^x_{\boldsymbol{r},A}\sigma^y_{\boldsymbol{r}+\boldsymbol{a}_1,B}\sigma^z_{\boldsymbol{r}+\boldsymbol{a}_2,B}+\sigma^x_{\boldsymbol{r},B}\sigma^y_{\boldsymbol{r},A}\sigma^z_{\boldsymbol{r}+\boldsymbol{a}_2,B}+\sigma^x_{\boldsymbol{r},B}\sigma^y_{\boldsymbol{r}+\boldsymbol{a}_1,B}\sigma^z_{\boldsymbol{r},A}\\&=-\mathrm{i}u_{\boldsymbol{r}+\boldsymbol{a}_1,B;\boldsymbol{r},A}u_{\boldsymbol{r}+\boldsymbol{a}_2,B;\boldsymbol{r},A}c_{\boldsymbol{r}+\boldsymbol{a}_1,B}c_{\boldsymbol{r}+\boldsymbol{a}_2,B}\\&-\mathrm{i}u_{\boldsymbol{r}+\boldsymbol{a}_2,B;\boldsymbol{r},A}u_{\boldsymbol{r},B;\boldsymbol{r},A}c_{\boldsymbol{r}+\boldsymbol{a}_2,B}c_{\boldsymbol{r},B}\\&-\mathrm{i}u_{\boldsymbol{r},B;\boldsymbol{r},A}u_{\boldsymbol{r}+\boldsymbol{a}_1,B;\boldsymbol{r},A}c_{\boldsymbol{r},B}c_{\boldsymbol{r}+\boldsymbol{a}_1,B}\\&=-\mathrm{i}\sum_{\substack{(\boldsymbol{\delta}_1,\boldsymbol{\delta}_2)\in\\\{(\boldsymbol{a}_1,\boldsymbol{a}_2),(\boldsymbol{a}_2,\boldsymbol{0}),(\boldsymbol{0},\boldsymbol{a}_1)\}}}u_{\boldsymbol{r}+\boldsymbol{\delta}_1,B;\boldsymbol{r},A}u_{\boldsymbol{r}+\boldsymbol{\delta}_2,B;\boldsymbol{r},A}c_{\boldsymbol{r}+\boldsymbol{\delta}_1,B}c_{\boldsymbol{r}+\boldsymbol{\delta}_2,B}\end{aligned} \tag{74}$$

$$\begin{aligned}\text{around}B&=\sigma^x_{\boldsymbol{r},B}\sigma^y_{\boldsymbol{r}-\boldsymbol{a}_1,A}\sigma^z_{\boldsymbol{r}-\boldsymbol{a}_2,A}+\sigma^x_{\boldsymbol{r},A}\sigma^y_{\boldsymbol{r},B}\sigma^z_{\boldsymbol{r}-\boldsymbol{a}_2,A}+\sigma^x_{\boldsymbol{r},A}\sigma^y_{\boldsymbol{r}-\boldsymbol{a}_1,A}\sigma^z_{\boldsymbol{r},B}\\&=\text{around}A\left(\boldsymbol{a}_1\leftrightarrow-\boldsymbol{a}_1,\boldsymbol{a}_2\leftrightarrow-\boldsymbol{a}_2,A\leftrightarrow B\right)\\&=-\mathrm{i}\sum_{\substack{\left(\boldsymbol{\delta}'_1,\boldsymbol{\delta}'_2\right)\in\\\{(-\boldsymbol{a}_1,-\boldsymbol{a}_2),(-\boldsymbol{a}_2,\boldsymbol{0}),(\boldsymbol{0},-\boldsymbol{a}_1)\}}}u_{\boldsymbol{r}+\boldsymbol{\delta}'_1,A;\boldsymbol{r},B}u_{\boldsymbol{r}+\boldsymbol{\delta}'_2,A;\boldsymbol{r},B}c_{\boldsymbol{r}+\boldsymbol{\delta}'_1,A}c_{\boldsymbol{r}+\boldsymbol{\delta}'_2,A}\end{aligned} \tag{75}$$

$$\begin{aligned}-\kappa\sum_{\boldsymbol{r}}\text{around}A&=\mathrm{i}\kappa\sum_{\boldsymbol{r}}\sum_{(\boldsymbol{\delta}_1,\boldsymbol{\delta}_2)}u_{\boldsymbol{r}+\boldsymbol{\delta}_1,B;\boldsymbol{r},A}u_{\boldsymbol{r}+\boldsymbol{\delta}_2,B;\boldsymbol{r},A}c_{\boldsymbol{r}+\boldsymbol{\delta}_1,B}c_{\boldsymbol{r}+\boldsymbol{\delta}_2,B}\\&=\mathrm{i}\kappa\sum_{(\boldsymbol{\delta}_1,\boldsymbol{\delta}_2)}\sum_{\boldsymbol{r}'}\sum_{\boldsymbol{r}''}\sum_{\boldsymbol{r}}\delta_{\boldsymbol{r}',\boldsymbol{r}+\boldsymbol{\delta}_1}\delta_{\boldsymbol{r}'',\boldsymbol{r}+\boldsymbol{\delta}_2}u_{\boldsymbol{r}',B;\boldsymbol{r},A}u_{\boldsymbol{r}'',B;\boldsymbol{r},A}c_{\boldsymbol{r}',B}c_{\boldsymbol{r}'',B}\\&=\mathrm{i}\kappa\sum_{(\boldsymbol{\delta}_1,\boldsymbol{\delta}_2)}\sum_{\boldsymbol{r}'}\sum_{\boldsymbol{r}''}\delta_{\boldsymbol{r}'-\boldsymbol{\delta}_1,\boldsymbol{r}''-\boldsymbol{\delta}_2}u_{\boldsymbol{r}',B;\boldsymbol{r}'-\boldsymbol{\delta}_1,A}u_{\boldsymbol{r}'',B;\boldsymbol{r}''-\boldsymbol{\delta}_2,A}c_{\boldsymbol{r}',B}c_{\boldsymbol{r}'',B}\\&=\mathrm{i}\kappa\sum_{\boldsymbol{r}'}\sum_{\boldsymbol{r}''}\left(\sum_{(\boldsymbol{\delta}_1,\boldsymbol{\delta}_2)}\delta_{\boldsymbol{r}'-\boldsymbol{\delta}_1,\boldsymbol{r}''-\boldsymbol{\delta}_2}u_{\boldsymbol{r}',B;\boldsymbol{r}'-\boldsymbol{\delta}_1,A}u_{\boldsymbol{r}'',B;\boldsymbol{r}''-\boldsymbol{\delta}_2,A}\right)c_{\boldsymbol{r}',B}c_{\boldsymbol{r}'',B}\\&=\mathrm{i}\kappa\sum_{i=1}^{N}\sum_{j=1}^{N}\left(\sum_{(\boldsymbol{\delta}_1,\boldsymbol{\delta}_2)}\delta_{\boldsymbol{r}_i-\boldsymbol{\delta}_1,\boldsymbol{r}_j-\boldsymbol{\delta}_2}u_{\boldsymbol{r}_i,B;\boldsymbol{r}_i-\boldsymbol{\delta}_1,A}u_{\boldsymbol{r}_j,B;\boldsymbol{r}_j-\boldsymbol{\delta}_2,A}\right)c_{i,B}c_{j,B}\end{aligned} \tag{76}$$

令

$$t_{ij}^{(+)}=\sum_{(\boldsymbol{\delta}_1,\boldsymbol{\delta}_2)}\delta_{\boldsymbol{r}_i-\boldsymbol{\delta}_1,\boldsymbol{r}_j-\boldsymbol{\delta}_2}u_{\boldsymbol{r}_i,B;\boldsymbol{r}_i-\boldsymbol{\delta}_1,A}u_{\boldsymbol{r}_j,B;\boldsymbol{r}_j-\boldsymbol{\delta}_2,A} \tag{77}$$

$$c_{\boldsymbol{r},A}=a_{\boldsymbol{r}}+a_{\boldsymbol{r}}^{\dagger},\quad c_{\boldsymbol{r},B}=\frac{1}{\mathrm{i}}\left(a_{\boldsymbol{r}}-a_{\boldsymbol{r}}^{\dagger}\right), \tag{78}$$

则

$$
\begin{aligned}
-\kappa \sum_{\boldsymbol{r}} \text{around} A &= \mathrm{i}\kappa \sum_{i=1}^{N}\sum_{j=1}^{N}\left(\sum_{(\boldsymbol{\delta}_1,\boldsymbol{\delta}_2)} \delta_{\boldsymbol{r}_i-\boldsymbol{\delta}_1,\boldsymbol{r}_j-\boldsymbol{\delta}_2} u_{\boldsymbol{r}_i,B;\boldsymbol{r}_i-\boldsymbol{\delta}_1,A} u_{\boldsymbol{r}_j,B;\boldsymbol{r}_j-\boldsymbol{\delta}_2,A}\right) c_{i,B} c_{j,B} \\
&= \mathrm{i}\kappa \sum_{i=1}^{N}\sum_{j=1}^{N} t_{ij}^{(+)} c_{i,B} c_{j,B} \\
&= -\mathrm{i}\kappa \sum_{i=1}^{N}\sum_{j=1}^{N} t_{ij}^{(+)} \left(a_i - a_i^\dagger\right)\left(a_j - a_j^\dagger\right) \\
&= -\mathrm{i}\kappa \sum_{i=1}^{N}\sum_{j=1}^{N} t_{ij}^{(+)} \left(a_i a_j + a_i^\dagger a_j^\dagger - a_i a_j^\dagger - a_i^\dagger a_j\right) \\
&= \mathrm{i}\kappa \sum_{i=1}^{N}\sum_{j=1}^{N} -\frac{\left(t_{ij}^{(+)} - t_{ji}^{(+)}\right)}{2}\left(a_i a_j + a_i^\dagger a_j^\dagger\right) + \mathrm{i}\kappa \sum_{i=1}^{N}\sum_{j=1}^{N} -\left(t_{ji}^{(+)} - t_{ij}^{(+)}\right) a_i^\dagger a_j + \mathrm{i}\kappa \sum_{i=1}^{N} t_{ii}^{(+)}
\end{aligned} \tag{79}
$$

令

$$
t_{ij}^{(-)} = \sum_{(\boldsymbol{\delta}_1',\boldsymbol{\delta}_2')} \delta_{\boldsymbol{r}_i-\boldsymbol{\delta}_1',\boldsymbol{r}_j-\boldsymbol{\delta}_2'} u_{\boldsymbol{r}_i,A;\boldsymbol{r}_i-\boldsymbol{\delta}_1',B} u_{\boldsymbol{r}_j,A;\boldsymbol{r}_j-\boldsymbol{\delta}_2',B} \tag{80}
$$

则

$$
\begin{aligned}
-\kappa \sum_{\boldsymbol{r}} \text{around} B &= \mathrm{i}\kappa \sum_{i=1}^{N}\sum_{j=1}^{N} t_{ij}^{(-)} c_{i,A} c_{j,A} \\
&= \mathrm{i}\kappa \sum_{i=1}^{N}\sum_{j=1}^{N} t_{ij}^{(-)} \left(a_i + a_i^\dagger\right)\left(a_j + a_j^\dagger\right) \\
&= \mathrm{i}\kappa \sum_{i=1}^{N}\sum_{j=1}^{N} t_{ij}^{(-)} \left(a_i a_j + a_i^\dagger a_j^\dagger + a_i a_j^\dagger + a_i^\dagger a_j\right) \\
&= \mathrm{i}\kappa \sum_{i=1}^{N}\sum_{j=1}^{N} \frac{\left(t_{ij}^{(-)} - t_{ji}^{(-)}\right)}{2}\left(a_i a_j + a_i^\dagger a_j^\dagger\right) - \mathrm{i}\kappa \sum_{i=1}^{N}\sum_{j=1}^{N} \left(t_{ji}^{(-)} - t_{ij}^{(-)}\right) a_i^\dagger a_j + \mathrm{i}\kappa \sum_{i=1}^{N} t_{ii}^{(-)}
\end{aligned} \tag{81}
$$

于是微扰哈密顿量为

$$
\begin{aligned}
\widetilde{H}_\kappa = &\frac{1}{2}\sum_{i,j} \mathrm{i}\kappa \left[\left(t_{ij}^{-} - t_{ij}^{+}\right) - \left(t_{ji}^{-} - t_{ji}^{+}\right)\right] a_i a_j \\
&+ \frac{1}{2}\sum_{i,j} \mathrm{i}\kappa \left[\left(t_{ij}^{-} - t_{ij}^{+}\right) - \left(t_{ji}^{-} - t_{ji}^{+}\right)\right] a_i^\dagger a_j^\dagger \\
&+ \frac{1}{2}\sum_{i,j} \mathrm{i}\kappa \left[\left(t_{ij}^{+} + t_{ij}^{-}\right) - \left(t_{ji}^{+} + t_{ji}^{-}\right)\right] a_i a_j^\dagger \\
&+ \frac{1}{2}\sum_{i,j} \mathrm{i}\kappa \left[\left(t_{ij}^{+} + t_{ij}^{-}\right) - \left(t_{ji}^{+} + t_{ji}^{-}\right)\right] a_i^\dagger a_j
\end{aligned} \tag{82}
$$

--- above revised

设

$$
\begin{aligned}
\widetilde{H}_{\text{eff}}^{(3)} &= \frac{1}{2}\begin{bmatrix} a_1^\dagger & \cdots & a_N^\dagger & a_1 & \cdots & a_N \end{bmatrix}\begin{bmatrix} \mathbf{h}'_{11} & \mathbf{h}'_{12} \\ \mathbf{h}'_{21} & \mathbf{h}'_{22} \end{bmatrix}\begin{bmatrix} a_1 \\ \vdots \\ a_N \\ a_1^\dagger \\ \vdots \\ a_N^\dagger \end{bmatrix} \\
&= \frac{1}{2}\sum_{i,j}\left(\mathbf{h}'_{11}\right)_{ij} a_i^\dagger a_j + \frac{1}{2}\sum_{i,j}\left(\mathbf{h}'_{12}\right)_{ij} a_i^\dagger a_j^\dagger + \frac{1}{2}\sum_{i,j}\left(\mathbf{h}'_{21}\right)_{ij} a_i a_j + \frac{1}{2}\sum_{i,j}\left(\mathbf{h}'_{22}\right)_{ij} a_i a_j^\dagger
\end{aligned} \tag{83}
$$

一种取法为

$$
(\mathbf{h}'_{11})_{ij} = \mathrm{i}\kappa\left[\left(t_{ij}^{+} + t_{ij}^{-}\right) - \left(t_{ji}^{+} + t_{ji}^{-}\right)\right] \tag{84}
$$

$$
(\mathbf{h}'_{12})_{ij} = \mathrm{i}\kappa\left[\left(t_{ij}^{-} - t_{ij}^{+}\right) - \left(t_{ji}^{-} - t_{ji}^{+}\right)\right] \tag{85}
$$

$$
(\mathbf{h}'_{21})_{ij} = \mathrm{i}\kappa\left[\left(t_{ij}^{-} - t_{ij}^{+}\right) - \left(t_{ji}^{-} - t_{ji}^{+}\right)\right] \tag{86}
$$

$$
(\mathbf{h}'_{22})_{ij} = \mathrm{i}\kappa\left[\left(t_{ij}^{+} + t_{ij}^{-}\right) - \left(t_{ji}^{+} + t_{ji}^{-}\right)\right] \tag{87}
$$

若令

$$
\Xi' = \mathbf{h}'_{11}, \quad \Delta' = \mathbf{h}'_{12} \tag{88}
$$

$$
\Xi'^\dagger = \Xi, \quad \Delta'^{\mathrm{T}} = -\Delta'^{\mathrm{T}} \tag{89}
$$

则

$$
\mathbf{h}'_{22} = -\Xi'^{\mathrm{T}} = \Xi' \tag{90}
$$

$$
\mathbf{h}'_{21} = \Delta'^\dagger = \Delta' \tag{91}
$$

则

$$
\mathbf{h}' = \begin{bmatrix} \mathbf{h}'_{11} & \mathbf{h}'_{12} \\ \mathbf{h}'_{21} & \mathbf{h}'_{22} \end{bmatrix} = \begin{bmatrix} \Xi' & \Delta' \\ \Delta' & \Xi' \end{bmatrix} \tag{92}
$$

--- above revises

计算基态宇称

已知

$$
\widetilde{H} = \frac{1}{2}\begin{bmatrix} a_1^\dagger & \cdots & a_N^\dagger & a_1 & \cdots & a_N \end{bmatrix}\begin{bmatrix} \Xi & \Delta \\ \Delta^\dagger & -\Xi^{\mathrm{T}} \end{bmatrix}\begin{bmatrix} a_1 \\ \vdots \\ a_N \\ a_1^\dagger \\ \vdots \\ a_N^\dagger \end{bmatrix} \tag{93}
$$

其中

$$
a_i \equiv \frac{1}{2}\left(c_{i,A} + \mathrm{i}c_{i,B}\right), \quad a_i^\dagger \equiv \frac{1}{2}\left(c_{i,A} - \mathrm{i}c_{i,B}\right), \tag{94}
$$

$$
c_{i,A} = a_i + a_i^\dagger, \quad c_{r,B} = \frac{1}{\mathrm{i}}\left(a_i - a_i^\dagger\right), \tag{95}
$$

设 $\widetilde{H}$ 可以写为

$$\widetilde{H}=\frac{\mathrm{i}}{2}\begin{bmatrix}c_{1,A} & c_{1,B} & \cdots & c_{N,A} & c_{N,B}\end{bmatrix}A\begin{bmatrix}c_{1,A}\\ c_{1,B}\\ \vdots\\ c_{N,A}\\ c_{N,B}\end{bmatrix}\tag{96}$$

则反对称的 A 怎么写?

设

$$\begin{bmatrix}a_1\\ \vdots\\ a_N\\ a_1^\dagger\\ \vdots\\ a_N^\dagger\end{bmatrix}=P\begin{bmatrix}a_1\\ a_1^\dagger\\ \vdots\\ a_N\\ a_N^\dagger\end{bmatrix}\tag{97}$$

则上面的矩阵方程可化为

$$\begin{cases}a_i=\sum_{j=1}^{N}\left(P_{i,2j-1}a_j+P_{i,2j}a_j^\dagger\right)\\ a_i^\dagger=\sum_{j=1}^{N}\left(P_{i+N,2j-1}a_j+P_{i+N,2j}a_j^\dagger\right)\end{cases},i=1,2,\cdots,N\tag{98}$$

因此，P 的非零矩阵元为：

$$P_{i,2i-1}=1,\quad P_{i+N,2i}=1,\quad i=1,2,\cdots,N\tag{99}$$

再设

$$\begin{bmatrix}a_1\\ a_1^\dagger\\ \vdots\\ a_N\\ a_N^\dagger\end{bmatrix}=P'\begin{bmatrix}c_{1,A}\\ c_{1,B}\\ \vdots\\ c_{N,A}\\ c_{N,B}\end{bmatrix}\tag{100}$$

注意到

$$\begin{bmatrix}a_i\\ a_i^\dagger\end{bmatrix}=\begin{bmatrix}\frac{1}{2}\left(c_{i,A}+\mathrm{i}c_{i,B}\right)\\ \frac{1}{2}\left(c_{i,A}-\mathrm{i}c_{i,B}\right)\end{bmatrix}=\frac{1}{2}\begin{bmatrix}1 & \mathrm{i}\\ 1 & -\mathrm{i}\end{bmatrix}\begin{bmatrix}c_{i,A}\\ c_{i,B}\end{bmatrix}\tag{101}$$

因此

$$P'=\bigoplus_{i=1}^{N}\frac{1}{2}\begin{bmatrix}1 & \mathrm{i}\\ 1 & -\mathrm{i}\end{bmatrix}\tag{102}$$

总的来说

$$
\begin{aligned}
\widetilde{H} &= \frac{1}{2}\begin{bmatrix} a_1^\dagger & \cdots & a_N^\dagger & a_1 & \cdots & a_N \end{bmatrix}\begin{bmatrix} \Xi & \Delta \\ \Delta^\dagger & -\Xi^\mathrm{T} \end{bmatrix}\begin{bmatrix} a_1 \\ \vdots \\ a_N \\ a_1^\dagger \\ \vdots \\ a_N^\dagger \end{bmatrix} \\
&= \frac{1}{2}\begin{bmatrix} c_{1,A} & c_{1,B} & \cdots & c_{N,A} & c_{N,B} \end{bmatrix}(PP')^\dagger h (PP')\begin{bmatrix} c_{1,A} \\ c_{1,B} \\ \vdots \\ c_{N,A} \\ c_{N,B} \end{bmatrix} \\
&= \frac{\mathrm{i}}{2}\begin{bmatrix} c_{1,A} & c_{1,B} & \cdots & c_{N,A} & c_{N,B} \end{bmatrix}\left[-\mathrm{i}(PP')^\dagger h (PP')\right]\begin{bmatrix} c_{1,A} \\ c_{1,B} \\ \vdots \\ c_{N,A} \\ c_{N,B} \end{bmatrix}
\end{aligned}
\tag{103}
$$

令

$$
A' = -\mathrm{i}(PP')^\dagger h (PP'), \tag{104}
$$

其中

$$
h = \begin{bmatrix} \Xi & \Delta \\ \Delta^\dagger & -\Xi^\mathrm{T} \end{bmatrix} \tag{105}
$$

$$
P_{i,2i-1} = 1, \quad P_{i+N,2i} = 1, \quad i = 1, 2, \cdots, N, \quad P\text{的其余矩阵元为}0 \tag{106}
$$

$$
P' = \bigoplus_{i=1}^{N} \frac{1}{2}\begin{bmatrix} 1 & \mathrm{i} \\ 1 & -\mathrm{i} \end{bmatrix} = I_N \otimes \frac{1}{2}\begin{bmatrix} 1 & \mathrm{i} \\ 1 & -\mathrm{i} \end{bmatrix} \tag{107}
$$

由 c-Majorana 反对易关系

$$
i \neq j, \quad c_i c_j = -c_j c_i \tag{108}
$$

可知

$$
\begin{aligned}
\widetilde{H} &= \frac{\mathrm{i}}{2}\mathbf{c}^\dagger A' \mathbf{c} = \frac{\mathrm{i}}{2}\sum_{i,j,i\neq j} A'_{ij} c_i c_j = \frac{\mathrm{i}}{2}\sum_{i,j,i\neq j} -A'_{ij} c_j c_i = \frac{\mathrm{i}}{2}\sum_{j,i,j\neq i} -A'_{ji} c_i c_j \\
&= \frac{\mathrm{i}}{2}\mathbf{c}^\dagger\left(-A'^\mathrm{T}\right)\mathbf{c}
\end{aligned}
\tag{109}
$$

于是

$$
\widetilde{H} = \frac{\mathrm{i}}{2}\mathbf{c}^\dagger A' \mathbf{c} = \frac{\mathrm{i}}{2}\mathbf{c}^\dagger\left[\frac{1}{2}\left(A' - A'^\mathrm{T}\right)\right]\mathbf{c} \tag{110}
$$

于是最终有

$$
A = \frac{1}{2}\left(A' - A'^\mathrm{T}\right) \tag{111}
$$

$$
\begin{aligned}
\widetilde{H} =& \frac{\mathrm{i}}{2}\begin{bmatrix}\cdots & c_{i,A} & c_{i,B} & \cdots\end{bmatrix} M \begin{bmatrix}\vdots \\ c_{i,A} \\ c_{i,B} \\ \vdots\end{bmatrix} \\
=& \frac{\mathrm{i}}{2}\sum_{i=1}^{N}\sum_{j=1}^{N}\left(M_{2i-1,2j-1}c_{i,A}c_{j,A} + M_{2i-1,2j}c_{i,A}c_{j,B} + M_{2i,2j-1}c_{i,B}c_{j,A} + M_{2i,2j}c_{i,B}c_{j,B}\right)
\end{aligned}
\tag{112}
$$

对无磁场哈密顿量，

$$
\begin{aligned}
\widetilde{H}_0 &= \frac{\mathrm{i}}{2}\sum_{i=1}^{N}\sum_{j=1}^{N}\left(2t_{ij}\right)c_{i,A}c_{j,B} \\
&= \frac{\mathrm{i}}{2}\sum_{i=1}^{N}\sum_{j=1}^{N}\left[\left(t_{ij}\right)c_{i,A}c_{j,B} - t_{ji}c_{i,B}c_{j,A}\right]
\end{aligned}
\tag{113}
$$

一种取法为

$$(M_0)_{2i-1,2j-1} = 0 \tag{114}$$

$$(M_0)_{2i-1,2j} = t_{ij} \tag{115}$$

$$(M_0)_{2i,2j-1} = -t_{ji} \tag{116}$$

$$(M_0)_{2i,2j} = 0 \tag{117}$$

对 κ 项，

$$\widetilde{H}_\kappa = \frac{\mathrm{i}}{2}\sum_{i=1}^{N}\sum_{j=1}^{N}\left[\kappa\left(t_{ij}^{+} - t_{ji}^{+}\right)c_{i,B}c_{j,B} + \kappa\left(t_{ij}^{-} - t_{ji}^{-}\right)c_{i,A}c_{j,A}\right] \tag{118}$$

M_κ 的一种取法为

$$(M_\kappa)_{2i-1,2j-1} = \kappa\left(t_{ij}^{-} - t_{ji}^{-}\right) \tag{119}$$

$$(M_\kappa)_{2i-1,2j} = 0 \tag{120}$$

$$(M_\kappa)_{2i,2j-1} = 0 \tag{121}$$

$$(M_\kappa)_{2i,2j} = \kappa\left(t_{ij}^{+} - t_{ji}^{+}\right) \tag{122}$$

总哈密顿量为

$$\widetilde{H} = \widetilde{H}_0 + \widetilde{H}_\kappa = \frac{\mathrm{i}}{2}\begin{bmatrix}\cdots & c_{i,A} & c_{i,B} & \cdots\end{bmatrix} M \begin{bmatrix}\vdots \\ c_{i,A} \\ c_{i,B} \\ \vdots\end{bmatrix} \tag{123}$$

$$M = M_0 + M_\kappa \tag{124}$$

h_{BdG} 的粒子-空穴对称性

设

$$h=\begin{bmatrix}\Xi & \Delta\\ \Delta^\dagger & -\Xi^{\mathrm{T}}\end{bmatrix}, \tag{125}$$

其中

$$\Xi^\dagger=\Xi,\quad \Delta^{\mathrm{T}}=-\Delta. \tag{126}$$

上面两式同取复共轭

$$\Xi^{\mathrm{T}}=\Xi^*,\quad \Delta^\dagger=-\Delta^*. \tag{127}$$

设 $E,(u,v)^{\mathrm{T}}$ 是 h 的一组本征解，可以证明 $-E,(v^*,u^*)^{\mathrm{T}}$ 也是 h 的一组本征解。

$$\begin{bmatrix}\Xi & \Delta\\ \Delta^\dagger & -\Xi^{\mathrm{T}}\end{bmatrix}\begin{bmatrix}u\\ v\end{bmatrix}=\begin{bmatrix}\Xi u+\Delta v\\ \Delta^\dagger u-\Xi^{\mathrm{T}}v\end{bmatrix}=E\begin{bmatrix}u\\ v\end{bmatrix} \tag{128}$$

$$\Xi u+\Delta v=Eu,\quad \Delta^\dagger u-\Xi^{\mathrm{T}}v=Ev \tag{129}$$

两边取复共轭

$$\Xi^*u^*+\Delta^*v^*=Eu^*,\quad \Delta^{\mathrm{T}}u^*-\Xi^\dagger v^*=Ev^* \tag{130}$$

也即

$$\Xi^{\mathrm{T}}u^*-\Delta^\dagger v^*=Eu^*,\quad -\Delta u^*-\Xi v^*=Ev^* \tag{131}$$

于是

$$\begin{bmatrix}\Xi & \Delta\\ \Delta^\dagger & -\Xi^{\mathrm{T}}\end{bmatrix}\begin{bmatrix}v^*\\ u^*\end{bmatrix}=\begin{bmatrix}\Xi v^*+\Delta u^*\\ \Delta^\dagger v^*-\Xi^{\mathrm{T}}u^*\end{bmatrix}=\begin{bmatrix}-Ev^*\\ -Eu^*\end{bmatrix}=-E\begin{bmatrix}v^*\\ u^*\end{bmatrix} \tag{132}$$

Bogoliubov变换与基态能量

$$\begin{aligned}\widetilde{H}&=\frac{1}{2}\begin{bmatrix}a^\dagger & a^{\mathrm{T}}\end{bmatrix}\mathbf{h}\begin{bmatrix}a\\ \left(a^\dagger\right)^{\mathrm{T}}\end{bmatrix}\\ &=\frac{1}{2}\begin{bmatrix}a^\dagger & a^{\mathrm{T}}\end{bmatrix}\mathbf{U}\mathbf{D}\mathbf{U}^\dagger\begin{bmatrix}a\\ \left(a^\dagger\right)^{\mathrm{T}}\end{bmatrix}\end{aligned} \tag{133}$$

$$\mathbf{D}=\operatorname{diag}(E_1,\cdots,E_N,-E_1,\cdots,-E_N) \tag{134}$$

$$\mathbf{U}=\begin{pmatrix}\mathbf{w} & \mathbf{v}^*\\ \mathbf{v} & \mathbf{w}^*\end{pmatrix} \tag{135}$$

$$\mathbf{w}=\begin{pmatrix}\mathbf{w}_1 & \cdots & \mathbf{w}_N\end{pmatrix} \tag{136}$$

$$\mathbf{v}=\begin{pmatrix}\mathbf{v}_1 & \cdots & \mathbf{v}_N\end{pmatrix} \tag{137}$$

$$\boldsymbol{\alpha}=\mathbf{w}^\dagger\mathbf{a}+\mathbf{v}^\dagger\left(\mathbf{a}^\dagger\right)^{\mathrm{T}} \tag{138}$$

$$\begin{aligned}\alpha_i=\left(\mathbf{w}_i\right)^\dagger\mathbf{a}+\left(\mathbf{v}_i\right)^\dagger\left(\mathbf{a}^\dagger\right)^{\mathrm{T}}=\sum_{j=1}^{N}\left[\left(\mathbf{w}_i\right)_j^*a_j+\left(\mathbf{v}_i\right)_j^*a_j^\dagger\right]\\ =\sum_{j=1}^{N}\left(w_{ji}^*a_j+v_{ji}^*a_j^\dagger\right)\end{aligned} \tag{139}$$

$$\alpha_i^\dagger=\sum_{j=1}^{N}\left(v_{ji}a_j+w_{ij}a_j^\dagger\right) \tag{140}$$

$$
\begin{aligned}
\widetilde{H} &= \frac{1}{2}\begin{pmatrix}\boldsymbol{\alpha}^{\dagger} & \boldsymbol{\alpha}^{\mathrm{T}}\end{pmatrix}\mathbf{D}\begin{pmatrix}\boldsymbol{\alpha}\\ \left(\boldsymbol{\alpha}^{\dagger}\right)^{\mathrm{T}}\end{pmatrix}\\
&= \frac{1}{2}\sum_{i=1}^{N}E_i\alpha_i^{\dagger}\alpha_i+\frac{1}{2}\sum_{i=1}^{N}\left(-E_i\right)\alpha_i\alpha_i^{\dagger}\\
&= \sum_{i=1}^{N}E_i\alpha_i^{\dagger}\alpha_i-\frac{1}{2}\sum_{i=1}^{N}E_i
\end{aligned}
\tag{141}
$$

基态能量为

$$
E_{\mathrm{GS}} = -\frac{1}{2}\sum_{i=1}^{N}E_i \tag{142}
$$

基态波函数

基态 $|\Omega\rangle$ 是 α 准粒子的真空态，满足:

$$
\alpha_i\left|\Omega\right\rangle = 0 \tag{143}
$$

也即

$$
\sum_{j=1}^{N}\left(w_{ji}^{*}a_j+v_{ji}^{*}a_j^{\dagger}\right)\left|\Omega\right\rangle = 0 \tag{144}
$$

基态形式

$$
\left|\Omega\right\rangle = \mathcal{N}\exp\left(\frac{1}{2}\sum_{i,j}f_{i,j}a_i^{\dagger}a_j^{\dagger}\right)\left|0_a\right\rangle \tag{145}
$$

其中 $|0_a\rangle$ 是 a 费米子真空态，$f_{i,j}=-f_{j,i}$

由于

$$
\left[a_i^{\dagger}a_j^{\dagger},a_k^{\dagger}a_l^{\dagger}\right] = 0 \tag{146}
$$

而

$$
[A,B]=0\Longrightarrow\exp(A+B)=\exp(A)\exp(B) \tag{147}
$$

于是

$$
\begin{aligned}
\left|\Omega\right\rangle &= \mathcal{N}\exp\left(\frac{1}{2}\sum_{i,j}f_{i,j}a_i^{\dagger}a_j^{\dagger}\right)\left|0_a\right\rangle\\
&= \mathcal{N}\prod_{i,j}\exp\left(\frac{1}{2}f_{i,j}a_i^{\dagger}a_j^{\dagger}\right)\left|0_a\right\rangle
\end{aligned}
\tag{148}
$$

注意到

$$
\begin{aligned}
\exp\left(\frac{1}{2}f_{i,j}a_i^{\dagger}a_j^{\dagger}\right)\left|0_a\right\rangle &= \sum_{k=0}^{\infty}\frac{1}{k!}\left(\frac{1}{2}f_{i,j}a_i^{\dagger}a_j^{\dagger}\right)^{k}\left|0_a\right\rangle\\
&= \left(1+\frac{1}{1!}\cdot\frac{1}{2^1}f_{i,j}a_i^{\dagger}a_j^{\dagger}+\frac{1}{2!}\cdot\frac{1}{2^2}a_i^{\dagger}a_j^{\dagger}a_i^{\dagger}a_j^{\dagger}+\cdots\right)\left|0_a\right\rangle\\
&= \left(1+\frac{1}{2}f_{i,j}a_i^{\dagger}a_j^{\dagger}\right)\left|0_a\right\rangle
\end{aligned}
\tag{149}
$$

于是

$$
\begin{aligned}
|\Omega\rangle &= \mathcal{N}\prod_{i,j}\exp\left(\frac{1}{2}f_{i,j}a_i^\dagger a_j^\dagger\right)|0_a\rangle \\
&= \mathcal{N}\prod_{i,j}\left(1+\frac{1}{2}f_{i,j}a_i^\dagger a_j^\dagger\right)|0_a\rangle
\end{aligned}
\tag{150}
$$

求基态波函数 $f_{i,j}$

$$
\alpha_i = \sum_{j=1}^{N}\left(w_{ji}^* a_j + v_{ji}^* a_j^\dagger\right)
$$

$$
|\Omega\rangle = \mathcal{N}\prod_{l,m}\left(1+\frac{1}{2}f_{l,m}a_l^\dagger a_m^\dagger\right)|0_a\rangle \tag{151}
$$

基态由

$$
\alpha_i|\Omega\rangle = 0 \tag{152}
$$

确定。

利用

$$
AB = [A,B] + BA \tag{153}
$$

$$
\left[A,\prod_i B_i\right] = \sum_k\left(\prod_{j<k}B_j\right)[A,B_k]\left(\prod_{j>k}B_j\right) \tag{154}
$$

$$
\left[1+\frac{1}{2}f_{i,j}a_i^\dagger a_j^\dagger, 1+\frac{1}{2}f_{l,m}a_l^\dagger a_m^\dagger\right] = 0 \tag{155}
$$

$$
\begin{aligned}
\left[a_j, 1+\frac{1}{2}f_{l',m'}a_{l'}^\dagger a_{m'}^\dagger\right] &= \frac{1}{2}f_{l',m'}\left[a_j, a_{l'}^\dagger a_{m'}^\dagger\right] \\
&= \frac{1}{2}f_{l',m'}\left(\left[a_j,a_{l'}^\dagger\right]a_{m'}^\dagger + a_{l'}^\dagger\left[a_j,a_{m'}^\dagger\right]\right) \\
&= \frac{1}{2}f_{l',m'}\left[\left(\left\{a_j,a_{l'}^\dagger\right\} - 2a_{l'}^\dagger a_j\right)a_{m'}^\dagger + a_{l'}^\dagger\left(\left\{a_j,a_{m'}^\dagger\right\} - 2a_{m'}^\dagger a_j\right)\right] \\
&= \frac{1}{2}f_{l',m'}\left[\left(\delta_{j,l'} - 2a_{l'}^\dagger a_j\right)a_{m'}^\dagger + a_{l'}^\dagger\left(\delta_{j,m'} - 2a_{m'}^\dagger a_j\right)\right] \\
&= \frac{1}{2}f_{l',m'}\left(\delta_{j,l'}a_{m'}^\dagger + \delta_{j,m'}a_{l'}^\dagger - 2a_{l'}^\dagger a_j a_{m'}^\dagger - 2a_{l'}^\dagger a_{m'}^\dagger a_j\right) \\
&= \frac{1}{2}f_{l',m'}\left[\delta_{j,l'}a_{m'}^\dagger + \delta_{j,m'}a_{l'}^\dagger - 2a_{l'}^\dagger\left(\delta_{j,m'} - a_{m'}^\dagger a_j\right) - 2a_{l'}^\dagger a_{m'}^\dagger a_j\right] \\
&= \frac{1}{2}f_{l',m'}\left(\delta_{j,l'}a_{m'}^\dagger - \delta_{j,m'}a_{l'}^\dagger\right)
\end{aligned}
\tag{156}
$$

$$
\left[a_{m'}^\dagger, 1+\frac{1}{2}f_{l,m}a_l^\dagger a_m^\dagger\right] = 0 \tag{157}
$$

$$
\begin{aligned}
&\frac{1}{2}f_{l',m'}\left(\delta_{j,l'}a_{m'}^\dagger - \delta_{j,m'}a_{l'}^\dagger\right)\cdot\left(1+\frac{1}{2}f_{l',m'}a_{l'}^\dagger a_{m'}^\dagger\right) \\
=&\frac{1}{2}f_{l',m'}\left(\delta_{j,l'}a_{m'}^\dagger - \delta_{j,m'}a_{l'}^\dagger\right) + \frac{1}{4}f_{l',m'}^2\left(\delta_{j,l'}a_{m'}^\dagger - \delta_{j,m'}a_{l'}^\dagger\right)a_{l'}^\dagger a_{m'}^\dagger \\
=&\frac{1}{2}f_{l',m'}\left(\delta_{j,l'}a_{m'}^\dagger - \delta_{j,m'}a_{l'}^\dagger\right)
\end{aligned}
\tag{158}
$$

有

$$
\begin{aligned}
a_j \prod_{l,m}\left(1+\frac{1}{2} f_{l,m} a_l^{\dagger} a_m^{\dagger}\right)\left|0_a\right\rangle &= \left[a_j, \prod_{l,m}\left(1+\frac{1}{2} f_{l,m} a_l^{\dagger} a_m^{\dagger}\right)\right]\left|0_a\right\rangle+\prod_{l,m}\left(1+\frac{1}{2} f_{l,m} a_l^{\dagger} a_m^{\dagger}\right) a_j\left|0_a\right\rangle \\
&= \left[a_j, \prod_{l,m}\left(1+\frac{1}{2} f_{l,m} a_l^{\dagger} a_m^{\dagger}\right)\right]\left|0_a\right\rangle \\
&= \sum_{l',m'}\left[a_j, 1+\frac{1}{2} f_{l',m'} a_{l'}^{\dagger} a_{m'}^{\dagger}\right] \prod_{(l,m)\backslash(l',m')}\left(1+\frac{1}{2} f_{l,m} a_l^{\dagger} a_m^{\dagger}\right) a_j\left|0_a\right\rangle \\
&= \sum_{l',m'} \frac{1}{2} f_{l',m'}\left(\delta_{j,l'} a_{m'}^{\dagger}-\delta_{j,m'} a_{l'}^{\dagger}\right) \prod_{(l,m)\backslash(l',m')}\left(1+\frac{1}{2} f_{l,m} a_l^{\dagger} a_m^{\dagger}\right) a_j\left|0_a\right\rangle \\
&= \sum_{l',m'} \frac{1}{2} f_{l',m'}\left(\delta_{j,l'} a_{m'}^{\dagger}-\delta_{j,m'} a_{l'}^{\dagger}\right) \cdot\left(1+\frac{1}{2} f_{l',m'} a_{l'}^{\dagger} a_{m'}^{\dagger}\right) \prod_{(l,m)\backslash(l',m')}\left(1+\frac{1}{2} f_{l,m} a_l^{\dagger} a_m^{\dagger}\right) a_j\left|0_a\right\rangle \\
&= \sum_{l',m'} \frac{1}{2} f_{l',m'}\left(\delta_{j,l'} a_{m'}^{\dagger}-\delta_{j,m'} a_{l'}^{\dagger}\right) \prod_{l,m}\left(1+\frac{1}{2} f_{l,m} a_l^{\dagger} a_m^{\dagger}\right) a_j\left|0_a\right\rangle \\
&= \left[\sum_{m'} \frac{1}{2} f_{j,m'} a_{m'}^{\dagger}-\sum_{l'} \frac{1}{2} f_{l',j} a_{l'}^{\dagger}\right] \prod_{l,m}\left(1+\frac{1}{2} f_{l,m} a_l^{\dagger} a_m^{\dagger}\right) a_j\left|0_a\right\rangle \\
&= \left[\sum_{m'} \frac{1}{2} f_{j,m'} a_{m'}^{\dagger}+\sum_{l'} \frac{1}{2} f_{j,l'} a_{l'}^{\dagger}\right] \prod_{l,m}\left(1+\frac{1}{2} f_{l,m} a_l^{\dagger} a_m^{\dagger}\right) a_j\left|0_a\right\rangle \\
&= \sum_k f_{j,k} a_k^{\dagger} \prod_{l,m}\left(1+\frac{1}{2} f_{l,m} a_l^{\dagger} a_m^{\dagger}\right) a_j\left|0_a\right\rangle
\end{aligned}
\tag{159}
$$

于是 a_j 对 $|\Omega\rangle$ 的作用为

$$
\begin{aligned}
a_j|\Omega\rangle &= \mathcal{N} a_j \prod_{l,m}\left(1+\frac{1}{2} f_{l,m} a_l^{\dagger} a_m^{\dagger}\right)\left|0_a\right\rangle \\
&= \mathcal{N} \sum_k f_{j,k} a_k^{\dagger} \prod_{l,m}\left(1+\frac{1}{2} f_{l,m} a_l^{\dagger} a_m^{\dagger}\right) a_j\left|0_a\right\rangle \\
&= \sum_k f_{j,k} a_k^{\dagger}|\Omega\rangle
\end{aligned}
\tag{160}
$$

基态由

$$
\alpha_i|\Omega\rangle=0 \tag{161}
$$

确定，也即

$$
\sum_{j=1}^N\left(w_{ji}^* a_j+v_{ji}^* a_j^{\dagger}\right)|\Omega\rangle=0 \tag{162}
$$

把 $a_j|\Omega\rangle$ 代入:

$$
\begin{aligned}
0 &= \sum_{j=1}^{N}\left(w_{ji}^{*}a_j + v_{ji}^{*}a_j^{\dagger}\right)|\Omega\rangle \\
&= \sum_{j=1}^{N}\left(w_{ji}^{*}\sum_k f_{j,k}a_k^{\dagger} + v_{ji}^{*}a_j^{\dagger}\right)|\Omega\rangle \\
&= \sum_{j=1}^{N}\left(w_{ji}^{*}\sum_k f_{j,k}a_k^{\dagger} + v_{ji}^{*}\sum_k \delta_{j,k}a_k^{\dagger}\right)|\Omega\rangle \\
&= \sum_{j=1}^{N}\left(\sum_k w_{ji}^{*}f_{j,k}a_k^{\dagger} + \sum_k v_{ji}^{*}\delta_{j,k}a_k^{\dagger}\right)|\Omega\rangle \\
&= \sum_{j=1}^{N}\sum_k\left(w_{ji}^{*}f_{j,k}a_k^{\dagger} + v_{ji}^{*}\delta_{j,k}a_k^{\dagger}\right)|\Omega\rangle \\
&= \sum_k\sum_{j=1}^{N}\left(w_{ji}^{*}f_{j,k}a_k^{\dagger} + v_{ji}^{*}\delta_{j,k}a_k^{\dagger}\right)|\Omega\rangle \\
&= \sum_k\left[\sum_{j=1}^{N}\left(w_{ji}^{*}f_{j,k} + v_{ji}^{*}\delta_{j,k}\right)\right]a_k^{\dagger}|\Omega\rangle
\end{aligned} \tag{163}
$$

因此有

$$
\sum_{j=1}^{N}\left(w_{ji}^{*}f_{j,k} + v_{ji}^{*}\delta_{j,k}\right) = 0, \quad \forall i,k \tag{164}
$$

利用 $f_{j,k}$ 的反对称性有

$$
\sum_{j=1}^{N}\left(-f_{k,j}w_{ji}^{*} + \delta_{k,j}v_{ji}^{*}\right) = 0, \quad \forall i,k \tag{165}
$$

构造 $\mathbf{f}$ 矩阵:

$$
\mathbf{f} = \begin{pmatrix} f_{1,1} & f_{1,2} & \cdots \\ f_{2,1} & \ddots & \vdots \\ \vdots & \cdots & \ddots \end{pmatrix} \tag{166}
$$

则化为

$$
-\left(\mathbf{f}\mathbf{w}^{*}\right)_{k,i} + \left(\mathbf{I}\mathbf{v}^{*}\right)_{k,i} = 0, \quad \forall i,k \tag{167}
$$

也即矩阵方程

$$
\mathbf{f}\mathbf{w}^{*} = \mathbf{v}^{*} \tag{168}
$$

于是

$$
\mathbf{f} = \mathbf{v}^{*}\left(\mathbf{w}^{*}\right)^{-1} \tag{169}
$$

求归一化系数 $\mathcal{N}$

$$
|\Omega\rangle = \mathcal{N}\exp\left(\frac{1}{2}\sum_{i,j}f_{i,j}a_i^{\dagger}a_j^{\dagger}\right)|0_a\rangle = \mathcal{N}\prod_{i,j}\left(1+\frac{1}{2}f_{i,j}a_i^{\dagger}a_j^{\dagger}\right)|0_a\rangle \tag{170}
$$

现在要求 $\mathcal{N}$.

令

$$\left|\widetilde{\Omega}\right\rangle = \prod_{i,j}\left(1+\frac{1}{2}f_{i,j}a_i^\dagger a_j^\dagger\right)|0_a\rangle \tag{171}$$

$|\Omega\rangle$ 的归一性

$$\langle\Omega\,|\,\Omega\rangle = 1 \tag{172}$$

给出

$$\mathcal{N}^2\left\langle\widetilde{\Omega}\,\middle|\,\widetilde{\Omega}\right\rangle = 1 \tag{173}$$

因此

$$\mathcal{N} = \sqrt{\frac{1}{\left\langle\widetilde{\Omega}\,\middle|\,\widetilde{\Omega}\right\rangle}} \tag{174}$$

于是只需要计算 $\left\langle\widetilde{\Omega}\,\middle|\,\widetilde{\Omega}\right\rangle$.

$$\left\langle 0_a\,\middle|\,a_{i'_{2n}}\cdots a_{i'_1}a_{i_1}^\dagger\cdots a_{i_{2n}}^\dagger\,\middle|\,0_a\right\rangle = \sum_{P\in S_{2n}}\operatorname{sgn}(P)\prod_{k=1}^{2n}\delta_{i'_k,i_{P(k)}} \tag{175}$$

$\left|\widetilde{\Omega}\right\rangle$ 的求和形式

$$\begin{aligned}\left|\widetilde{\Omega}\right\rangle &= \prod_{i,j}\left(1+\frac{1}{2}f_{i,j}a_i^\dagger a_j^\dagger\right)|0_a\rangle \\ &= \sum_{n=0}^{N}\frac{1}{2^n}\sum_{i_{\{1\to 2n\}}=1}^{N}\prod_{j=1}^{n}f_{i_{2j-1},i_{2j}}a_{i_1}^\dagger\cdots a_{i_{2n}}^\dagger|0_a\rangle\end{aligned} \tag{176}$$

$$\left\langle\widetilde{\Omega}\right| = \sum_{n'=0}^{N}\frac{1}{2^{n'}}\sum_{i'_{\{1\to 2n'\}}=1}^{N}\prod_{j'=1}^{n'}f^*_{i'_{2j'-1},i'_{2j'}}\langle 0_a|\,a_{i'_{2n'}}\cdots a_{i'_1} \tag{177}$$

内积为

$$\begin{aligned}\left\langle\widetilde{\Omega}\,\middle|\,\widetilde{\Omega}\right\rangle &= \sum_{n=0}^{N}\sum_{n'=0}^{N}\frac{1}{2^{n+n'}}\sum_{i_{\{1\to 2n\}}=1}^{N}\sum_{i'_{\{1\to 2n'\}}=1}^{N}\prod_{j=1}^{n}f_{i_{2j-1},i_{2j}}\prod_{j'=1}^{n'}f^*_{i'_{2j'-1},i'_{2j'}}\left\langle 0_a\,\middle|\,a_{i'_{2n'}}\cdots a_{i'_1}a_{i_1}^\dagger\cdots a_{i_{2n}}^\dagger\,\middle|\,0_a\right\rangle \\ &= \sum_{n=0}^{N}\frac{1}{2^{2n}}\sum_{i_{\{1\to 2n\}}=1}^{N}\sum_{i'_{\{1\to 2n\}}=1}^{N}\prod_{j=1}^{n}f_{i_{2j-1},i_{2j}}\prod_{j'=1}^{n}f^*_{i'_{2j'-1},i'_{2j'}}\left\langle 0_a\,\middle|\,a_{i'_{2n}}\cdots a_{i'_1}a_{i_1}^\dagger\cdots a_{i_{2n}}^\dagger\,\middle|\,0_a\right\rangle \\ &= \sum_{n=0}^{N}\frac{1}{2^{2n}}\sum_{i_{\{1\to 2n\}}=1}^{N}\sum_{i'_{\{1\to 2n\}}=1}^{N}\prod_{j=1}^{n}f^*_{i'_{2j-1},i'_{2j}}f_{i_{2j-1},i_{2j}}\left\langle 0_a\,\middle|\,a_{i'_{2n}}\cdots a_{i'_1}a_{i_1}^\dagger\cdots a_{i_{2n}}^\dagger\,\middle|\,0_a\right\rangle \\ &= \sum_{n=0}^{N}\frac{1}{2^{2n}}\sum_{i_{\{1\to 2n\}}=1}^{N}\sum_{P\in S_{2n}}\operatorname{sgn}(P)\prod_{j=1}^{n}f^*_{i_{P(2j-1)},i_{P(2j)}}f_{i_{2j-1},i_{2j}}\end{aligned} \tag{178}$$

$$\left\langle\widetilde{\Omega}\,\middle|\,\widetilde{\Omega}\right\rangle = \sum_{n=0}^{N}\frac{n!}{2^n}\sum_{i_1,\cdots,i_{2n}}\left(\prod_{j=1}^{n}f_{i_{2j-1},i_{2j}}\right)\operatorname{Pf}\left(M^{i_{\{1\to 2n\}}}\right) \tag{179}$$

$$M_{j,k}^{i_{\{1\to 2n\}}} = f^*_{i_j,i_k},\quad f_{i,j} = -f_{j,k},\quad f_{i,j}\text{已知} \tag{180}$$

overlap

现在已知

$$\left|\Omega_0\right\rangle = \mathcal{N}_0 \exp\left(\frac{1}{2}\sum_{i,j} f_{i,j}^{(0)} a_i^\dagger a_j^\dagger\right)|0\rangle \tag{181}$$

$$\left|\Omega_1\right\rangle = \mathcal{N}_1 \exp\left(\frac{1}{2}\sum_{i,j} f_{i,j}^{(1)} a_i^\dagger a_j^\dagger\right)|0\rangle \tag{182}$$

定义

$$\left|\widetilde{\Omega}_0\right\rangle = \exp\left(\frac{1}{2}\sum_{i,j} f_{i,j}^{(0)} a_i^\dagger a_j^\dagger\right)|0\rangle \tag{183}$$

$$\left|\widetilde{\Omega}_1\right\rangle = \exp\left(\frac{1}{2}\sum_{i,j} f_{i,j}^{(1)} a_i^\dagger a_j^\dagger\right)|0\rangle \tag{184}$$

先求 overlap

$$\left\langle\widetilde{\Omega}_0 \middle| \widetilde{\Omega}_1\right\rangle \tag{185}$$

Grassmann

费米子相干态

单模相干态：

$$|z_i\rangle \equiv \exp\left(-z_i a_i^\dagger\right)|0\rangle \tag{186}$$

$$\langle z_i| \equiv \langle 0|\exp\left(-a_i \bar{z}_i\right) \tag{187}$$

多模相干态：

$$|z\rangle \equiv \exp\left(-\sum_i z_i a_i^\dagger\right)|0\rangle \tag{188}$$

$$\langle z| \equiv \langle 0|\exp\left(-\sum_i a_i \bar{z}_i\right) \tag{189}$$

相干态是湮灭算符本征态：

$$a_i|z\rangle = z_i|z\rangle \tag{190}$$

$$\langle z| a_i^\dagger = \langle z|\bar{z}_i \tag{191}$$

相干态与真空态overlap

$$\langle 0 \mid z\rangle = 1 \tag{192}$$

$$\langle z \mid 0\rangle = 1 \tag{193}$$

费米子相干态表象完备性关系

$$\int\left(\prod_i \mathrm{d}\bar{z}_i \mathrm{d}z_i\right)\exp\left(-\sum_j \bar{z}_j z_j\right)|z\rangle\langle z| = 1 \tag{194}$$

Grassmann高斯积分

反对称矩阵 $A_{2N\times 2N}, \Theta=(\theta_1,\cdots,\theta_{2N})^\top$ 实Grassmann高斯积分:

$$\int\left(\prod_{i=1}^{2N}\mathrm{d}\theta_i\right)\exp\left(-\frac{1}{2}\Theta^\top A\Theta\right)=\mathrm{Pf}(A) \tag{195}$$

$$\int\left(\prod_{i=1}^{2N}\mathrm{d}\theta_i\right)\exp\left(\frac{1}{2}\Theta^\top A\Theta\right)=(-1)^N\mathrm{Pf}(A) \tag{196}$$

$A_{N\times N}, \Theta=(\theta_1,\cdots,\theta_N)^\top, \bar{\Theta}=(\bar{\theta}_1,\cdots,\bar{\theta}_N)^\top$ 复Grassmann高斯积分:

$$\int\left(\prod_i \mathrm{d}\bar{\theta}_i\mathrm{d}\theta_i\right)\exp\left(-\bar{\Theta}^\top A\Theta\right)=\det(A) \tag{197}$$

复Grassmann数高斯积分更一般形式:

在费米子相干态表象计算overlap

$$\left|\tilde{\Omega}_1\right\rangle=\exp\left(\frac{1}{2}\sum_{i,j}f_{i,j}^{(1)}a_i^\dagger a_j^\dagger\right)|0\rangle\,,\quad f_{i,j}^{(1)}=-f_{j,i}^{(1)} \tag{198}$$

$$\left|\tilde{\Omega}_2\right\rangle=\exp\left(\frac{1}{2}\sum_{i,j}f_{i,j}^{(2)}a_i^\dagger a_j^\dagger\right)|0\rangle\,,\quad f_{i,j}^{(2)}=-f_{j,i}^{(2)} \tag{199}$$

$$\begin{aligned}
\left\langle\widetilde{\Omega}_1\middle|\widetilde{\Omega}_2\right\rangle&=\int\left(\prod_i\mathrm{d}\bar{z}_i\mathrm{d}z_i\right)\exp\left(-\sum_j\bar{z}_jz_j\right)\left\langle\widetilde{\Omega}_1\middle|z\right\rangle\left\langle z\middle|\widetilde{\Omega}_2\right\rangle\\
&=\int\mathrm{d}(\bar{z},z)\exp\left(-\bar{z}^\top z\right)\left\langle 0\middle|\exp\left(\frac{1}{2}\sum_{i,j}f_{i,j}^{(1)*}a_ja_i\right)\middle|z\right\rangle\left\langle z\middle|\exp\left(\frac{1}{2}\sum_{i,j}f_{i,j}^{(2)}a_i^\dagger a_j^\dagger\right)\middle|0\right\rangle\\
&=\int\mathrm{d}(\bar{z},z)\exp\left(-\bar{z}^\top z\right)\exp\left(\frac{1}{2}\sum_{i,j}f_{i,j}^{(1)*}z_jz_i\right)\exp\left(\frac{1}{2}\sum_{i,j}f_{i,j}^{(2)}\bar{z}_i\bar{z}_j\right)\langle 0\,|\,z\rangle\,\langle z\,|\,0\rangle\\
&=\int\mathrm{d}(\bar{z},z)\exp\left(-\bar{z}^\top z\right)\exp\left(-\frac{1}{2}\sum_{i,j}f_{i,j}^{(1)*}z_iz_j\right)\exp\left(\frac{1}{2}\sum_{i,j}f_{i,j}^{(2)}\bar{z}_i\bar{z}_j\right)\\
&=\int\mathrm{d}(\bar{z},z)\exp\left(-\bar{z}^\top z\right)\exp\left(-\frac{1}{2}z^\top f^{(1)*}z\right)\exp\left(\frac{1}{2}\bar{z}^\top f^{(2)}\bar{z}\right)
\end{aligned} \tag{200}$$

为了用实Grassmann高斯积分的结果，构造

$$Z\equiv(\bar{z}_1,\cdots,\bar{z}_N,z_1,\cdots,z_N)^\top \tag{201}$$

从

$$\bar{z}_1,z_1,\bar{z}_2,z_2,\cdots,\bar{z}_N,z_N \tag{202}$$

到

$$\bar{z}_1,\cdots,\bar{z}_N,z_1,\cdots,z_N \tag{203}$$

共需要多少次最近邻交换?

以

$$\bar{z}_1\bar{z}_2\cdots\bar{z}_Nz_1z_2\cdots z_N \tag{204}$$

为正序，则逆序对数量为

$$(N-1)+(N-2)+\cdots+1=\frac{N(N-1)}{2} \tag{205}$$

因此

$$\begin{aligned}
\mathrm{d}(\bar{z},z) \equiv \prod_i \mathrm{d}\bar{z}_i \mathrm{d}z_i &= (\mathrm{d}\bar{z}_1 \mathrm{d}z_1)\cdots(\mathrm{d}\bar{z}_N \mathrm{d}z_N) \\
&= (-1)^{N(N-1)/2}\, \mathrm{d}\bar{z}_1 \cdots \mathrm{d}\bar{z}_N \mathrm{d}z_1 \mathrm{d}z_N \\
&= (-1)^{N(N-1)/2} \left(\prod_i \mathrm{d}\bar{z}_i\right) \left(\prod_j \mathrm{d}z_j\right) \\
&= (-1)^{N(N-1)/2} \prod_{i=1}^{2N} \mathrm{d}Z_i
\end{aligned} \tag{206}$$

而

$$\begin{aligned}
&\exp\left(-\bar{z}^\top z\right)\exp\left(-\frac{1}{2}z^\top f^{(1)*}z\right)\exp\left(\frac{1}{2}\bar{z}^\top f^{(2)}\bar{z}\right) \\
=&\exp\left(-\bar{z}^\top z-\frac{1}{2}z^\top f^{(1)*}z+\frac{1}{2}\bar{z}^\top f^{(2)}\bar{z}\right) \\
=&\exp\left(-\frac{1}{2}\bar{z}^\top z-\frac{1}{2}\bar{z}^\top z-\frac{1}{2}z^\top f^{(1)*}z+\frac{1}{2}\bar{z}^\top f^{(2)}\bar{z}\right) \\
=&\exp\left(-\frac{1}{2}\bar{z}^\top z+\frac{1}{2}z^\top \bar{z}-\frac{1}{2}z^\top f^{(1)*}z+\frac{1}{2}\bar{z}^\top f^{(2)}\bar{z}\right)
\end{aligned} \tag{207}$$

$$\begin{aligned}
-\frac{1}{2}\bar{z}^\top z+\frac{1}{2}z^\top \bar{z}-\frac{1}{2}z^\top f^{(1)*}z+\frac{1}{2}\bar{z}^\top f^{(2)}\bar{z} &= \frac{1}{2}\begin{pmatrix}\bar{z}^\top & z^\top\end{pmatrix}\begin{pmatrix} f^{(2)} & -I \\ I & -f^{(1)*}\end{pmatrix}\begin{pmatrix}\bar{z} \\ z\end{pmatrix} \\
&= \frac{1}{2}Z^\top M Z
\end{aligned} \tag{208}$$

$$M_{i,j}=-M_{j,i} \tag{209}$$

于是

$$\begin{aligned}
\left\langle \widetilde{\Omega}_1 \middle| \widetilde{\Omega}_2 \right\rangle &= \int \mathrm{d}\left(\bar{z},z\right)\exp\left(-\bar{z}^\top z\right)\exp\left(-\frac{1}{2}z^\top f^{(1)*}z\right)\exp\left(\frac{1}{2}\bar{z}^\top f^{(2)}\bar{z}\right) \\
&= (-1)^{N(N-1)/2}\int\prod_{i=1}^{2N}\mathrm{d}Z_i \exp\left(\frac{1}{2}Z^\top M Z\right) \\
&= (-1)^{N(N-1)/2}\int\prod_{i=1}^{2N}\mathrm{d}Z_i \exp\left(-\frac{1}{2}Z^\top\left(-M\right)Z\right) \\
&= (-1)^{N(N-1)/2}\,\mathrm{Pf}(-M) \\
&= (-1)^{N(N-1)/2}\cdot(-1)^N \mathrm{Pf}(M) \\
&= (-1)^{N(N+1)/2}\,\mathrm{Pf}(M)
\end{aligned} \tag{210}$$

Pf的基本性质

$$A^\top=-A \tag{211}$$

与行列式关系

$$\mathrm{Pf}^2(A)=\det(A) \tag{212}$$

块对角矩阵的Pf

若

$$A=\begin{pmatrix} A_1 & 0 \\ 0 & A_2 \end{pmatrix} \tag{213}$$

则

$$\mathrm{Pf}(A)=\mathrm{Pf}(A_1)\mathrm{Pf}(A_2) \tag{214}$$

正交变换

若 $O \in \mathrm{O}(2N)$，则

$$\mathrm{Pf}\left(OAO^{\top}\right)=\det(O)\mathrm{Pf}(A) \tag{215}$$

$$\mathrm{Pf}(A)=\frac{1}{\det(O)}\mathrm{Pf}\left(OAO^{\top}\right), \quad O \in \mathrm{O}(2N) \tag{216}$$

归一化系数$\mathcal{N}$

特别地，

$$\left\langle\widetilde{\Omega}_1 \middle| \widetilde{\Omega}_1\right\rangle=(-1)^{N(N+1)/2}\,\mathrm{Pf}\begin{pmatrix} f^{(1)} & -I \\ I & -f^{(1)*} \end{pmatrix} \tag{217}$$

令

$$M=\begin{pmatrix} f^{(1)} & -I \\ I & -f^{(1)*} \end{pmatrix}, \tag{218}$$

$$\begin{aligned} \left\langle\widetilde{\Omega}_1 \middle| \widetilde{\Omega}_1\right\rangle^2 &=(-1)^{N(N+1)}\,\mathrm{Pf}^2(M) \\ &=(-1)^{N(N+1)}\det(M) \end{aligned} \tag{219}$$

利用

$$\det\begin{pmatrix} A & B \\ C & D \end{pmatrix}=\det(A)\det\left(D-CA^{-1}B\right) \tag{220}$$

可得

$$\begin{aligned} \left\langle\widetilde{\Omega}_1 \middle| \widetilde{\Omega}_1\right\rangle^2 &=(-1)^{N(N+1)}\det(M) \\ &=(-1)^{N(N+1)}\det\left(f^{(1)}\right)\det\left(-f^{(1)*}-I\left(f^{(1)}\right)^{-1}(-I)\right) \\ &=(-1)^{N(N+1)}\det\left(I-f^{(1)}f^{(1)*}\right) \\ &=(-1)^{N(N+1)}\det\left(\left(I-f^{(1)}f^{(1)*}\right)^{\top}\right) \\ &=(-1)^{N(N+1)}\det\left(I-f^{(1)*}f^{(1)}\right) \\ &=(-1)^{N(N+1)}\det\left(I+f^{(1)\dagger}f^{(1)}\right) \\ &=\det\left(I+f^{(1)\dagger}f^{(1)}\right) \end{aligned} \tag{221}$$

由归一化条件

$$1=\mathcal{N}_1^2\left\langle\widetilde{\Omega}_1 \middle| \widetilde{\Omega}_1\right\rangle \tag{222}$$

归一化系数 $\mathcal{N}_1$ 可以取为

$$\mathrm{Pf}(I+f^{\dagger}f), \quad f^{\top}=-f \tag{223}$$

两点关联函数

用Grassmann积分表达 $\left\langle\Psi_1\,\middle|\,F\left(a,a^{\dagger}\right)\,\middle|\,\Psi_2\right\rangle$

构造

$$\tilde{z}\equiv\left(\bar{z}_1,\cdots,\bar{z}_N,z_1,\cdots,z_N\right)^{\top}, \tag{224}$$

完备性关系

$$\int\left(\prod_i \mathrm{d}\bar{z}_i\mathrm{d}z_i\right)\exp\left(-\sum_j\bar{z}_jz_j\right)|z\rangle\langle z|=1 \tag{225}$$

可化为

$$(-1)^{N(N-1)/2}\int\left(\prod_{i=1}^{2N}\mathrm{d}\tilde{z}_i\right)\exp\left(-\sum_j\bar{z}_iz_j\right)|z\rangle\langle z|=1 \tag{226}$$

$\left\langle\Psi_1\,\middle|\,a_la_m\,\middle|\,\Psi_2\right\rangle$

$$\begin{aligned}
&\left\langle\Psi_1\,\middle|\,a_la_m\,\middle|\,\Psi_2\right\rangle\\
=&\left\langle\Psi_1\,\middle|\,a_la_m1\,\middle|\,\Psi_2\right\rangle\\
=&(-1)^{N(N+1)/2}\int\left(\prod_{i=1}^{2N}\mathrm{d}\tilde{z}_i\right)\exp\left(-\sum_j\bar{z}_jz_j\right)\left\langle\Psi_1\,\middle|\,a_la_m\,\middle|\,z\right\rangle\left\langle z\,\middle|\,\Psi_2\right\rangle\\
=&(-1)^{N(N+1)/2}\int\left(\prod_{i=1}^{2N}\mathrm{d}\tilde{z}_i\right)\exp\left(-\sum_j\bar{z}_jz_j\right)\left\langle\Psi_1\,\middle|\,a_la_m\,\middle|\,z\right\rangle\left\langle z\,\middle|\,\Psi_2\right\rangle\\
=&(-1)^{N(N+1)/2}\mathcal{N}_1^*\mathcal{N}_2\int\left(\prod_{i=1}^{2N}\mathrm{d}\tilde{z}_i\right)\exp\left(-\sum_j\bar{z}_jz_j\right)\left\langle 0\,\middle|\,\exp\left(\frac{1}{2}\sum_{i,j}f_{i,j}^{(1)*}a_ja_i\right)\,\middle|\,a_la_m\,\middle|\,z\right\rangle\left\langle z\,\middle|\,\exp\left(\frac{1}{2}\sum_{i,j}f_{i,j}^{(2)}a_i^{\dagger}a_j^{\dagger}\right)\,\middle|\,0\right\rangle\\
=&(-1)^{N(N+1)/2}\mathcal{N}_1^*\mathcal{N}_2\int\left(\prod_{i=1}^{2N}\mathrm{d}\tilde{z}_i\right)\exp\left(-\sum_j\bar{z}_jz_j\right)\exp\left(\frac{1}{2}\sum_{i,j}f_{i,j}^{(1)*}z_jz_i\right)z_lz_m\exp\left(\frac{1}{2}\sum_{i,j}f_{i,j}^{(2)}\bar{z}_i\bar{z}_j\right)\langle 0\,|\,z\rangle\langle z\,|\,0\rangle\\
=&(-1)^{N(N+1)/2}\mathcal{N}_1^*\mathcal{N}_2\int\left(\prod_{i=1}^{2N}\mathrm{d}\tilde{z}_i\right)z_lz_m\exp\left(-\sum_j\bar{z}_jz_j\right)\exp\left(-\frac{1}{2}\sum_{i,j}f_{i,j}^{(1)*}z_iz_j\right)\exp\left(\frac{1}{2}\sum_{i,j}f_{i,j}^{(2)}\bar{z}_i\bar{z}_j\right)\\
=&(-1)^{N(N+1)/2}\mathcal{N}_1^*\mathcal{N}_2\int\left(\prod_{i=1}^{2N}\mathrm{d}\tilde{z}_i\right)z_lz_m\exp\left(\frac{1}{2}\begin{pmatrix}\bar{z} & z\end{pmatrix}\begin{pmatrix}f^{(2)} & -I\\ I & -f^{(1)*}\end{pmatrix}\begin{pmatrix}\bar{z}\\ z\end{pmatrix}\right)\\
=&(-1)^{N(N+1)/2}\mathcal{N}_1^*\mathcal{N}_2\int\left(\prod_{i=1}^{2N}\mathrm{d}\tilde{z}_i\right)z_lz_m\exp\left(\frac{1}{2}\tilde{z}^{\top}M\tilde{z}\right)
\end{aligned} \tag{227}$$

其中

$$M\equiv\begin{pmatrix}f^{(2)} & -I\\ I & -f^{(1)*}\end{pmatrix} \tag{228}$$

$\left\langle \Psi_1 \,\middle|\, a_l a_m^\dagger \,\middle|\, \Psi_2 \right\rangle$

$$
\begin{aligned}
&\left\langle \Psi_1 \,\middle|\, a_l a_m^\dagger \,\middle|\, \Psi_2 \right\rangle \\
=&\left\langle \Psi_1 \,\middle|\, a_l 1 a_m^\dagger \,\middle|\, \Psi_2 \right\rangle \\
=&(-1)^{N(N+1)/2}\mathcal{N}_1^*\mathcal{N}_2 \int \left(\prod_{i=1}^{2N}\mathrm{d}\tilde{z}_i\right)\exp\left(-\sum_j \bar{z}_j z_j\right)\left\langle 0 \,\middle|\, \exp\left(\frac{1}{2}\sum_{i,j} f_{i,j}^{(1)*} a_j a_i\right) \,\middle|\, a_l \,\middle|\, z \right\rangle \left\langle z \,\middle|\, a_m^\dagger \exp\left(\frac{1}{2}\sum_{i,j} f_{i,j}^{(2)} a_i^\dagger a_j^\dagger\right) \,\middle|\, 0 \right\rangle \\
=&(-1)^{N(N+1)/2}\mathcal{N}_1^*\mathcal{N}_2 \int \left(\prod_{i=1}^{2N}\mathrm{d}\tilde{z}_i\right) z_l \bar{z}_m \exp\left(\frac{1}{2}\tilde{z}^\top M \tilde{z}\right)
\end{aligned}
\tag{229}
$$

$\left\langle \Psi_1 \,\middle|\, a_l^\dagger a_m \,\middle|\, \Psi_2 \right\rangle$

$$
\begin{aligned}
\left\langle \Psi_1 \,\middle|\, a_l^\dagger a_m \,\middle|\, \Psi_2 \right\rangle &= \left\langle \Psi_1 \,\middle|\, \left(\delta_{l,m} - a_m a_l^\dagger\right) \,\middle|\, \Psi_2 \right\rangle \\
&= (-1)^{N(N+1)/2}\mathcal{N}_1^*\mathcal{N}_2 \int \left(\prod_{i=1}^{2N}\mathrm{d}\tilde{z}_i\right)(\delta_{l,m} - z_m\bar{z}_l)\exp\left(\frac{1}{2}\tilde{z}^\top M \tilde{z}\right) \\
(l \neq m) &= (-1)^{N(N+1)/2}\mathcal{N}_1^*\mathcal{N}_2 \int \left(\prod_{i=1}^{2N}\mathrm{d}\tilde{z}_i\right)\bar{z}_l z_m \exp\left(\frac{1}{2}\tilde{z}^\top M \tilde{z}\right)
\end{aligned}
\tag{230}
$$

$\left\langle \Psi_1 \,\middle|\, a_l^\dagger a_m^\dagger \,\middle|\, \Psi_2 \right\rangle$

$$
\begin{aligned}
\left\langle \Psi_1 \,\middle|\, a_l^\dagger a_m^\dagger \,\middle|\, \Psi_2 \right\rangle &= \left\langle \Psi_1 \,\middle|\, 1 a_l^\dagger a_m^\dagger \,\middle|\, \Psi_2 \right\rangle \\
&= (-1)^{N(N+1)/2}\mathcal{N}_1^*\mathcal{N}_2 \int \left(\prod_{i=1}^{2N}\mathrm{d}\tilde{z}_i\right)\bar{z}_l \bar{z}_m \exp\left(\frac{1}{2}\tilde{z}^\top M \tilde{z}\right)
\end{aligned}
\tag{231}
$$

如果定义

$$
\tilde{a} \equiv \left(a_1, \cdots, a_N, a_1^\dagger, \cdots, a_N^\dagger\right)^\top,
\tag{232}
$$

则

- $1 \leqslant i \leqslant N, 1 \leqslant j \leqslant N$

$$
\begin{aligned}
\langle \Psi_1 \,|\, \tilde{a}_i \tilde{a}_j \,|\, \Psi_2 \rangle &= \langle \Psi_1 \,|\, a_i a_j \,|\, \Psi_2 \rangle \\
&= (-1)^{N(N+1)/2}\mathcal{N}_1^*\mathcal{N}_2 \int \left(\prod_{i=1}^{2N}\mathrm{d}\tilde{z}_i\right) z_i z_j \exp\left(\frac{1}{2}\tilde{z}^\top M \tilde{z}\right) \\
&= (-1)^{N(N+1)/2}\mathcal{N}_1^*\mathcal{N}_2 \int \left(\prod_{i=1}^{2N}\mathrm{d}\tilde{z}_i\right) \tilde{z}_{i+N} \tilde{z}_{j+N} \exp\left(\frac{1}{2}\tilde{z}^\top M \tilde{z}\right)
\end{aligned}
\tag{233}
$$

- $1 \leqslant i \leqslant N, N+1 \leqslant j \leqslant 2N$

$$
\begin{aligned}
\langle \Psi_1 \,|\, \tilde{a}_i \tilde{a}_j \,|\, \Psi_2 \rangle &= \left\langle \Psi_1 \,\middle|\, a_i a_{j-N}^\dagger \,\middle|\, \Psi_2 \right\rangle \\
&= (-1)^{N(N+1)/2}\mathcal{N}_1^*\mathcal{N}_2 \int \left(\prod_{i=1}^{2N}\mathrm{d}\tilde{z}_i\right) z_i \bar{z}_{j-N} \exp\left(\frac{1}{2}\tilde{z}^\top M \tilde{z}\right) \\
&= (-1)^{N(N+1)/2}\mathcal{N}_1^*\mathcal{N}_2 \int \left(\prod_{i=1}^{2N}\mathrm{d}\tilde{z}_i\right) \tilde{z}_{i+N} \tilde{z}_{j-N} \exp\left(\frac{1}{2}\tilde{z}^\top M \tilde{z}\right)
\end{aligned}
\tag{234}
$$

- $N+1 \leqslant i \leqslant 2N, 1 \leqslant j \leqslant N, i-N \neq j$

$$
\begin{aligned}
\langle\Psi_1\,|\,\tilde a_i\tilde a_j\,|\,\Psi_2\rangle &= \left\langle\Psi_1\,\middle|\,a_{i-N}^\dagger a_j\,\middle|\,\Psi_2\right\rangle \\
&= (-1)^{N(N+1)/2}\mathcal{N}_1^*\mathcal{N}_2\int\left(\prod_{i=1}^{2N}\mathrm{d}\tilde z_i\right)\bar z_{i-N}z_j\exp\left(\frac{1}{2}\tilde z^\top M\tilde z\right) \\
&= (-1)^{N(N+1)/2}\mathcal{N}_1^*\mathcal{N}_2\int\left(\prod_{i=1}^{2N}\mathrm{d}\tilde z_i\right)\tilde z_{i-N}\tilde z_{j+N}\exp\left(\frac{1}{2}\tilde z^\top M\tilde z\right)
\end{aligned}
\tag{235}
$$

- $N+1\leqslant i\leqslant 2N, N+1\leqslant j\leqslant 2N$

$$
\begin{aligned}
\langle\Psi_1\,|\,\tilde a_i\tilde a_j\,|\,\Psi_2\rangle &= \left\langle\Psi_1\,\middle|\,a_{i-N}^\dagger a_{j-N}^\dagger\,\middle|\,\Psi_2\right\rangle \\
&= (-1)^{N(N+1)/2}\mathcal{N}_1^*\mathcal{N}_2\int\left(\prod_{i=1}^{2N}\mathrm{d}\tilde z_i\right)\bar z_{i-N}\bar z_{j-N}\exp\left(\frac{1}{2}\tilde z^\top M\tilde z\right) \\
&= (-1)^{N(N+1)/2}\mathcal{N}_1^*\mathcal{N}_2\int\left(\prod_{i=1}^{2N}\mathrm{d}\tilde z_i\right)\tilde z_{i-N}\tilde z_{j-N}\exp\left(\frac{1}{2}\tilde z^\top M\tilde z\right)
\end{aligned}
\tag{236}
$$

计算 $\exp$ 前有Grassmann数的积分

现在要计算形如

$$
\int\left(\prod_{i=1}^{2N}\mathrm{d}\tilde z_i\right)\tilde z_l\tilde z_m\exp\left(\frac{1}{2}\tilde z^\top M\tilde z\right)
\tag{237}
$$

的积分。

根据

$$
\int\left(\prod_i\mathrm{d}\theta_i\right)\exp\left(\frac{1}{2}\Theta^\top A\Theta\right)\exp\left(\eta^\top\Theta\right) = \mathrm{Pf}(A)\exp\left(\frac{1}{2}\eta^\top A^{-1}\eta\right)
\tag{238}
$$

两边同时求偏导 $\partial^2/\partial\eta_m\partial\eta_l$，左边：

$$
\begin{aligned}
\mathrm{LHS} &= \frac{\partial^2}{\partial\eta_m\partial\eta_l}\int\left(\prod_i\mathrm{d}\theta_i\right)\exp\left(\frac{1}{2}\Theta^\top A\Theta\right)\exp\left(\eta^\top\Theta\right) \\
&= \int\left(\prod_i\mathrm{d}\theta_i\right)\exp\left(\frac{1}{2}\Theta^\top A\Theta\right)\frac{\partial^2}{\partial\eta_m\partial\eta_l}\exp\left(\eta^\top\Theta\right) \\
&= \int\left(\prod_i\mathrm{d}\theta_i\right)\exp\left(\frac{1}{2}\Theta^\top A\Theta\right)(-\theta_l\theta_m)\exp\left(\eta^\top\Theta\right)
\end{aligned}
\tag{239}
$$

右边：

$$
\begin{aligned}
\mathrm{RHS} &= \frac{\partial^2}{\partial\eta_m\partial\eta_l}\mathrm{Pf}(A)\exp\left(\frac{1}{2}\eta^\top A^{-1}\eta\right) \\
&= \mathrm{Pf}(A)\frac{\partial^2}{\partial\eta_m\partial\eta_l}\exp\left(\frac{1}{2}\sum_{i,j}\left(A^{-1}\right)_{ij}\eta_i\eta_j\right) \\
&= \mathrm{Pf}(A)\left(A^{-1}\right)_{l,m}\exp\left(\frac{1}{2}\eta^\top A^{-1}\eta\right)
\end{aligned}
\tag{240}
$$

于是

$$
\int\left(\prod_i\mathrm{d}\theta_i\right)\exp\left(\frac{1}{2}\Theta^\top A\Theta\right)(-\theta_l\theta_m)\exp\left(\eta^\top\Theta\right) = \mathrm{Pf}(A)\left(A^{-1}\right)_{l,m}\exp\left(\frac{1}{2}\eta^\top A^{-1}\eta\right)
\tag{241}
$$

对比两边关于 η 的零次项，得

$$\int\left(\prod_i \mathrm{d}\theta_i\right)\exp\left(\frac{1}{2}\Theta^\top A\Theta\right)(-\theta_l\theta_m)=\operatorname{Pf}(A)\left(A^{-1}\right)_{l,m} \tag{242}$$

也即

$$\int\left(\prod_i \mathrm{d}\theta_i\right)\theta_l\theta_m\exp\left(\frac{1}{2}\Theta^\top A\Theta\right)=\operatorname{Pf}(A)(-1)\left(A^{-1}\right)_{l,m} \tag{243}$$

$$\langle\Psi_1\,|\,\mathrm{i}c_{i,A}c_{j,B}\,|\,\Psi_2\rangle=\left[\mathcal{N}_1^*\mathcal{N}_2(-1)^{N(N+1)/2}\operatorname{Pf}(M)\right]\left[-\left(M^{-1}\right)_{i+N,j+N}+\left(M^{-1}\right)_{i+N,j}-\left(M^{-1}\right)_{i,j+N}+\left(M^{-1}\right)_{i,j}\right] \tag{244}$$

$$\langle\Psi_1\,|\,c_{i,B}c_{j,B}\,|\,\Psi_2\rangle=\left[\mathcal{N}_1^*\mathcal{N}_2(-1)^{N(N+1)/2}\operatorname{Pf}(M)\right]\left[\left(M^{-1}\right)_{i+N,j+N}-\left(M^{-1}\right)_{i+N,j}-\left(M^{-1}\right)_{i,j+N}+\left(M^{-1}\right)_{i,j}\right] \tag{245}$$

- $1\leqslant i\leqslant N, 1\leqslant j\leqslant N$

$$\begin{aligned}\langle\Psi_1\,|\,\tilde{a}_i\tilde{a}_j\,|\,\Psi_2\rangle&=\langle\Psi_1\,|\,a_ia_j\,|\,\Psi_2\rangle\\&=(-1)^{N(N+1)/2}\mathcal{N}_1^*\mathcal{N}_2\int\left(\prod_{i=1}^{2N}\mathrm{d}\tilde{z}_i\right)\tilde{z}_{i+N}\tilde{z}_{j+N}\exp\left(\frac{1}{2}\tilde{z}^\top M\tilde{z}\right)\\&=(-1)^{N(N+1)/2}\mathcal{N}_1^*\mathcal{N}_2\operatorname{Pf}(M)(-1)\left(M^{-1}\right)_{i+N,j+N}\end{aligned} \tag{246}$$

- $1\leqslant i\leqslant N, N+1\leqslant j\leqslant 2N$

$$\begin{aligned}\langle\Psi_1\,|\,\tilde{a}_i\tilde{a}_j\,|\,\Psi_2\rangle&=\left\langle\Psi_1\,\middle|\,a_ia_{j-N}^\dagger\,\middle|\,\Psi_2\right\rangle\\&=(-1)^{N(N+1)/2}\mathcal{N}_1^*\mathcal{N}_2\int\left(\prod_{i=1}^{2N}\mathrm{d}\tilde{z}_i\right)\tilde{z}_{i+N}\tilde{z}_{j-N}\exp\left(\frac{1}{2}\tilde{z}^\top M\tilde{z}\right)\\&=(-1)^{N(N+1)/2}\mathcal{N}_1^*\mathcal{N}_2\operatorname{Pf}(M)(-1)\left(M^{-1}\right)_{i+N,j-N}\end{aligned} \tag{247}$$

- $N+1\leqslant i\leqslant 2N, 1\leqslant j\leqslant N, i-N\neq j$

$$\begin{aligned}\langle\Psi_1\,|\,\tilde{a}_i\tilde{a}_j\,|\,\Psi_2\rangle&=\left\langle\Psi_1\,\middle|\,a_{i-N}^\dagger a_j\,\middle|\,\Psi_2\right\rangle\\&=(-1)^{N(N+1)/2}\mathcal{N}_1^*\mathcal{N}_2\int\left(\prod_{i=1}^{2N}\mathrm{d}\tilde{z}_i\right)\tilde{z}_{i-N}\tilde{z}_{j+N}\exp\left(\frac{1}{2}\tilde{z}^\top M\tilde{z}\right)\\&=(-1)^{N(N+1)/2}\mathcal{N}_1^*\mathcal{N}_2\operatorname{Pf}(M)(-1)\left(M^{-1}\right)_{i-N,j+N}\end{aligned} \tag{248}$$

- $N+1\leqslant i\leqslant 2N, N+1\leqslant j\leqslant 2N$

$$\begin{aligned}\langle\Psi_1\,|\,\tilde{a}_i\tilde{a}_j\,|\,\Psi_2\rangle&=\left\langle\Psi_1\,\middle|\,a_{i-N}^\dagger a_{j-N}^\dagger\,\middle|\,\Psi_2\right\rangle\\&=(-1)^{N(N+1)/2}\mathcal{N}_1^*\mathcal{N}_2\int\left(\prod_{i=1}^{2N}\mathrm{d}\tilde{z}_i\right)\tilde{z}_{i-N}\tilde{z}_{j-N}\exp\left(\frac{1}{2}\tilde{z}^\top M\tilde{z}\right)\\&=(-1)^{N(N+1)/2}\mathcal{N}_1^*\mathcal{N}_2\operatorname{Pf}(M)(-1)\left(M^{-1}\right)_{i-N,j-N}\end{aligned} \tag{249}$$

两点关联函数

$$\langle\tilde{a}_i\tilde{a}_j\rangle\equiv\frac{\left\langle 0\,\middle|\,\exp\left(\frac{1}{2}\sum_{l,m}f_{l,m}^*(\lambda_1)a_ma_l\right)\tilde{a}_i\tilde{a}_j\exp\left(\frac{1}{2}\sum_{l,m}f_{l,m}(\lambda_2)a_l^\dagger a_m^\dagger\right)\,\middle|\,0\right\rangle}{\left\langle 0\,\middle|\,\exp\left(\frac{1}{2}\sum_{l,m}f_{l,m}^*(\lambda_1)a_ma_l\right)\exp\left(\frac{1}{2}\sum_{l,m}f_{l,m}(\lambda_2)a_l^\dagger a_m^\dagger\right)\,\middle|\,0\right\rangle} \tag{250}$$

$$\mathcal{Z} \equiv \left\langle 0 \left| \exp\left(\frac{1}{2}\sum_{l,m} f^*_{l,m}(\lambda_1) a_m a_l\right) \exp\left(\frac{1}{2}\sum_{l,m} f_{l,m}(\lambda_2) a^\dagger_l a^\dagger_m\right) \right| 0 \right\rangle = (-1)^{N(N+1)/2} \mathrm{Pf}(M) \tag{251}$$

- $1 \leqslant i \leqslant N, 1 \leqslant j \leqslant N$

$$\begin{aligned} \langle \tilde{a}_i \tilde{a}_j \rangle &= \frac{1}{(-1)^{N(N+1)/2}\mathrm{Pf}(M)} \cdot (-1)^{N(N+1)/2}\, \mathrm{Pf}(M)(-1)\left(M^{-1}\right)_{i+N,j+N} \\ &= (-1)\left(M^{-1}\right)_{i+N,j+N} \end{aligned} \tag{252}$$

- $1 \leqslant i \leqslant N, N+1 \leqslant j \leqslant 2N$

$$\langle \tilde{a}_i \tilde{a}_j \rangle = (-1)\left(M^{-1}\right)_{i+N,j-N} \tag{253}$$

- $N+1 \leqslant i \leqslant 2N, 1 \leqslant j \leqslant N, i-N \neq j$

$$\langle \tilde{a}_i \tilde{a}_j \rangle = (-1)\left(M^{-1}\right)_{i-N,j+N} \tag{254}$$

- $N+1 \leqslant i \leqslant 2N, N+1 \leqslant j \leqslant 2N$

$$\langle \tilde{a}_i \tilde{a}_j \rangle = (-1)\left(M^{-1}\right)_{i-N,j-N} \tag{255}$$

关联函数矩阵

$$\left\langle \begin{pmatrix} c_1^\dagger \\ \vdots \\ c_N^\dagger \\ c_1 \\ \vdots \\ c_N \end{pmatrix} \begin{pmatrix} c_1^\dagger & \cdots & c_N^\dagger & c_1 & \cdots & c_N \end{pmatrix} \right\rangle \tag{256}$$

如何用 M 表达?

χ费米子

低能激发态

矩阵元

已知费米型 vison pair 湮灭、产生算符:

$$\chi_{\boldsymbol{r},\alpha} \equiv \frac{1}{2}\left(b^\alpha_{\boldsymbol{r}} + \mathrm{i} b^\alpha_{\boldsymbol{r}+\boldsymbol{\delta}_\alpha}\right), \quad \boldsymbol{r} \in A \tag{257}$$

$$\chi^\dagger_{\boldsymbol{r},\alpha} \equiv \frac{1}{2}\left(b^\alpha_{\boldsymbol{r}} - \mathrm{i} b^\alpha_{\boldsymbol{r}+\boldsymbol{\delta}_\alpha}\right), \quad \boldsymbol{r} \in A \tag{258}$$

如何证明

$$u_{i,j} \equiv -\mathrm{i} b^\alpha_i b^\alpha_j = (-1)^{\chi^\dagger_{i,\alpha}\chi_{i,\alpha}}, \quad i \in A \tag{259}$$

$$u_{\boldsymbol{r},\boldsymbol{r}+\boldsymbol{\delta}_\alpha} \equiv -\mathrm{i} b^\alpha_{\boldsymbol{r}} b^\alpha_{\boldsymbol{r}+\boldsymbol{\delta}_\alpha} = 1 - 2\chi^\dagger_{\boldsymbol{r},\alpha}\chi_{\boldsymbol{r},\alpha} = (-1)^{\chi^\dagger_{\boldsymbol{r},\alpha}\chi_{\boldsymbol{r},\alpha}} \tag{260}$$

u 算符本征值为 $+1$ 的本征态是 $\chi^\dagger\chi$ 本征值为 0 的本征态，u 算符本征值为 -1 的本征态是 $\chi^\dagger\chi$ 本征值为 1 的本征态。因此，u 取 -1 相当于 bond 上占据了一个 χ 费米子。u 取 $+1$ 相当于 bond 上没有 χ 费米子。

χ 与 vison 的联系是什么?

若用 $|\Omega\rangle$ 表示无磁场基态（α 准粒子零占据、所有 u_{ij} 全为 $+1$，也就是所有 χ 费米子也零占据），则 $\chi_{\boldsymbol{r},\alpha}^{\dagger}|\Omega\rangle$ 表示产生一个 χ 费米子的态，也就是翻转某个 $u_{i,j}$ 使得 $u_{i,j}=-1$ 的态。这条键两边的 W_p 也反号，因此产生一对 vison

玻色型 vison pair 产生算符:

$$d_{\boldsymbol{r},\alpha,j}^{\dagger}|\Omega\rangle \equiv \left(\prod_{\text{boundary}}\chi^{\dagger}\right)\chi_{\boldsymbol{r},\alpha}^{\dagger}\tilde{\alpha}_{j}^{\dagger}|\Omega\rangle \tag{261}$$

如何计算

$$\left\langle \Omega \middle| d_{\boldsymbol{r},\beta,m}H_h d_{\boldsymbol{r},\alpha,l}^{\dagger} \middle| \Omega \right\rangle \tag{262}$$

考虑

$$\left(-\vec{h}\cdot\sum_{\boldsymbol{r}}\vec{\sigma}_{\boldsymbol{r}}\right)\left(\prod\chi^{\dagger}\right)\chi_{\boldsymbol{r},\alpha}^{\dagger}\tilde{\alpha}_{j}^{\dagger}|0_{\chi},0_{\alpha}\rangle \tag{263}$$

$\left(\prod\chi^{\dagger}\right)\chi_{\boldsymbol{r},\alpha}^{\dagger}\tilde{\alpha}_{j}^{\dagger}|0_{\chi},0_{\alpha}\rangle$ 是 $\hat{W}_p$ 的本征态。

$\sigma_{\boldsymbol{r}}^{\alpha}d_{\boldsymbol{r},\beta,l}^{\dagger}|\Omega\rangle$ 仍是 $\hat{W}_p$ 的本征态。相对于 $d_{\boldsymbol{r},\beta,l}^{\dagger}|\Omega\rangle$，$\sigma_{\boldsymbol{r}}^{\alpha}d_{\boldsymbol{r},\beta,l}^{\dagger}|\Omega\rangle$ 由 $(\boldsymbol{r},\alpha)$ 确定的 bond 所连接的两个 W_p 的本征值反号。

$$\left\langle \Omega \middle| d_{\boldsymbol{r},\alpha,m}\left(-\vec{h}\cdot\sum_{\boldsymbol{r}'}\vec{\sigma}_{\boldsymbol{r}'}\right)d_{\boldsymbol{r},\beta,l}^{\dagger} \middle| \Omega \right\rangle = -\sum_{\gamma}\varepsilon^{\alpha\beta\gamma}h_{\gamma}\left\langle \Omega \middle| d_{\boldsymbol{r},\alpha,m}\left(\sigma_{\boldsymbol{r}}^{\gamma}+\sigma_{\boldsymbol{r}+\boldsymbol{\delta}_{\gamma}}^{\gamma}\right)d_{\boldsymbol{r},\beta,l}^{\dagger} \middle| \Omega \right\rangle \tag{264}$$

- $\alpha,\beta=x,y,$ 非零 $\gamma=z$

$$\left\langle \Omega \middle| d_{\boldsymbol{r},x,m}H_h d_{\boldsymbol{r},y,l}^{\dagger} \middle| \Omega \right\rangle = -h_z\left\langle \Omega \middle| d_{\boldsymbol{r},x,m}\left(\sigma_{\boldsymbol{r}}^{z}+\sigma_{\boldsymbol{r}+\boldsymbol{\delta}_z}^{z}\right)d_{\boldsymbol{r},y,l}^{\dagger} \middle| \Omega \right\rangle \tag{265}$$

$$\begin{aligned}\sigma_{\boldsymbol{r}}^{z} &= \mathrm{i}b_{\boldsymbol{r}}^{z}c_{\boldsymbol{r}}\\ &= \mathrm{i}b_{\boldsymbol{r}}^{z}c_{\boldsymbol{r}}\left(b_{\boldsymbol{r}}^{x}b_{\boldsymbol{r}}^{y}b_{\boldsymbol{r}}^{z}c_{\boldsymbol{r}}\right)\\ &= -\mathrm{i}b_{\boldsymbol{r}}^{x}b_{\boldsymbol{r}}^{y}\\ &= -\mathrm{i}\left(\chi_{\boldsymbol{r},x}+\chi_{\boldsymbol{r},x}^{\dagger}\right)\left(\chi_{\boldsymbol{r},y}+\chi_{\boldsymbol{r},y}^{\dagger}\right)\end{aligned} \tag{266}$$

$$\begin{aligned}\chi_{\boldsymbol{r},x}\sigma_{\boldsymbol{r}}^{z}\chi_{\boldsymbol{r},y}^{\dagger} &= -\mathrm{i}\chi_{\boldsymbol{r},x}\left(\chi_{\boldsymbol{r},x}+\chi_{\boldsymbol{r},x}^{\dagger}\right)\left(\chi_{\boldsymbol{r},y}+\chi_{\boldsymbol{r},y}^{\dagger}\right)\chi_{\boldsymbol{r},y}^{\dagger}\\ &= -\mathrm{i}\chi_{\boldsymbol{r},x}\chi_{\boldsymbol{r},x}^{\dagger}\chi_{\boldsymbol{r},y}\chi_{\boldsymbol{r},y}^{\dagger}\\ &= -\mathrm{i}\left(1-\chi_{\boldsymbol{r},x}^{\dagger}\chi_{\boldsymbol{r},x}\right)\left(1-\chi_{\boldsymbol{r},y}^{\dagger}\chi_{\boldsymbol{r},y}\right)\end{aligned} \tag{267}$$

$$-h_z\left\langle \Omega \middle| d_{\boldsymbol{r},x,m}\left(\sigma_{\boldsymbol{r}}^{z}\right)d_{\boldsymbol{r},y,l}^{\dagger} \middle| \Omega \right\rangle = -h_z\left\langle \Psi_0^c(\boldsymbol{r},x) \middle| \tilde{\alpha}_m(\boldsymbol{r},x)\left(-\mathrm{i}\right)\tilde{\alpha}_l^{\dagger}(\boldsymbol{r},y) \middle| \Psi_0^c(\boldsymbol{r},y) \right\rangle \tag{268}$$

$$|\Omega\rangle \equiv |0_{\chi}\rangle \otimes \left|\Psi_0^c\left[\left\{u_{ij}^{\text{std}}\right\}\right]\right\rangle? \tag{269}$$

$$d_{\boldsymbol{r},y,l}^{\dagger}|\Omega\rangle \equiv \chi_{\boldsymbol{r},y}^{\dagger}|0_{\chi}\rangle \otimes \tilde{a}_l^{\dagger}\left|\Psi_0^c\left(\boldsymbol{r},y\right)\right\rangle? \tag{270}$$

$$\begin{aligned}\sigma_{\boldsymbol{r}+\boldsymbol{\delta}_z}^{z} &= \mathrm{i}b_{\boldsymbol{r}+\boldsymbol{\delta}_z}^{z}c_{\boldsymbol{r}+\boldsymbol{\delta}_z}\\ &= b_{\boldsymbol{r}}^{x}b_{\boldsymbol{r}}^{y}b_{\boldsymbol{r}}^{z}c_{\boldsymbol{r}}\left(\mathrm{i}b_{\boldsymbol{r}+\boldsymbol{\delta}_z}^{z}c_{\boldsymbol{r}+\boldsymbol{\delta}_z}\right)\\ &= -\mathrm{i}b_{\boldsymbol{r}}^{x}b_{\boldsymbol{r}}^{y}\left(-\mathrm{i}c_{\boldsymbol{r}}c_{\boldsymbol{r}+\boldsymbol{\delta}_z}\right)\left(\mathrm{i}b_{\boldsymbol{r}}^{z}b_{\boldsymbol{r}+\boldsymbol{\delta}_z}^{z}\right)\\ &= \sigma_{\boldsymbol{r}}^{z}\left(\mathrm{i}c_{\boldsymbol{r}}c_{\boldsymbol{r}+\boldsymbol{\delta}_z}\right)\left(-\mathrm{i}b_{\boldsymbol{r}}^{z}b_{\boldsymbol{r}+\boldsymbol{\delta}_z}^{z}\right)\end{aligned} \tag{271}$$

$$\begin{aligned}&-h_z\left\langle \Omega \middle| d_{\boldsymbol{r},x,m}\left[\sigma_{\boldsymbol{r}}^{z}\left(\mathrm{i}c_{\boldsymbol{r}}c_{\boldsymbol{r}+\boldsymbol{\delta}_z}\right)\left(-\mathrm{i}b_{\boldsymbol{r}}^{z}b_{\boldsymbol{r}+\boldsymbol{\delta}_z}^{z}\right)\right]d_{\boldsymbol{r},y,l}^{\dagger} \middle| \Omega \right\rangle\\ =&-h_z\left\langle \Omega \middle| d_{\boldsymbol{r},x,m}\left[\sigma_{\boldsymbol{r}}^{z}\left(\mathrm{i}c_{\boldsymbol{r}}c_{\boldsymbol{r}+\boldsymbol{\delta}_z}\right)(+1)\right]d_{\boldsymbol{r},y,l}^{\dagger} \middle| \Omega \right\rangle\\ =&-h_z\left\langle \Psi_0^c(\boldsymbol{r},x) \middle| \tilde{\alpha}_m(\boldsymbol{r},x)\left(-\mathrm{i}\right)\left(\mathrm{i}c_{\boldsymbol{r}}c_{\boldsymbol{r}+\boldsymbol{\delta}_z}\right)\tilde{\alpha}_l^{\dagger}(\boldsymbol{r},y) \middle| \Psi_0^c(\boldsymbol{r},y) \right\rangle\end{aligned} \tag{272}$$

$$\left\langle\Omega\left|d_{\boldsymbol{r},x,m}H_h d^{\dagger}_{\boldsymbol{r},y,l}\right|\Omega\right\rangle=\mathrm{i}h_z\left\langle\Psi_0^c(\boldsymbol{r},x)\left|\tilde{\alpha}_m(\boldsymbol{r},x)\left(1+\mathrm{i}c_{\boldsymbol{r}}c_{\boldsymbol{r}+\boldsymbol{\delta}_z}\right)\tilde{\alpha}^{\dagger}_l(\boldsymbol{r},y)\right|\Psi_0^c(\boldsymbol{r},y)\right\rangle \tag{273}$$

α,β 更一般情况的写法为

$$\left\langle\Omega\left|d_{\boldsymbol{r},\alpha,m}H_h d^{\dagger}_{\boldsymbol{r},\beta,l}\right|\Omega\right\rangle=\sum_{\gamma}\mathrm{i}\varepsilon^{\alpha\beta\gamma}h_{\gamma}\left\langle\Psi_0^c(\boldsymbol{r},\alpha)\left|\tilde{\alpha}_m(\boldsymbol{r},\alpha)\left(1+\mathrm{i}c_{\boldsymbol{r}}c_{\boldsymbol{r}+\boldsymbol{\delta}_{\gamma}}\right)\tilde{\alpha}^{\dagger}_l(\boldsymbol{r},\beta)\right|\Psi_0^c(\boldsymbol{r},\beta)\right\rangle \tag{274}$$

- $|\Psi_0^c\left[\{u_{ij}\}\right]\rangle=\mathcal{N}\exp\left(\frac{1}{2}\sum_{i,j}f_i^{\dagger}f_j^{\dagger}\right)|0_f\rangle$ 如何用 $\left|\Psi_0^c\left[\left\{u_{ij}^{\mathrm{std}}\right\}\right]\right\rangle=|0_f\rangle$ 表达?
- 用overlap算矩阵元的具体数值?
- $\left\langle\Omega\left|H_h d^{\dagger}_{\boldsymbol{r},\mu}\right|\Omega\right\rangle=?$
- $H_{\mathrm{B}}=?$