

标准规范 $\{u_{ij} = +1\}$ 下, 哈密顿量

$$\begin{aligned}
H(0) &= \frac{1}{2} \begin{pmatrix} a^\dagger & a^\top \end{pmatrix} h(0) \begin{pmatrix} a \\ (a^\dagger)^\top \end{pmatrix} \\
&= \frac{1}{2} \begin{pmatrix} a^\dagger & a^\top \end{pmatrix} U(0) D(0) U^\dagger(0) \begin{pmatrix} a \\ (a^\dagger)^\top \end{pmatrix} \\
&= \frac{1}{2} \begin{pmatrix} \alpha^\dagger(0) & \alpha^\top(0) \end{pmatrix} D(0) \begin{pmatrix} \alpha(0) \\ (\alpha^\dagger(0))^\top \end{pmatrix}
\end{aligned} \tag{1}$$

$$U(0) = \begin{pmatrix} W(0) & V^*(0) \\ V(0) & W^*(0) \end{pmatrix}, \quad D(0) = \text{diag}(E_1(0), \dots, E_N(0), -E_1(0), \dots, -E_N(0)) \tag{2}$$

$$\begin{pmatrix} \alpha(0) \\ (\alpha^\dagger(0))^\top \end{pmatrix} = U^\dagger(0) \begin{pmatrix} a \\ (a^\dagger)^\top \end{pmatrix}, \quad \begin{pmatrix} \alpha^\dagger(0) & \alpha^\top(0) \end{pmatrix} = \begin{pmatrix} a^\dagger & a^\top \end{pmatrix} U(0) \tag{3}$$

$$\begin{pmatrix} a \\ (a^\dagger)^\top \end{pmatrix} = U(0) \begin{pmatrix} \alpha(0) \\ (\alpha^\dagger(0))^\top \end{pmatrix}, \quad \begin{pmatrix} a^\dagger & a^\top \end{pmatrix} = \begin{pmatrix} \alpha^\dagger(0) & \alpha^\top(0) \end{pmatrix} U^\dagger(0) \tag{4}$$

则 $H(0)$ 的基态是 $\alpha(0)$ 的真空态 $|0_{\alpha(0)}\rangle$, 可以由 a 的真空 $|0_a\rangle$ 生成:

$$|0_{\alpha(0)}\rangle = \mathcal{N}(0) \exp\left(\frac{1}{2} \sum_{i,j} F_{i,j}(0) a_i^\dagger a_j\right) |0_a\rangle \tag{5}$$

$$F(0) = V(0)^* [W^*(0)]^{-1} \tag{6}$$

$$\mathcal{N}(0) = \det^{-1/4} (I + F^\dagger(0) F(0)) \tag{7}$$

考虑构型 $\{u_{ij}\}$ 下, 哈密顿量

$$\begin{aligned}
H &= \frac{1}{2} \begin{pmatrix} a^\dagger & a^\top \end{pmatrix} h \begin{pmatrix} a \\ (a^\dagger)^\top \end{pmatrix} \\
&= \frac{1}{2} \begin{pmatrix} a^\dagger & a^\top \end{pmatrix} U D U^\dagger \begin{pmatrix} a \\ (a^\dagger)^\top \end{pmatrix} \\
&= \frac{1}{2} \begin{pmatrix} \alpha^\dagger(0) & \alpha^\top(0) \end{pmatrix} U^\dagger(0) U D U^\dagger U(0) \begin{pmatrix} \alpha(0) \\ (\alpha^\dagger(0))^\top \end{pmatrix} \\
&\equiv \frac{1}{2} \begin{pmatrix} \alpha^\dagger(0) & \alpha^\top(0) \end{pmatrix} \tilde{U} D \tilde{U}^\dagger \begin{pmatrix} \alpha(0) \\ (\alpha^\dagger(0))^\top \end{pmatrix} \\
&\equiv \frac{1}{2} \begin{pmatrix} \alpha^\dagger & \alpha^\top \end{pmatrix} D \begin{pmatrix} \alpha \\ (\alpha^\dagger)^\top \end{pmatrix}
\end{aligned} \tag{8}$$

$$\tilde{U} \equiv U^\dagger(0) U, \quad \tilde{U}^\dagger = U^\dagger U(0) \tag{9}$$

$$\tilde{U} = \begin{pmatrix} \widetilde{W} & \widetilde{V}^* \\ \widetilde{V} & \widetilde{W}^* \end{pmatrix}, \quad \tilde{U}^\dagger = \begin{pmatrix} \widetilde{W}^\dagger & \widetilde{V}^\dagger \\ \widetilde{V}^\top & \widetilde{W}^\top \end{pmatrix} \tag{10}$$

$$\begin{pmatrix} \alpha^\dagger & \alpha^\top \end{pmatrix} = \begin{pmatrix} \alpha^\dagger(0) & \alpha^\top(0) \end{pmatrix} \tilde{U} = \begin{pmatrix} \alpha^\dagger(0) & \alpha^\top(0) \end{pmatrix} \begin{pmatrix} \widetilde{W} & \widetilde{V}^* \\ \widetilde{V} & \widetilde{W}^* \end{pmatrix}, \tag{11}$$

$$\begin{pmatrix} \alpha \\ (\alpha^\dagger)^\top \end{pmatrix} = \tilde{U}^\dagger \begin{pmatrix} \alpha(0) \\ (\alpha^\dagger(0))^\top \end{pmatrix} = \begin{pmatrix} \widetilde{W}^\dagger & \widetilde{V}^\dagger \\ \widetilde{V}^\top & \widetilde{W}^\top \end{pmatrix} \begin{pmatrix} \alpha(0) \\ (\alpha^\dagger(0))^\top \end{pmatrix} \tag{12}$$

H 的基态是 α 的真空态 $|0_\alpha\rangle$, 可以由 $\alpha(0)$ 的真空态 $|0_{\alpha(0)}\rangle$ 生成:

$$|0_\alpha\rangle = \tilde{\mathcal{N}} \exp\left(\frac{1}{2} \sum_{i,j} \tilde{F}_{i,j} \alpha_i^\dagger(0) \alpha_j^\dagger(0)\right) |0_{\alpha(0)}\rangle \quad (13)$$

$$\tilde{F} = \tilde{V}^* \left(\tilde{W}^*\right)^{-1} \quad (14)$$

$$\tilde{\mathcal{N}} = \det^{-1/4} \left(I + \tilde{F}^\dagger \tilde{F}\right) \quad (15)$$

实际上 $\tilde{\mathcal{N}}$ 可以化简。

$$\tilde{N} = \left| \det \left(\tilde{W}\right) \right|^{1/2} \quad (16)$$

c-Majorana如何换成 $\alpha(0)$

$$c_{i,A} = a_i + a_i^\dagger, \quad c_{i,B} = \frac{1}{i} \left(a_i - a_i^\dagger\right), \quad (17)$$

$$\begin{pmatrix} a \\ (a^\dagger)^\top \end{pmatrix} = U(0) \begin{pmatrix} \alpha(0) \\ (\alpha^\dagger(0))^\top \end{pmatrix} \quad (18)$$

$$U(0) = \begin{pmatrix} \mathbf{W}(0) & \mathbf{V}^*(0) \\ \mathbf{V}(0) & \mathbf{W}^*(0) \end{pmatrix} \quad (19)$$

$$a_i = \frac{1}{2} (c_{i,A} + i c_{i,B}), \quad a_i^\dagger = \frac{1}{2} (c_{i,A} - i c_{i,B}) \quad (20)$$

$$a \equiv \begin{pmatrix} a_1 \\ \vdots \\ a_N \end{pmatrix} = \frac{1}{2} c_A + \frac{i}{2} c_B \quad (21)$$

$$(a^\dagger)^\top = \frac{1}{2} c_A - \frac{i}{2} c_B \quad (22)$$

一方面

$$\begin{pmatrix} a \\ (a^\dagger)^\top \end{pmatrix} = \begin{pmatrix} \frac{1}{2}I & \frac{i}{2}I \\ \frac{1}{2}I & -\frac{i}{2}I \end{pmatrix} \begin{pmatrix} c_A \\ c_B \end{pmatrix} \quad (23)$$

另一方面

$$\begin{pmatrix} a \\ (a^\dagger)^\top \end{pmatrix} = U(0) \begin{pmatrix} \alpha(0) \\ (\alpha^\dagger(0))^\top \end{pmatrix} \quad (24)$$

$$U(0) = \begin{pmatrix} \mathbf{W}(0) & \mathbf{V}^*(0) \\ \mathbf{V}(0) & \mathbf{W}^*(0) \end{pmatrix} \quad (25)$$

于是

$$\begin{aligned} \begin{pmatrix} c_A \\ c_B \end{pmatrix} &= \begin{pmatrix} \frac{1}{2}I & \frac{i}{2}I \\ \frac{1}{2}I & -\frac{i}{2}I \end{pmatrix}^{-1} \begin{pmatrix} \mathbf{W}(0) & \mathbf{V}^*(0) \\ \mathbf{V}(0) & \mathbf{W}^*(0) \end{pmatrix} \begin{pmatrix} \alpha(0) \\ (\alpha^\dagger(0))^\top \end{pmatrix} = \begin{pmatrix} I & I \\ -iI & iI \end{pmatrix} \begin{pmatrix} \mathbf{W}(0) & \mathbf{V}^*(0) \\ \mathbf{V}(0) & \mathbf{W}^*(0) \end{pmatrix} \begin{pmatrix} \alpha(0) \\ (\alpha^\dagger(0))^\top \end{pmatrix} \\ &\equiv U'(0) \begin{pmatrix} \alpha(0) \\ (\alpha^\dagger(0))^\top \end{pmatrix} = \begin{pmatrix} W(0) + V(0) & V^*(0) + W^*(0) \\ i(-W(0) + V(0)) & i(-V^*(0) + W^*(0)) \end{pmatrix} \begin{pmatrix} \alpha(0) \\ (\alpha^\dagger(0))^\top \end{pmatrix} \\ &\equiv \begin{pmatrix} \mathbf{U}'_{11}(0) & \mathbf{U}'_{12}(0) \\ \mathbf{U}'_{21}(0) & \mathbf{U}'_{22}(0) \end{pmatrix} \begin{pmatrix} \alpha(0) \\ (\alpha^\dagger(0))^\top \end{pmatrix} \end{aligned} \quad (26)$$

$$c_{i,A} = U'_{i,}(0) \begin{pmatrix} \alpha(0) \\ (\alpha^\dagger(0))^\top \end{pmatrix} = \mathbf{U}'_{11}(0)_{i,} \alpha(0) + \mathbf{U}'_{12}(0)_{i,} (\alpha^\dagger(0))^\top \quad (27)$$

$$c_{i,A} = c_{i,A}^\dagger = \alpha^\dagger(0) [\mathbf{U}'_{11}(0)_{i,}]^\dagger + \alpha^\top(0) [\mathbf{U}'_{12}(0)_{i,}]^\dagger \quad (28)$$

$$c_{j,B} = U'_{j+N,}(0) \begin{pmatrix} \alpha(0) \\ (\alpha^\dagger(0))^\top \end{pmatrix} = \mathbf{U}'_{21}(0)_{j,} \alpha(0) + \mathbf{U}'_{22}(0)_{j,} (\alpha^\dagger(0))^\top \quad (29)$$

$$c_{j,B} = c_{j,B}^\dagger = \alpha^\dagger(0) [\mathbf{U}'_{21}(0)_{j,}]^\dagger + \alpha^\top(0) [\mathbf{U}'_{22}(0)_{j,}]^\dagger \quad (30)$$

跃迁振幅

$$\begin{aligned} & \langle 0_\chi, 0_{\alpha(1)} | d_{\mathbf{r},x}(1) H_h d_{\mathbf{r},y}^\dagger(2) | 0_\chi, 0_{\alpha(2)} \rangle \\ &= \langle \chi(\mathbf{r}, x), 0_{\alpha(1)} | \alpha(1) [-h_z (\sigma_{\mathbf{r}}^z + \sigma_{\mathbf{r}+\delta_z}^z)] \alpha^\dagger(2) | \chi(\mathbf{r}, y), 0_{\alpha(2)} \rangle \\ &= -h_z \langle \chi(\mathbf{r}, x), 0_{\alpha(1)} | \alpha(1) (\sigma_{\mathbf{r}}^z + \sigma_{\mathbf{r}+\delta_z}^z) \alpha^\dagger(2) | \chi(\mathbf{r}, y), 0_{\alpha(2)} \rangle \\ &= -h_z \langle \chi, 0_{\alpha(1)} | \alpha(1) [-i(1 + i c_{i,A} c_{j,B})] \alpha^\dagger(2) | \chi, 0_{\alpha(2)} \rangle \\ &= i h_z \langle \chi, 0_{\alpha(1)} | \alpha(1) (1 + i c_{i,A} c_{j,B}) \alpha^\dagger(2) | \chi, 0_{\alpha(2)} \rangle \\ &= i h_z \tilde{\mathcal{N}}(1) \tilde{\mathcal{N}}(2) \left\langle \chi, 0_{\alpha(0)} \left| \exp \left(\frac{1}{2} F_{i,j}^*(1) \alpha_i(0) \alpha_j(0) \right) \alpha(1) (1 + i c_{i,A} c_{j,B}) \alpha^\dagger(2) \exp \left(\frac{1}{2} \sum_{i,j} F_{i,j}(2) \alpha_i^\dagger(0) \alpha_j^\dagger(0) \right) \right| \chi, 0_{\alpha(0)} \right\rangle \quad (31) \\ &\equiv i h_z \langle \Psi(1) | \alpha(1) (1 + i c_{i,A} c_{j,B}) \alpha^\dagger(2) | \Psi(2) \rangle \\ &= i h_z \langle \Psi(1) | \Psi(2) \rangle \langle \alpha(1) (1 + i c_{i,A} c_{j,B}) \alpha^\dagger(2) \rangle \\ &= h_z \langle \Psi(1) | \Psi(2) \rangle [i \langle \alpha(1) \alpha^\dagger(2) \rangle - \langle \alpha(1) c_{i,A} c_{j,B} \alpha^\dagger(2) \rangle] \end{aligned}$$

$$\bullet \langle \Psi(1) | \Psi(2) \rangle$$

$$\langle \Psi(1) | \Psi(2) \rangle = \tilde{N}(1) \tilde{N}(2) (-1)^{N(N+1)/2} \text{Pf}(M) \quad (32)$$

$$M \equiv \begin{pmatrix} \tilde{F}(2) & -I \\ I & -\tilde{F}^*(1) \end{pmatrix} \quad (33)$$

$$\tilde{N} = \left| \det(\tilde{W}) \right|^{1/2} \quad (34)$$

$$\tilde{F} = \tilde{V}^* (\tilde{W}^*)^{-1} \quad (35)$$

$$\tilde{U} \equiv U^\dagger(0)U, \quad \tilde{U}^\dagger = U^\dagger U(0) \quad (36)$$

$$\tilde{U} = \begin{pmatrix} \tilde{W} & \tilde{V}^* \\ \tilde{V} & \tilde{W}^* \end{pmatrix}, \quad \tilde{U}^\dagger = \begin{pmatrix} \tilde{W}^\dagger & \tilde{V}^\dagger \\ \tilde{V}^\top & \tilde{W}^\top \end{pmatrix} \quad (37)$$

$$\bullet \langle \alpha(1) \alpha^\dagger(2) \rangle$$

$$\begin{pmatrix} \alpha(1) \\ (\alpha^\dagger(1))^\top \end{pmatrix} = \tilde{U}^\dagger(1) \begin{pmatrix} \alpha(0) \\ (\alpha^\dagger(0))^\top \end{pmatrix} = \begin{pmatrix} \tilde{W}^\dagger(1) & \tilde{V}^\dagger(1) \\ \tilde{V}^\top(1) & \tilde{W}^\top(1) \end{pmatrix} \begin{pmatrix} \alpha(0) \\ (\alpha^\dagger(0))^\top \end{pmatrix} \quad (38)$$

$$\alpha(1) = \tilde{W}^\dagger(1) \alpha(0) + \tilde{V}^\dagger(1) (\alpha^\dagger(0))^\top \quad (39)$$

$$\begin{pmatrix} \alpha^\dagger(2) & \alpha^\top(2) \end{pmatrix} = \begin{pmatrix} \alpha^\dagger(0) & \alpha^\top(0) \end{pmatrix} \tilde{U}(2) = \begin{pmatrix} \alpha^\dagger(0) & \alpha^\top(0) \end{pmatrix} \begin{pmatrix} \tilde{W}(2) & \tilde{V}^*(2) \\ \tilde{V}(2) & \tilde{W}^*(2) \end{pmatrix}, \quad (40)$$

$$\alpha^\dagger(2) = \alpha^\dagger(0) \tilde{W}(2) + \alpha^\top(0) \tilde{V}(2) \quad (41)$$

$$\begin{aligned}
& \langle \alpha(1) \alpha^\dagger(2) \rangle \\
&= \left\langle \left[\widetilde{W}^\dagger(1) \alpha(0) + \widetilde{V}^\dagger(1) (\alpha^\dagger(0))^\top \right] \left[\alpha^\dagger(0) \widetilde{W}(2) + \alpha^\top(0) \widetilde{V}(2) \right] \right\rangle \\
&= \left\langle \begin{pmatrix} \widetilde{V}^\dagger(1) & \widetilde{W}^\dagger(1) \end{pmatrix} \begin{pmatrix} (\alpha^\dagger(0))^\top \\ \alpha(0) \end{pmatrix} \begin{pmatrix} \alpha^\dagger(0) & \alpha^\top(0) \end{pmatrix} \begin{pmatrix} \widetilde{W}(2) \\ \widetilde{V}(2) \end{pmatrix} \right\rangle \\
&= \begin{pmatrix} \widetilde{V}^\dagger(1) & \widetilde{W}^\dagger(1) \end{pmatrix} \left\langle \begin{pmatrix} (\alpha^\dagger(0))^\top \alpha^\dagger(0) & (\alpha^\dagger(0))^\top \alpha^\top(0) \\ \alpha(0) \alpha^\dagger(0) & \alpha(0) \alpha^\top(0) \end{pmatrix} \right\rangle \begin{pmatrix} \widetilde{W}(2) \\ \widetilde{V}(2) \end{pmatrix} \\
&= \begin{pmatrix} \widetilde{V}^\dagger(1) & \widetilde{W}^\dagger(1) \end{pmatrix} \left(-M^{-1} + \begin{pmatrix} 0 & I \\ 0 & 0 \end{pmatrix} \right) \begin{pmatrix} \widetilde{W}(2) \\ \widetilde{V}(2) \end{pmatrix}
\end{aligned} \tag{42}$$

$$\bullet \langle \alpha(1) c_{i,A} c_{j,B} \alpha^\dagger(2) \rangle$$

Wick定理给出

$$\begin{aligned}
& \langle \alpha(1) c_{i,A} c_{j,B} \alpha^\dagger(2) \rangle \\
&= \langle \alpha(1) c_{i,A} \rangle \langle c_{j,B} \alpha^\dagger(2) \rangle - \langle \alpha(1) c_{j,B} \rangle \langle c_{i,A} \alpha^\dagger(2) \rangle + \langle \alpha(1) \alpha^\dagger(2) \rangle \langle c_{i,A} c_{j,B} \rangle
\end{aligned} \tag{43}$$

$$\bullet \circ \langle \alpha(1) c_{i,A} \rangle$$

$$\boxed{\alpha(1) = \widetilde{W}^\dagger(1) \alpha(0) + \widetilde{V}^\dagger(1) (\alpha^\dagger(0))^\top} \tag{44}$$

$$\boxed{c_{i,A} = c_{i,A}^\dagger = \alpha^\dagger(0) [\mathbf{U}'_{11}(0)_{i,}]^\dagger + \alpha^\top(0) [\mathbf{U}'_{12}(0)_{i,}]^\dagger} \tag{45}$$

$$\begin{aligned}
& \langle \alpha(1) c_{i,A} \rangle \\
&= \left\langle \left\{ \widetilde{W}^\dagger(1) \alpha(0) + \widetilde{V}^\dagger(1) (\alpha^\dagger(0))^\top \right\} \left\{ \alpha^\dagger(0) [\mathbf{U}'_{11}(0)_{i,}]^\dagger + \alpha(0)^\top [\mathbf{U}'_{12}(0)_{i,}]^\dagger \right\} \right\rangle \\
&= \begin{pmatrix} \widetilde{V}^\dagger(1) & \widetilde{W}^\dagger(1) \end{pmatrix} \left\langle \begin{pmatrix} (\alpha^\dagger(0))^\top \\ \alpha(0) \end{pmatrix} \begin{pmatrix} \alpha^\dagger(0) & \alpha^\top(0) \end{pmatrix} \right\rangle \begin{pmatrix} [\mathbf{U}'_{11}(0)_{i,}]^\dagger \\ [\mathbf{U}'_{12}(0)_{i,}]^\dagger \end{pmatrix} \\
&= \begin{pmatrix} \widetilde{V}^\dagger(1) & \widetilde{W}^\dagger(1) \end{pmatrix} \left(-M^{-1} + \begin{pmatrix} 0 & I \\ 0 & 0 \end{pmatrix} \right) \begin{pmatrix} [\mathbf{U}'_{11}(0)_{i,}]^\dagger \\ [\mathbf{U}'_{12}(0)_{i,}]^\dagger \end{pmatrix}
\end{aligned} \tag{46}$$

$$\bullet \circ \langle \alpha(1) c_{j,B} \rangle$$

$$\boxed{\alpha(1) = \widetilde{W}^\dagger(1) \alpha(0) + \widetilde{V}^\dagger(1) (\alpha^\dagger(0))^\top} \tag{47}$$

$$\boxed{c_{j,B} = c_{j,B}^\dagger = \alpha^\dagger(0) [\mathbf{U}'_{21}(0)_{j,}]^\dagger + \alpha^\top(0) [\mathbf{U}'_{22}(0)_{j,}]^\dagger} \tag{48}$$

$$\begin{aligned}
& \langle \alpha(1) c_{j,B} \rangle \\
&= \left\langle \left\{ \widetilde{W}^\dagger(1) \alpha(0) + \widetilde{V}^\dagger(1) (\alpha^\dagger(0))^\top \right\} \left\{ \alpha^\dagger(0) [\mathbf{U}'_{21}(0)_{j,}]^\dagger + \alpha^\top(0) [\mathbf{U}'_{22}(0)_{j,}]^\dagger \right\} \right\rangle \\
&= \begin{pmatrix} \widetilde{V}^\dagger(1) & \widetilde{W}^\dagger(1) \end{pmatrix} \left\langle \begin{pmatrix} (\alpha^\dagger(0))^\top \\ \alpha(0) \end{pmatrix} \begin{pmatrix} \alpha^\dagger(0) & \alpha^\top(0) \end{pmatrix} \right\rangle \begin{pmatrix} [\mathbf{U}'_{21}(0)_{j,}]^\dagger \\ [\mathbf{U}'_{22}(0)_{j,}]^\dagger \end{pmatrix} \\
&= \begin{pmatrix} \widetilde{V}^\dagger(1) & \widetilde{W}^\dagger(1) \end{pmatrix} \left(-M^{-1} + \begin{pmatrix} 0 & I \\ 0 & 0 \end{pmatrix} \right) \begin{pmatrix} [\mathbf{U}'_{21}(0)_{j,}]^\dagger \\ [\mathbf{U}'_{22}(0)_{j,}]^\dagger \end{pmatrix}
\end{aligned} \tag{49}$$

$$\bullet \circ \langle c_{i,A} \alpha^\dagger(2) \rangle$$

$$\boxed{\alpha^\dagger(2) = \alpha^\dagger(0) \widetilde{W}(2) + \alpha^\top(0) \widetilde{V}(2)} \tag{50}$$

$$c_{i,A} = U'_{i,}(0) \begin{pmatrix} \alpha(0) \\ (\alpha^\dagger(0))^\top \end{pmatrix} = \mathbf{U}'_{11}(0)_{i,} \alpha(0) + \mathbf{U}'_{12}(0)_{i,} (\alpha^\dagger(0))^\top \quad (51)$$

$$\begin{aligned} & \langle c_{i,A} \alpha^\dagger(2) \rangle \\ &= \left\langle \left\{ \mathbf{U}'_{11}(0)_{i,} \alpha(0) + \mathbf{U}'_{12}(0)_{i,} (\alpha^\dagger(0))^\top \right\} \left\{ \alpha^\dagger(0) \widetilde{W}(2) + \alpha^\top(0) \widetilde{V}(2) \right\} \right\rangle \\ &= (\mathbf{U}'_{12}(0)_{i,} \quad \mathbf{U}'_{11}(0)_{i,}) \left\langle \begin{pmatrix} (\alpha^\dagger(0))^\top \\ \alpha(0) \end{pmatrix} (\alpha^\dagger(0) \quad \alpha^\top(0)) \right\rangle \begin{pmatrix} \widetilde{W}(2) \\ \widetilde{V}(2) \end{pmatrix} \\ &= (\mathbf{U}'_{12}(0)_{i,} \quad \mathbf{U}'_{11}(0)_{i,}) \left(-M^{-1} + \begin{pmatrix} 0 & I \\ 0 & 0 \end{pmatrix} \right) \begin{pmatrix} \widetilde{W}(2) \\ \widetilde{V}(2) \end{pmatrix} \end{aligned} \quad (52)$$

$$\bullet \quad \circ \quad \langle c_{j,B} \alpha^\dagger(2) \rangle$$

$$\alpha^\dagger(2) = \alpha^\dagger(0) \widetilde{W}(2) + \alpha^\top(0) \widetilde{V}(2) \quad (53)$$

$$c_{j,B} = U'_{j+N,}(0) \begin{pmatrix} \alpha(0) \\ (\alpha^\dagger(0))^\top \end{pmatrix} = \mathbf{U}'_{21}(0)_{j,} \alpha(0) + \mathbf{U}'_{22}(0)_{j,} (\alpha^\dagger(0))^\top \quad (54)$$

$$\begin{aligned} & \langle c_{j,B} \alpha^\dagger(2) \rangle \\ &= \left\langle \left\{ \mathbf{U}'_{21}(0)_{j,} \alpha(0) + \mathbf{U}'_{22}(0)_{j,} (\alpha^\dagger(0))^\top \right\} \left\{ \alpha^\dagger(0) \widetilde{W}(2) + \alpha^\top(0) \widetilde{V}(2) \right\} \right\rangle \\ &= (\mathbf{U}'_{22}(0)_{j,} \quad \mathbf{U}'_{21}(0)_{j,}) \left\langle \begin{pmatrix} (\alpha^\dagger(0))^\top \\ \alpha(0) \end{pmatrix} (\alpha^\dagger(0) \quad \alpha^\top(0)) \right\rangle \begin{pmatrix} \widetilde{W}(2) \\ \widetilde{V}(2) \end{pmatrix} \\ &= (\mathbf{U}'_{22}(0)_{j,} \quad \mathbf{U}'_{21}(0)_{j,}) \left(-M^{-1} + \begin{pmatrix} 0 & I \\ 0 & 0 \end{pmatrix} \right) \begin{pmatrix} \widetilde{W}(2) \\ \widetilde{V}(2) \end{pmatrix} \end{aligned} \quad (55)$$

$$\bullet \quad \circ \quad \langle c_{i,A} c_{j,B} \rangle$$

$$c_{i,A} = U'_{i,}(0) \begin{pmatrix} \alpha(0) \\ (\alpha^\dagger(0))^\top \end{pmatrix} = \mathbf{U}'_{11}(0)_{i,} \alpha(0) + \mathbf{U}'_{12}(0)_{i,} (\alpha^\dagger(0))^\top \quad (56)$$

$$c_{j,B} = c_{j,B}^\dagger = \alpha^\dagger(0) [\mathbf{U}'_{21}(0)_{j,}]^\dagger + \alpha^\top(0) [\mathbf{U}'_{22}(0)_{j,}]^\dagger \quad (57)$$

$$\begin{aligned} & \langle c_{i,A} c_{j,B} \rangle \\ &= \left\langle \left\{ \mathbf{U}'_{11}(0)_{i,} \alpha(0) + \mathbf{U}'_{12}(0)_{i,} (\alpha^\dagger(0))^\top \right\} \left\{ \alpha^\dagger(0) [\mathbf{U}'_{21}(0)_{j,}]^\dagger + \alpha^\top(0) [\mathbf{U}'_{22}(0)_{j,}]^\dagger \right\} \right\rangle \\ &= (\mathbf{U}'_{12}(0)_{i,} \quad \mathbf{U}'_{11}(0)_{i,}) \left\langle \begin{pmatrix} (\alpha^\dagger(0))^\top \alpha^\dagger(0) & (\alpha^\dagger(0))^\top \alpha^\top(0) \\ \alpha(0) \alpha^\dagger(0) & \alpha(0) \alpha^\top(0) \end{pmatrix} \right\rangle \begin{pmatrix} [\mathbf{U}'_{21}(0)_{j,}]^\dagger \\ [\mathbf{U}'_{22}(0)_{j,}]^\dagger \end{pmatrix} \\ &= (\mathbf{U}'_{12}(0)_{i,} \quad \mathbf{U}'_{11}(0)_{i,}) \left(-M^{-1} + \begin{pmatrix} 0 & I \\ 0 & 0 \end{pmatrix} \right) \begin{pmatrix} [\mathbf{U}'_{21}(0)_{j,}]^\dagger \\ [\mathbf{U}'_{22}(0)_{j,}]^\dagger \end{pmatrix} \end{aligned} \quad (58)$$

以B子格为中心

要算

$$\begin{aligned} & \left\langle 0_\chi, 0_{\alpha(1)} \left| \chi_{\mathbf{r}+\mathbf{a}_2, x} \alpha(1) H_h \alpha^\dagger(2) \chi_{\mathbf{r}-\mathbf{a}_1+\mathbf{a}_2, y}^\dagger \right| 0_\chi, 0_{\alpha(2)} \right\rangle \\ &= \left\langle 0_\chi, 0_{\alpha(1)} \left| \chi_{\mathbf{r}+\mathbf{a}_2, x} \alpha(1) [-\hbar_z (\sigma_{\mathbf{r}} + \sigma_{\mathbf{r}+\delta_z})] \alpha^\dagger(2) \chi_{\mathbf{r}-\mathbf{a}_1+\mathbf{a}_2, y}^\dagger \right| 0_\chi, 0_{\alpha(2)} \right\rangle \end{aligned} \quad (59)$$

注意到

$$\chi_{r,\alpha} \equiv \frac{1}{2} (b_r^\alpha + i b_{r+\delta_\alpha}^\alpha), \quad \chi_{r,\alpha}^\dagger \equiv \frac{1}{2} (b_r^\alpha - i b_{r+\delta_\alpha}^\alpha), \quad r \in A \quad (60)$$

$$b_r^\alpha = \chi_{r,\alpha} + \chi_{r,\alpha}^\dagger, \quad b_{r+\delta_\alpha}^\alpha = \frac{1}{i} (\chi_{r,\alpha} - \chi_{r,\alpha}^\dagger) \quad (61)$$

于是

$$\begin{aligned} \sigma_{r+\delta_z}^z &= i b_{r+\delta_z}^z c_{r+\delta_z} = -i b_{r+\delta_z}^x b_{r+\delta_z}^y \\ &= -i b_{r+a_2+\delta_x}^x b_{r-a_1+a_2+\delta_y}^y \\ &= -i \cdot \frac{1}{i} \left(\chi_{r+a_2,x} - \chi_{r+a_2,x}^\dagger \right) \cdot \frac{1}{i} \left(\chi_{r-a_1+a_2,y} - \chi_{r-a_1+a_2,y}^\dagger \right) \\ &= i \left(\chi_{r+a_2,x} - \chi_{r+a_2,x}^\dagger \right) \left(\chi_{r-a_1+a_2,y} - \chi_{r-a_1+a_2,y}^\dagger \right) \end{aligned} \quad (62)$$

$$\begin{aligned} \sigma_{r+\delta_z} \chi_{r-a_1+a_2,y}^\dagger &= i \left(\chi_{r+a_2,x} - \chi_{r+a_2,x}^\dagger \right) \left(\chi_{r-a_1+a_2,y} - \chi_{r-a_1+a_2,y}^\dagger \right) \cdot \chi_{r-a_1+a_2,y}^\dagger \\ &= i \left(\chi_{r+a_2,x} - \chi_{r+a_2,x}^\dagger \right) \end{aligned} \quad (63)$$

在braket中 $= -i \chi_{r+a_2,x}^\dagger$

$$\begin{aligned} \sigma_r^z &= i b_r^z c_r = b_{r+\delta_z}^x b_{r+\delta_z}^y b_{r+\delta_z}^z c_{r+\delta_z} (i b_r^z c_r) \\ &= (-i b_{r+\delta_z}^x b_{r+\delta_z}^y) (i c_r c_{r+\delta_z}) (-i b_r^z b_{r+\delta_z}^z) \\ &= (-i b_{r+\delta_z}^x b_{r+\delta_z}^y) (i c_r c_{r+\delta_z}) \cdot 1 \end{aligned} \quad (64)$$

$$\begin{aligned} \sigma_r^z \chi_{r-a_1+a_2,y}^\dagger &= (-i b_{r+\delta_z}^x b_{r+\delta_z}^y) (i c_r c_{r+\delta_z}) \chi_{r-a_1+a_2,y}^\dagger \\ &= (i c_r c_{r+\delta_z}) (-i b_{r+\delta_z}^x b_{r+\delta_z}^y) \chi_{r-a_1+a_2,y}^\dagger \\ &= (i c_r c_{r+\delta_z}) \left[i \left(\chi_{r+a_2,x} - \chi_{r+a_2,x}^\dagger \right) \right] \\ &= -c_r c_{r+\delta_z} \left(\chi_{r+a_2,x} - \chi_{r+a_2,x}^\dagger \right) \end{aligned} \quad (65)$$

在braket中 $= c_r c_{r+\delta_z} \chi_{r+a_2,x}^\dagger$

因此

$$\begin{aligned} &\left\langle 0_\chi, 0_{\alpha(1)} \left| \chi_{r+a_2,x} \alpha(1) H_h \alpha^\dagger(2) \chi_{r-a_1+a_2,y}^\dagger \right| 0_\chi, 0_{\alpha(2)} \right\rangle \\ &= \left\langle 0_\chi, 0_{\alpha(1)} \left| \chi_{r+a_2,x} \alpha(1) [-h_z (\sigma_r + \sigma_{r+\delta_z})] \alpha^\dagger(2) \chi_{r-a_1+a_2,y}^\dagger \right| 0_\chi, 0_{\alpha(2)} \right\rangle \\ &= -h_z \left\langle 0_\chi, 0_{\alpha(1)} \left| \chi_{r+a_2,x} \alpha(1) [(c_r c_{r+\delta_z} - i)] \alpha^\dagger(2) \chi_{r+a_2,x}^\dagger \right| 0_\chi, 0_{\alpha(2)} \right\rangle \\ &= i h_z \left\langle 0_\chi, 0_{\alpha(1)} \left| \chi_{r+a_2,x} \alpha(1) (1 + i c_r c_{r+\delta_z}) \alpha^\dagger(2) \chi_{r+a_2,x}^\dagger \right| 0_\chi, 0_{\alpha(2)} \right\rangle \\ &= i h_z \left\langle 0_\chi, 0_{\alpha(1)} \left| \alpha(1) (1 + i c_r c_{r+\delta_z}) \alpha^\dagger(2) \right| 0_\chi, 0_{\alpha(2)} \right\rangle \\ &= i h_z \left\langle 0_\chi, 0_{\alpha(1)} \left| \alpha(1) (1 + i c_{i,A} c_{j,B}) \alpha^\dagger(2) \right| 0_\chi, 0_{\alpha(2)} \right\rangle \end{aligned} \quad (66)$$

$T(\mathbf{a}_1)$ 的作用

$$\begin{aligned} &T(\mathbf{a}_1) (a_1 \ a_2 \ \cdots \ a_{N_1} \ a_{N_1+1} \ a_{N_1+2} \ \cdots \ a_{2N_1} \ \cdots \ \cdots) T^{-1}(\mathbf{a}_1) \\ &= (a_2 \ a_3 \ \cdots \ -a_1 \ a_{N_1+2} \ a_{N_1+3} \ \cdots \ -a_{N_1} \ \cdots \ \cdots) \\ &= (a_1 \ a_2 \ \cdots \ a_{N_1} \ a_{N_1+1} \ a_{N_1+2} \ \cdots \ a_{2N_1} \ \cdots \ \cdots) \bigoplus_{i=1}^{N_2} \begin{pmatrix} 0 & 0 & 0 & 0 & \cdots & -1 \\ 1 & 0 & 0 & 0 & \cdots & 0 \\ 0 & 1 & 0 & 0 & \cdots & 0 \\ 0 & 0 & 1 & 0 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & 1 & 0 \end{pmatrix} \end{aligned} \quad (67)$$

$$T_1 \equiv \bigoplus_{i=1}^{N_2} \begin{pmatrix} 0 & 0 & 0 & 0 & \cdots & -1 \\ 1 & 0 & 0 & 0 & \cdots & 0 \\ 0 & 1 & 0 & 0 & \cdots & 0 \\ 0 & 0 & 1 & 0 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & 1 & 0 \end{pmatrix} \quad (68)$$

$$T(\mathbf{a}_1) \begin{pmatrix} a^\dagger & a^\top \end{pmatrix} T^{-1}(\mathbf{a}_1) = \begin{pmatrix} a^\dagger & a^\top \end{pmatrix} \begin{pmatrix} T_1 & 0 \\ 0 & T_1 \end{pmatrix} \quad (69)$$

$$\begin{aligned} T(\mathbf{a}_1) \begin{pmatrix} a \\ (a^\dagger)^\top \end{pmatrix} T^{-1}(\mathbf{a}_1) &= \begin{pmatrix} T_1^\dagger & 0 \\ 0 & T_1^\dagger \end{pmatrix} \begin{pmatrix} a \\ (a^\dagger)^\top \end{pmatrix} \\ &= \begin{pmatrix} T_1^\top & 0 \\ 0 & T_1^\top \end{pmatrix} \begin{pmatrix} a \\ (a^\dagger)^\top \end{pmatrix} \end{aligned} \quad (70)$$

$$\begin{aligned} \begin{pmatrix} a^\dagger & a^\top \end{pmatrix} &= T(\mathbf{a}_1) \begin{pmatrix} a^\dagger & a^\top \end{pmatrix} T^{-1}(\mathbf{a}_1) \begin{pmatrix} T_1 & 0 \\ 0 & T_1 \end{pmatrix}^{-1} \\ &= T(\mathbf{a}_1) \begin{pmatrix} a^\dagger & a^\top \end{pmatrix} T^{-1}(\mathbf{a}_1) \begin{pmatrix} T_1 & 0 \\ 0 & T_1 \end{pmatrix}^\dagger \\ &= T(\mathbf{a}_1) \begin{pmatrix} a^\dagger & a^\top \end{pmatrix} T^{-1}(\mathbf{a}_1) \begin{pmatrix} T_1^\top & 0 \\ 0 & T_1^\top \end{pmatrix} \end{aligned} \quad (71)$$

$$\boxed{\begin{aligned} T(-\mathbf{a}_1) \begin{pmatrix} a^\dagger & a^\top \end{pmatrix} T^{-1}(-\mathbf{a}_1) &= T^{-1}(\mathbf{a}_1) \begin{pmatrix} a^\dagger & a^\top \end{pmatrix} T(\mathbf{a}_1) \\ &= \begin{pmatrix} a^\dagger & a^\top \end{pmatrix} \begin{pmatrix} T_1^\top & 0 \\ 0 & T_1^\top \end{pmatrix} \end{aligned}} \quad (72)$$

$$T(-\mathbf{a}_1) \begin{pmatrix} a^\top \\ (a^\dagger)^\top \end{pmatrix} T^{-1}(-\mathbf{a}_1) = \begin{pmatrix} T_1 & 0 \\ 0 & T_1 \end{pmatrix} \begin{pmatrix} a \\ (a^\dagger)^\top \end{pmatrix} \quad (73)$$

$T(\mathbf{a}_2)$ 的作用

$$\begin{aligned} &T(\mathbf{a}_2) \begin{pmatrix} a_1 & a_2 & \cdots & a_{N_1} & a_{N_1+1} & a_{N_1+2} & \cdots & a_{2N_1} & \cdots & \cdots \end{pmatrix} T^{-1}(\mathbf{a}_2) \\ &= T(\mathbf{a}_1) \begin{pmatrix} a_{N_1+1} & a_{N_1+2} & \cdots & a_{2N_1} & a_{2N_1+1} & a_{2N_1+2} & \cdots & a_{3N_1} & \cdots & -a_1 & -a_2 & \cdots & -a_{N_1} \end{pmatrix} T^{-1}(\mathbf{a}_1) \\ &= \begin{pmatrix} a_1 & a_2 & \cdots & a_{N_1} & a_{N_1+1} & a_{N_1+2} & \cdots & a_{2N_1} & \cdots & \cdots \end{pmatrix} \begin{pmatrix} 0 & 0 & 0 & 0 & \cdots & -I_{N_1} \\ I_{N_1} & 0 & 0 & 0 & \cdots & 0 \\ 0 & I_{N_1} & 0 & 0 & \cdots & 0 \\ 0 & 0 & \ddots & \cdots & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \cdots & 0 \\ 0 & 0 & 0 & \cdots & I_{N_1} & 0 \end{pmatrix} \end{aligned} \quad (74)$$

$$T_2 \equiv \begin{pmatrix} 0 & 0 & 0 & 0 & \cdots & -I_{N_1} \\ I_{N_1} & 0 & 0 & 0 & \cdots & 0 \\ 0 & I_{N_1} & 0 & 0 & \cdots & 0 \\ 0 & 0 & \ddots & \cdots & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \cdots & 0 \\ 0 & 0 & 0 & \cdots & I_{N_1} & 0 \end{pmatrix} \quad (75)$$

$$T(\mathbf{a}_2) \begin{pmatrix} a^\dagger & a^\top \end{pmatrix} T^{-1}(\mathbf{a}_2) = \begin{pmatrix} a^\dagger & a^\top \end{pmatrix} \begin{pmatrix} T_2 & 0 \\ 0 & T_2 \end{pmatrix} \quad (76)$$

$$\begin{aligned}
T(\mathbf{a}_2) \begin{pmatrix} \mathbf{a} \\ (\mathbf{a}^\dagger)^\top \end{pmatrix} T^{-1}(\mathbf{a}_2) &= \begin{pmatrix} T_2^\dagger & 0 \\ 0 & T_2^\dagger \end{pmatrix} \begin{pmatrix} \mathbf{a} \\ (\mathbf{a}^\dagger)^\top \end{pmatrix} \\
&= \begin{pmatrix} T_2^\top & 0 \\ 0 & T_2^\top \end{pmatrix} \begin{pmatrix} \mathbf{a} \\ (\mathbf{a}^\dagger)^\top \end{pmatrix}
\end{aligned} \tag{77}$$

哈密顿量的关系

已知 $H(\mathbf{r}, x/y/z)$, 要求 $H(\mathbf{r} + \mathbf{a}_2, x)$ 和 $H(\mathbf{r} - \mathbf{a}_1 + \mathbf{a}_2, y)$

$$\begin{aligned}
H(\mathbf{r} + \mathbf{a}_2, x) &= T(\mathbf{a}_2)H(\mathbf{r}, x)T^{-1}(\mathbf{a}_2) \\
&= \frac{1}{2}T(\mathbf{a}_2) \begin{pmatrix} \mathbf{a}^\dagger & \mathbf{a}^\top \end{pmatrix} T^{-1}(\mathbf{a}_2)h(\mathbf{r}, x)T(\mathbf{a}_2) \begin{pmatrix} \mathbf{a} \\ (\mathbf{a}^\dagger)^\top \end{pmatrix} T^{-1}(\mathbf{a}_2) \\
&= \frac{1}{2} \begin{pmatrix} \mathbf{a}^\dagger & \mathbf{a}^\top \end{pmatrix} \begin{pmatrix} T_2 & 0 \\ 0 & T_2 \end{pmatrix} h(\mathbf{r}, x) \begin{pmatrix} T_2^\top & 0 \\ 0 & T_2^\top \end{pmatrix} \begin{pmatrix} \mathbf{a} \\ (\mathbf{a}^\dagger)^\top \end{pmatrix}
\end{aligned} \tag{78}$$

$$\boxed{h(\mathbf{r} + \mathbf{a}_2) = \begin{pmatrix} T_2 & 0 \\ 0 & T_2 \end{pmatrix} h(\mathbf{r}, x) \begin{pmatrix} T_2^\top & 0 \\ 0 & T_2^\top \end{pmatrix}} \tag{79}$$

$$h(\mathbf{r}, x)U = UD \implies h(\mathbf{r} + \mathbf{a}_2) (\mathbf{T}_2 U) = (\mathbf{T}_2 U) D \tag{80}$$

$$\begin{aligned}
H(\mathbf{r} - \mathbf{a}_1 + \mathbf{a}_2, y) &= T(-\mathbf{a}_1)T(\mathbf{a}_2)H(\mathbf{r}, y)T^{-1}(\mathbf{a}_2)T^{-1}(-\mathbf{a}_1) \\
&= \frac{1}{2}T(-\mathbf{a}_1)T(\mathbf{a}_2) \begin{pmatrix} \mathbf{a}^\dagger & \mathbf{a}^\top \end{pmatrix} T^{-1}(\mathbf{a}_2)T^{-1}(-\mathbf{a}_1)h(\mathbf{r}, y)T(-\mathbf{a}_1)T(\mathbf{a}_2) \begin{pmatrix} \mathbf{a} \\ (\mathbf{a}^\dagger)^\top \end{pmatrix} T^{-1}(\mathbf{a}_2)T^{-1}(-\mathbf{a}_1) \\
&= \frac{1}{2} \begin{pmatrix} \mathbf{a}^\dagger & \mathbf{a}^\top \end{pmatrix} \begin{pmatrix} T_2 & 0 \\ 0 & T_2 \end{pmatrix} \begin{pmatrix} T_1^\top & 0 \\ 0 & T_1^\top \end{pmatrix} h(\mathbf{r}, y) \begin{pmatrix} T_1 & 0 \\ 0 & T_1 \end{pmatrix} \begin{pmatrix} T_2^\top & 0 \\ 0 & T_2^\top \end{pmatrix} \begin{pmatrix} \mathbf{a} \\ (\mathbf{a}^\dagger)^\top \end{pmatrix}
\end{aligned} \tag{81}$$

$$\boxed{h(\mathbf{r} - \mathbf{a}_1 + \mathbf{a}_2, y) = \begin{pmatrix} T_2 & 0 \\ 0 & T_2 \end{pmatrix} \begin{pmatrix} T_1^\top & 0 \\ 0 & T_1^\top \end{pmatrix} h(\mathbf{r}, y) \begin{pmatrix} T_1 & 0 \\ 0 & T_1 \end{pmatrix} \begin{pmatrix} T_2^\top & 0 \\ 0 & T_2^\top \end{pmatrix}} \tag{82}$$

$$h(\mathbf{r}, y)U = UD \implies h(\mathbf{r} - \mathbf{a}_1 + \mathbf{a}_2) (\mathbf{T}_2 \mathbf{T}_1^\top U) = (\mathbf{T}_2 \mathbf{T}_1^\top U) D \tag{83}$$