

标准规范 $\{u_{ij} = +1\}$ 下, 哈密顿量

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

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

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

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

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:

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

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

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

考虑构型 $\{u_{ij}\}$ 下, 哈密顿量

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

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

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

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

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

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 $\alpha(0)$

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Wick定理给出

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

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

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

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

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

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

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

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

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

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

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

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

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

• ◦ $\langle c_{j,B} \alpha^\dagger(2) \rangle$

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

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

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

• ◦ $\langle c_{i,A} c_{j,B} \rangle$

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

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

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

以B子格为中心

要算

$$\begin{aligned} & \left\langle 0_\chi, 0_{\alpha(1)} \middle| \chi_{r+a_2,x} \alpha(1) H_h \alpha^\dagger(2) \chi_{r-a_1+a_2,y}^\dagger \middle| 0_\chi, 0_{\alpha(2)} \right\rangle \\ &= \left\langle 0_\chi, 0_{\alpha(1)} \middle| \chi_{r+a_2,x} \alpha(1) [-h_z (\sigma_r + \sigma_{r+\delta_z})] \alpha^\dagger(2) \chi_{r-a_1+a_2,y}^\dagger \middle| 0_\chi, 0_{\alpha(2)} \right\rangle \end{aligned} \quad (59)$$

注意到

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

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

于是

$$\begin{aligned} \sigma_{\mathbf{r}+\delta_z}^z &= ib_{\mathbf{r}+\delta_z}^z c_{\mathbf{r}+\delta_z} = -ib_{\mathbf{r}+\delta_z}^x b_{\mathbf{r}+\delta_z}^y \\ &= -ib_{\mathbf{r}+\mathbf{a}_2+\delta_z}^x b_{\mathbf{r}-\mathbf{a}_1+\mathbf{a}_2+\delta_y}^y \\ &= -i \cdot \frac{1}{i} (\chi_{\mathbf{r}+\mathbf{a}_2,x} - \chi_{\mathbf{r}+\mathbf{a}_2,x}^\dagger) \cdot \frac{1}{i} (\chi_{\mathbf{r}-\mathbf{a}_1+\mathbf{a}_2,y} - \chi_{\mathbf{r}-\mathbf{a}_1+\mathbf{a}_2,y}^\dagger) \\ &= i (\chi_{\mathbf{r}+\mathbf{a}_2,x} - \chi_{\mathbf{r}+\mathbf{a}_2,x}^\dagger) (\chi_{\mathbf{r}-\mathbf{a}_1+\mathbf{a}_2,y} - \chi_{\mathbf{r}-\mathbf{a}_1+\mathbf{a}_2,y}^\dagger) \end{aligned} \quad (62)$$

$$\begin{aligned} \sigma_{\mathbf{r}+\delta_z} \chi_{\mathbf{r}-\mathbf{a}_1+\mathbf{a}_2,y}^\dagger &= i (\chi_{\mathbf{r}+\mathbf{a}_2,x} - \chi_{\mathbf{r}+\mathbf{a}_2,x}^\dagger) (\chi_{\mathbf{r}-\mathbf{a}_1+\mathbf{a}_2,y} - \chi_{\mathbf{r}-\mathbf{a}_1+\mathbf{a}_2,y}^\dagger) \cdot \chi_{\mathbf{r}-\mathbf{a}_1+\mathbf{a}_2,y}^\dagger \\ &= i (\chi_{\mathbf{r}+\mathbf{a}_2,x} - \chi_{\mathbf{r}+\mathbf{a}_2,x}^\dagger) \end{aligned} \quad (63)$$

在braket中 = $-i \chi_{\mathbf{r}+\mathbf{a}_2,x}^\dagger$

$$\begin{aligned} \sigma_{\mathbf{r}}^z &= ib_{\mathbf{r}}^z c_{\mathbf{r}} = b_{\mathbf{r}+\delta_z}^x b_{\mathbf{r}+\delta_z}^y b_{\mathbf{r}+\delta_z}^z c_{\mathbf{r}+\delta_z} (ib_{\mathbf{r}}^z c_{\mathbf{r}}) \\ &= (-ib_{\mathbf{r}+\delta_z}^x b_{\mathbf{r}+\delta_z}^y) (ic_{\mathbf{r}} c_{\mathbf{r}+\delta_z}) (-ib_{\mathbf{r}}^z b_{\mathbf{r}+\delta_z}^z) \\ &= (-ib_{\mathbf{r}+\delta_z}^x b_{\mathbf{r}+\delta_z}^y) (ic_{\mathbf{r}} c_{\mathbf{r}+\delta_z}) \cdot 1 \end{aligned} \quad (64)$$

$$\begin{aligned} \sigma_{\mathbf{r}}^z \chi_{\mathbf{r}-\mathbf{a}_1+\mathbf{a}_2,y}^\dagger &= (-ib_{\mathbf{r}+\delta_z}^x b_{\mathbf{r}+\delta_z}^y) (ic_{\mathbf{r}} c_{\mathbf{r}+\delta_z}) \chi_{\mathbf{r}-\mathbf{a}_1+\mathbf{a}_2,y}^\dagger \\ &= (ic_{\mathbf{r}} c_{\mathbf{r}+\delta_z}) (-ib_{\mathbf{r}+\delta_z}^x b_{\mathbf{r}+\delta_z}^y) \chi_{\mathbf{r}-\mathbf{a}_1+\mathbf{a}_2,y}^\dagger \\ &= (ic_{\mathbf{r}} c_{\mathbf{r}+\delta_z}) [i (\chi_{\mathbf{r}+\mathbf{a}_2,x} - \chi_{\mathbf{r}+\mathbf{a}_2,x}^\dagger)] \\ &= -c_{\mathbf{r}} c_{\mathbf{r}+\delta_z} (\chi_{\mathbf{r}+\mathbf{a}_2,x} - \chi_{\mathbf{r}+\mathbf{a}_2,x}^\dagger) \end{aligned} \quad (65)$$

在braket中 = $c_{\mathbf{r}} c_{\mathbf{r}+\delta_z} \chi_{\mathbf{r}+\mathbf{a}_2,x}^\dagger$

因此

$$\begin{aligned} &\left\langle 0_\chi, 0_{\alpha(1)} \mid \chi_{\mathbf{r}+\mathbf{a}_2,x} \alpha(1) H_h \alpha^\dagger(2) \chi_{\mathbf{r}-\mathbf{a}_1+\mathbf{a}_2,y}^\dagger \mid 0_\chi, 0_{\alpha(2)} \right\rangle \\ &= \left\langle 0_\chi, 0_{\alpha(1)} \mid \chi_{\mathbf{r}+\mathbf{a}_2,x} \alpha(1) [-h_z (\sigma_{\mathbf{r}} + \sigma_{\mathbf{r}+\delta_z})] \alpha^\dagger(2) \chi_{\mathbf{r}-\mathbf{a}_1+\mathbf{a}_2,y}^\dagger \mid 0_\chi, 0_{\alpha(2)} \right\rangle \\ &= -h_z \left\langle 0_\chi, 0_{\alpha(1)} \mid \chi_{\mathbf{r}+\mathbf{a}_2,x} \alpha(1) [(c_{\mathbf{r}} c_{\mathbf{r}+\delta_z} - i)] \alpha^\dagger(2) \chi_{\mathbf{r}+\mathbf{a}_2,x}^\dagger \mid 0_\chi, 0_{\alpha(2)} \right\rangle \\ &= ih_z \left\langle 0_\chi, 0_{\alpha(1)} \mid \chi_{\mathbf{r}+\mathbf{a}_2,x} \alpha(1) (1 + ic_{\mathbf{r}} c_{\mathbf{r}+\delta_z}) \alpha^\dagger(2) \chi_{\mathbf{r}+\mathbf{a}_2,x}^\dagger \mid 0_\chi, 0_{\alpha(2)} \right\rangle \\ &= ih_z \left\langle 0_\chi, 0_{\alpha(1)} \mid \alpha(1) (1 + ic_{\mathbf{r}} c_{\mathbf{r}+\delta_z}) \alpha^\dagger(2) \mid 0_\chi, 0_{\alpha(2)} \right\rangle \\ &= ih_z \left\langle 0_\chi, 0_{\alpha(1)} \mid \alpha(1) (1 + ic_{i,A} c_{j,B}) \alpha^\dagger(2) \mid 0_\chi, 0_{\alpha(2)} \right\rangle \end{aligned} \quad (66)$$

$T(\mathbf{a}_1)$ 的作用

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

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

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

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

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

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

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

$T(\mathbf{a}_2)$ 的作用

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

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

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

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

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 $H(\mathbf{r} - \mathbf{a}_1 + \mathbf{a}_2, y)$

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

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

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

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

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

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