Hubbard dimer : Green function and EKT

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Table des matières

1 Introduction

We chosed the spin-up configuration for $N = 1, 3$.

We used $\beta_{i,j}$ as coefficients for the eigenvector table for $N = 1$, we did the same with $\alpha_{i,j}$ and $\gamma_{i,j}$ for $N = 2$ and $N = 3$.

By symmetry, we have $G_{ij\sigma} = G_{ji\sigma}$ for all i, j, σ

2 N=1 electron

2.1 One particle Green's function

2.1.1 General case : $U_1 \neq U_2$ and $\epsilon_1 \neq \epsilon_2$

$$G_{ij\sigma}(\omega) = \sum_{\psi} \frac{\left\langle \psi \left| c_{i\sigma}^{\dagger} \right| \chi_0 \right\rangle \left\langle \chi_0 \left| c_{j\sigma} \right| \psi \right\rangle}{\omega - (E_{\psi} - E_0) + i\eta} + \frac{\left\langle 0 \quad 0 \left| c_{i\sigma} \right| \chi_0 \right\rangle \left\langle \chi_0 \left| c_{j\sigma}^{\dagger} \right| 0 \quad 0 \right\rangle}{\omega - E_0 - i\eta}$$

With $E_0 = (\epsilon_1 + \epsilon_2)/2 - d$

And with

$$A_{ij\sigma}^{N=1} = \left\langle 0 \quad 0 \left| c_{i\sigma} \right| \chi_0 \right\rangle \left\langle \chi_0 \left| c_{j\sigma}^{\dagger} \right| 0 \quad 0 \right\rangle$$

and

$$B_{m,ij\sigma}^{N=1} = \left\langle \psi_m \left| c_{i\sigma}^{\dagger} \right| \chi_0 \right\rangle \left\langle \chi_0 \left| c_{j\sigma} \right| \psi_m \right\rangle$$

$$G_{ij\sigma}(\omega) = \sum_{m} \frac{B_{m,ij\sigma}^{N=1}}{\omega - (E_{\psi_m} - E_0) + i\eta} + \frac{A_{ij\sigma}^{N=1}}{\omega - E_0 - i\eta}$$

2.1.2 Basic case : $U_1 = U_2 = U$ and $\epsilon_1 = \epsilon_2 = \epsilon_0$

$$\begin{aligned}
G_{ij\uparrow}(\omega) &= \frac{(-1)^{(i-j)}}{2} \left[\frac{1}{\omega - (\epsilon_0 + t) + i\eta} + \frac{(-1)^{(i-j)}}{\omega - (\epsilon_0 - t) - i\eta} \right] \\
G_{ij\downarrow}(\omega) &= \frac{(-1)^{(i-j)}}{4} \left[\frac{1}{\omega - (\epsilon_0 + t) + i\eta} + \frac{1}{\omega - (\epsilon_0 + t + U) + i\eta} \right] \\
&\quad + \frac{1}{2} \left[\frac{\frac{1}{a^2}\left(1 + \frac{4t}{(c-U)}\right)^2}{\omega - (\epsilon_0 + t - (c-U)/2) + i\eta} + \frac{\frac{1}{b^2}\left(1 - \frac{4t}{(c+U)}\right)^2}{\omega - (\epsilon_0 + t + (c+U)/2) + i\eta} \right]
\end{aligned}$$

2.2 Density matrix

2.2.1 General case : $U_1 \neq U_2$ and $\epsilon_1 \neq \epsilon_2$

$$\gamma_{ij\sigma} = \sum_{m} A_{m,ji\sigma}^{N=1}$$

2.2.2 Basic case : $U_1 = U_2 = U$ and $\epsilon_1 = \epsilon_2 = \epsilon_0$

3 N=2 electrons

3.1 One particle Green's function

3.1.1 General case : $U_1 \neq U_2$ and $\epsilon_1 \neq \epsilon_2$

$$G_{ij\sigma}(\omega) = \sum_{\phi} \frac{\left\langle \phi \left| c^{\dagger}_{i\sigma} \right| \psi_0 \right\rangle \langle \psi_0 \left| c_{j\sigma} \right| \phi \rangle}{\omega - (E_\phi - E_0) + i\eta} + \sum_{\chi} \frac{\langle \chi \left| c_{i\sigma} \right| \psi_0 \rangle \left\langle \psi_0 \left| c^{\dagger}_{j\sigma} \right| \chi \right\rangle}{\omega + (E_\chi - E_0) - i\eta}$$

And with

$$A^{N=2}_{m,ij\sigma} = \langle \chi_m \left| c_{i\sigma} \right| \psi_0 \rangle \left\langle \psi_0 \left| c^{\dagger}_{j\sigma} \right| \chi_m \right\rangle$$

and

$$B^{N=2}_{m,ij\sigma} = \left\langle \phi_m \left| c^{\dagger}_{i\sigma} \right| \psi_0 \right\rangle \langle \psi_0 \left| c_{j\sigma} \right| \phi_m \rangle$$

$$G_{ij\sigma}(\omega) = \sum_{m} \frac{B^{N=2}_{m,ij\sigma}}{\omega - (E_{\phi_m} - E_0) + i\eta} + \sum_{m} \frac{A^{N=2}_{m,ij\sigma}}{\omega + (E_{\chi_m} - E_0) - i\eta}$$

3.1.2 Basic case : $U_1 = U_2 = U$ and $\epsilon_1 = \epsilon_2 = \epsilon_0$

$$\begin{aligned} G_d(\omega) = {} & \frac{1}{2a^2}\left[\frac{\left(1+\frac{4t}{(c-U)}\right)^2}{\omega - (\epsilon_0 - t + (c+U)/2) + i\eta} + \frac{\left(1-\frac{4t}{(c-U)}\right)^2}{\omega - (\epsilon_0 + t + (c+U)/2) + i\eta}\right] \\ & + \frac{1}{2a^2}\left[\frac{\left(1+\frac{4t}{(c-U)}\right)^2}{\omega - (\epsilon_0 + t - (c-U)/2) - i\eta} + \frac{\left(1-\frac{4t}{(c-U)}\right)^2}{\omega - (\epsilon_0 - t - (c-U)/2) - i\eta}\right] \end{aligned}$$

$$\begin{aligned} G_a(\omega) = {} & -\frac{1}{2a^2}\left[\frac{\left(1+\frac{4t}{(c-U)}\right)^2}{\omega - (\epsilon_0 - t + (c+U)/2) + i\eta} - \frac{\left(1-\frac{4t}{(c-U)}\right)^2}{\omega - (\epsilon_0 + t + (c+U)/2) + i\eta}\right] \\ & + \frac{1}{2a^2}\left[\frac{\left(1+\frac{4t}{(c-U)}\right)^2}{\omega - (\epsilon_0 + t - (c-U)/2) - i\eta} - \frac{\left(1-\frac{4t}{(c-U)}\right)^2}{\omega - (\epsilon_0 - t - (c-U)/2) - i\eta}\right] \end{aligned}$$

$$G^{N=2}(\omega) = \begin{pmatrix} G_{11\uparrow} & G_{12\uparrow} & 0 & 0 \\ G_{21\uparrow} & G_{22\uparrow} & 0 & 0 \\ 0 & 0 & G_{11\downarrow} & G_{12\downarrow} \\ 0 & 0 & G_{21\downarrow} & G_{22\downarrow} \end{pmatrix} = \begin{pmatrix} G_d & G_a & 0 & 0 \\ G_a & G_d & 0 & 0 \\ 0 & 0 & G_d & G_a \\ 0 & 0 & G_a & G_d \end{pmatrix}$$

3.2 Density matrix

3.2.1 General case : $U_1 \neq U_2$ and $\epsilon_1 \neq \epsilon_2$

$$\gamma^{N=2}_{ij\sigma} = \sum_{m} A^{N=2}_{m,ij\sigma}$$

$$\gamma^{N=2} = \begin{pmatrix} A^2_{1,11\uparrow} + A^2_{3,11\uparrow} & A_{1,11\uparrow}A_{1,22\uparrow} + A_{3,11\uparrow}A_{3,22\uparrow} & 0 & 0 \\ A_{1,11\uparrow}A_{1,22\uparrow} + A_{3,11\uparrow}A_{3,22\uparrow} & A^2_{1,22\uparrow} + A^2_{3,22\uparrow} & 0 & 0 \\ 0 & 0 & A^2_{2,11\downarrow} + A^2_{4,11\downarrow} & A_{2,11\downarrow}A_{2,22\downarrow} + A_{4,11\downarrow}A_{4,22\downarrow} \\ 0 & 0 & A_{2,11\downarrow}A_{2,22\downarrow} + A_{4,11\downarrow}A_{4,22\downarrow} & A^2_{2,22\downarrow} + A^2_{4,22\downarrow} \end{pmatrix}$$

We can only focus either on the top left block of the matrix or the bottom right because it's a block matrix. Here are the eigenvalues and eigenvectors for the top left block :

$$\lambda_\pm = \frac{A^2_{1,11\uparrow} + A^2_{3,11\uparrow} + A^2_{1,22\uparrow} + A^2_{3,22\uparrow} \pm S}{2}$$

With :

$$S = \sqrt{(A^2_{1,11\uparrow} + A^2_{3,11\uparrow} + A^2_{1,22\uparrow} + A^2_{3,22\uparrow})^2 + 4(A_{1,11\uparrow}A_{1,22\uparrow} + A_{3,11\uparrow} + A_{3,22\uparrow})^2 - 4(A^2_{1,11\uparrow} + A^2_{3,11\uparrow})(A^2_{1,22\uparrow} + A^2_{3,22\uparrow})}$$

$$v_\pm = \begin{pmatrix} \sin(\rho_\pm) \\ \cos(\rho_\pm) \end{pmatrix}$$

With :

$$\tan(\rho_\pm) = \frac{A^2_{1,11\uparrow} + A^2_{3,11\uparrow} - A^2_{1,22\uparrow} - A^2_{3,22\uparrow} \pm S}{2(A_{1,11\uparrow}A_{1,22\uparrow} + A_{3,11\uparrow}A_{3,22\uparrow})}$$

This calculus is not optimal, we can directly get γ with the eigenvectors : here α_i are the coefficients of the eigenvector from the groundstate !

$$\gamma^{N=2} = \begin{pmatrix} \alpha_1^2 + \alpha_3^2 & 0 & \alpha_1\alpha_4 - \alpha_2\alpha_3 & 0 \\ 0 & \alpha_2^2 + \alpha_3^2 & 0 & \alpha_1\alpha_3 - \alpha_2\alpha_4 \\ \alpha_1\alpha_4 - \alpha_2\alpha_3 & 0 & \alpha_2^2 + \alpha_4^2 & 0 \\ 0 & \alpha_1\alpha_3 - \alpha_2\alpha_4 & 0 & \alpha_1^2 + \alpha_4^2 \end{pmatrix}$$

3.2.2 Basic case : $U_1 = U_2 = U$ and $\epsilon_1 = \epsilon_2 = \epsilon_0$

$$\gamma_d(\omega) = \frac{1}{2a^2}\left(1 + \frac{4t}{(c-U)}\right)^2 + \frac{1}{2a^2}\left(1 - \frac{4t}{(c-U)}\right)^2$$

$$\gamma_a(\omega) = \frac{1}{2a^2}\left(1 + \frac{4t}{(c-U)}\right)^2 - \frac{1}{2a^2}\left(1 - \frac{4t}{(c-U)}\right)^2$$

We have :

$$\lambda_\pm = \frac{1}{a^2}\left(1 \pm \frac{4t}{(c-U)}\right)^2$$

and

$$\tan(\rho_\pm) = \pm 1$$

3.3 EKT

3.3.1 General case : $U_1 \neq U_2$ and $\epsilon_1 \neq \epsilon_2$

$$V_{ij}^{\nu} = \sum_m (E_0 - E_m^{N-1}) A_{m,ij\sigma}$$

$$\epsilon_\nu = \frac{\sum_m \sum_i \sum_j C_{i\nu}^* C_{j\nu} (E_0 - E_m^{N-1}) A_{m,ij\sigma}^{N=2}}{\sum_m \sum_i \sum_j C_{i\nu}^* C_{j\nu} A_{m,ij\sigma}^{N=2}}$$

$$\epsilon_\nu = \frac{\sum_i \sum_j C_{i\nu}^* C_{j\nu} V_{ij}^{\nu}}{\sum_i \sum_j C_{i\nu}^* C_{j\nu} \gamma_{ij\sigma}^{N=2}}$$

3.3.2 Basic case : $U_1 = U_2 = U$ and $\epsilon_1 = \epsilon_2 = \epsilon_0$

4 N=3 electrons

4.1 One particle Green's function

4.1.1 General case : $U_1 \neq U_2$ and $\epsilon_1 \neq \epsilon_2$

$$G_{ij\sigma}(\omega) = \frac{\left\langle \uparrow\downarrow\uparrow\downarrow \left| c^\dagger_{i\sigma} \right| \phi_0 \right\rangle \langle \phi_0 \left| c_{j\sigma} \right| \uparrow\downarrow\uparrow\downarrow \rangle}{\omega - (E_{\uparrow\downarrow\uparrow\downarrow} - E_0) + i\eta} + \sum_\psi \frac{\langle \psi \left| c_{i\sigma} \right| \phi_0 \rangle \left\langle \phi_0 \left| c^\dagger_{j\sigma} \right| \psi \right\rangle}{\omega + (E_\psi - E_0) - i\eta}$$

With $E_0 = \frac{1}{2}(3\epsilon_1 + 3\epsilon_2 + U_1 + U_2 - g)$ and $E_{\uparrow\downarrow\uparrow\downarrow} = (2\epsilon_1 + 2\epsilon_2 + U_1 + U_2)$

$$\begin{aligned} G_{11\uparrow}(\omega) = &\frac{\gamma_{1,2}^2}{\omega - (E_{\uparrow\downarrow\uparrow\downarrow} - E_0) + i\eta} + \frac{(\alpha_{0,2}\gamma_{2,3} + \alpha_{0,4}\gamma_{2,1})^2}{\omega + (E_{\psi_1} - E_0) - i\eta} + \frac{(\alpha_{1,2}\gamma_{2,3} + \alpha_{1,4}\gamma_{2,1})^2}{\omega + (E_{\psi_2} - E_0) - i\eta} \\ &+ \frac{(\alpha_{2,2}\gamma_{2,3} + \alpha_{2,4}\gamma_{2,1})^2}{\omega + (E_{\psi_3} - E_0) - i\eta} + \frac{\gamma_{1,4}^2}{\omega + (E_{\psi_4} - E_0) - i\eta} + \frac{\gamma_{2,3}^2/2}{\omega + (E_{\psi_6} - E_0) - i\eta} \end{aligned}$$

$$\begin{aligned} G_{22\uparrow}(\omega) = &\frac{\gamma_{1,4}^2}{\omega - (E_{\uparrow\downarrow\uparrow\downarrow} - E_0) + i\eta} + \frac{(\alpha_{0,3}\gamma_{2,3} - \alpha_{0,1}\gamma_{2,1})^2}{\omega + (E_{\psi_1} - E_0) - i\eta} + \frac{(\alpha_{1,3}\gamma_{2,3} - \alpha_{1,1}\gamma_{2,1})^2}{\omega + (E_{\psi_2} - E_0) - i\eta} \\ &+ \frac{(\alpha_{2,3}\gamma_{2,3} - \alpha_{2,1}\gamma_{2,1})^2}{\omega + (E_{\psi_3} - E_0) - i\eta} + \frac{\gamma_{1,2}^2}{\omega + (E_{\psi_4} - E_0) - i\eta} + \frac{\gamma_{2,1}^2/2}{\omega + (E_{\psi_6} - E_0) - i\eta} \end{aligned}$$

$$\begin{aligned} G_{12\uparrow}(\omega) = &\frac{\gamma_{1,2}\gamma_{1,4}}{\omega - (E_{\uparrow\downarrow\uparrow\downarrow} - E_0) + i\eta} + \frac{(\alpha_{0,2}\gamma_{2,3} + \alpha_{0,4}\gamma_{2,1})(\alpha_{0,3}\gamma_{2,3} - \alpha_{0,1}\gamma_{2,1})}{\omega + (E_{\psi_1} - E_0) - i\eta} \\ &+ \frac{(\alpha_{1,2}\gamma_{2,3} + \alpha_{1,4}\gamma_{2,1})(\alpha_{1,3}\gamma_{2,3} - \alpha_{1,1}\gamma_{2,1})}{\omega + (E_{\psi_2} - E_0) - i\eta} + \frac{(\alpha_{2,2}\gamma_{2,3} + \alpha_{2,4}\gamma_{2,1})(\alpha_{2,3}\gamma_{2,3} - \alpha_{2,1}\gamma_{2,1})}{\omega + (E_{\psi_3} - E_0) - i\eta} \\ &- \frac{\gamma_{1,4}\gamma_{1,2}}{\omega + (E_{\psi_4} - E_0) - i\eta} - \frac{\gamma_{2,3}\gamma_{2,1}/2}{\omega + (E_{\psi_6} - E_0) - i\eta} \end{aligned}$$

$$\begin{aligned} G_{11\downarrow}(\omega) = &\frac{\gamma_{2,1}^2}{\omega - (E_{\uparrow\downarrow\uparrow\downarrow} - E_0) + i\eta} + \frac{(\alpha_{0,4}\gamma_{1,2} - \alpha_{0,1}\gamma_{1,4})^2}{\omega + (E_{\psi_1} - E_0) - i\eta} + \frac{(\alpha_{1,4}\gamma_{1,2} - \alpha_{1,1}\gamma_{1,4})^2}{\omega + (E_{\psi_2} - E_0) - i\eta} \\ &+ \frac{(\alpha_{2,4}\gamma_{1,2} - \alpha_{2,1}\gamma_{1,4})^2}{\omega + (E_{\psi_3} - E_0) - i\eta} + \frac{\gamma_{2,3}^2}{\omega + (E_{\psi_5} - E_0) - i\eta} + \frac{\gamma_{1,4}^2/2}{\omega + (E_{\psi_6} - E_0) - i\eta} \end{aligned}$$

$$\begin{aligned} G_{22\downarrow}(\omega) = &\frac{\gamma_{2,3}^2}{\omega - (E_{\uparrow\downarrow\uparrow\downarrow} - E_0) + i\eta} + \frac{(\alpha_{0,2}\gamma_{1,2} + \alpha_{0,3}\gamma_{1,4})^2}{\omega + (E_{\psi_1} - E_0) - i\eta} + \frac{(\alpha_{1,2}\gamma_{1,2} + \alpha_{1,3}\gamma_{1,4})^2}{\omega + (E_{\psi_2} - E_0) - i\eta} \\ &+ \frac{(\alpha_{2,2}\gamma_{1,2} + \alpha_{2,3}\gamma_{1,4})^2}{\omega + (E_{\psi_3} - E_0) - i\eta} + \frac{\gamma_{2,1}^2}{\omega + (E_{\psi_5} - E_0) - i\eta} + \frac{\gamma_{1,2}^2/2}{\omega + (E_{\psi_6} - E_0) - i\eta} \end{aligned}$$

$$\begin{aligned} G_{12\downarrow}(\omega) = &\frac{\gamma_{2,1}\gamma_{2,3}}{\omega - (E_{\uparrow\downarrow\uparrow\downarrow} - E_0) + i\eta} + \frac{(\alpha_{0,4}\gamma_{1,2} - \alpha_{0,1}\gamma_{1,4})(\alpha_{0,2}\gamma_{1,2} + \alpha_{0,3}\gamma_{1,4})}{\omega + (E_{\psi_1} - E_0) - i\eta} \\ &+ \frac{(\alpha_{1,4}\gamma_{1,2} - \alpha_{1,1}\gamma_{1,4})(\alpha_{1,2}\gamma_{1,2} + \alpha_{1,3}\gamma_{1,4})}{\omega + (E_{\psi_2} - E_0) - i\eta} + \frac{(\alpha_{2,4}\gamma_{1,2} - \alpha_{2,1}\gamma_{1,4})(\alpha_{2,2}\gamma_{1,2} + \alpha_{2,3}\gamma_{1,4})}{\omega + (E_{\psi_3} - E_0) - i\eta} \\ &- \frac{\gamma_{2,3}\gamma_{2,1}}{\omega + (E_{\psi_5} - E_0) - i\eta} - \frac{\gamma_{1,4}\gamma_{1,2}/2}{\omega + (E_{\psi_6} - E_0) - i\eta} \end{aligned}$$

4.1.2 Basic case : $U_1 = U_2 = U$ and $\epsilon_1 = \epsilon_2 = \epsilon_0$

$$\begin{aligned}
G_{ij\uparrow}(\omega) &= \frac{(-1)^{(i-j)}}{4}\left[\frac{1}{\omega-(\epsilon_0-t)+i\eta}+\frac{1}{\omega-(\epsilon_0+U-t)+i\eta}\right] \\
&+\frac{1}{2}\left[\frac{\frac{1}{a^2}\left(1-\frac{4t}{(c-U)}\right)^2}{\omega-(\epsilon_0+(U+c)/2-t)+i\eta}+\frac{\frac{1}{b^2}\left(1+\frac{4t}{(c+U)}\right)^2}{\omega-(\epsilon_0+(U-c)/2-t)+i\eta}\right] \\
G_{ij\downarrow}(\omega) &= \frac{(-1)^{(i-j)}}{2}\left[\frac{1}{\omega-(\epsilon_0+U-t)-i\eta}+\frac{(-1)^{(i-j)}}{\omega-(\epsilon_0+U+t)-i\eta}\right]
\end{aligned}$$

4.2 Density matrix

5 Annexes

5.1 General case : calculus on eigenvectors

5.1.1 $N = 1$ electron : $|\chi_i\rangle$

For $i = 1,3$: $|\chi_i\rangle = \beta_{i,2}|\downarrow \quad 0\rangle + \beta_{i,4}|0 \quad \downarrow\rangle$:

$$
\begin{aligned}
c^\dagger_{1\uparrow}|\chi_i\rangle &= -\beta_{i,2}|\uparrow\downarrow \quad 0\rangle - \beta_{i,4}|\uparrow \quad \downarrow\rangle \\
c_{1\uparrow}|\chi_i\rangle &= 0 \\
c^\dagger_{2\uparrow}|\chi_i\rangle &= \beta_{i,2}|\downarrow \quad \uparrow\rangle - \beta_{i,4}|0 \quad \uparrow\downarrow\rangle \\
c_{2\uparrow}|\chi_i\rangle &= 0 \\
c^\dagger_{1\downarrow}|\chi_i\rangle &= -\beta_{i,4}|\downarrow \quad \downarrow\rangle \\
c_{1\downarrow}|\chi_i\rangle &= \beta_{i,2}|0 \quad 0\rangle \\
c^\dagger_{2\downarrow}|\chi_i\rangle &= \beta_{i,2}|\downarrow \quad \downarrow\rangle \\
c_{2\downarrow}|\chi_i\rangle &= \beta_{i,4}|0 \quad 0\rangle
\end{aligned}
$$

For $i = 2,4$: $|\chi_i\rangle = \beta_{i,1}|\uparrow \quad 0\rangle + \beta_{i,3}|0 \quad \uparrow\rangle$:

$$
\begin{aligned}
c^\dagger_{1\uparrow}|\chi_i\rangle &= -\beta_{i,3}|\uparrow \quad \uparrow\rangle \\
c_{1\uparrow}|\chi_i\rangle &= \beta_{i,1}|0 \quad 0\rangle \\
c^\dagger_{2\uparrow}|\chi_i\rangle &= \beta_{i,1}|\uparrow \quad \uparrow\rangle \\
c_{2\uparrow}|\chi_i\rangle &= \beta_{i,3}|0 \quad 0\rangle \\
c^\dagger_{1\downarrow}|\chi_i\rangle &= \beta_{i,1}|\uparrow\downarrow \quad 0\rangle - \beta_{i,3}|\downarrow \quad \uparrow\rangle \\
c_{1\downarrow}|\chi_i\rangle &= 0 \\
c^\dagger_{2\downarrow}|\chi_i\rangle &= \beta_{i,1}|\uparrow \quad \downarrow\rangle + \beta_{i,3}|0 \quad \uparrow\downarrow\rangle \\
c_{2\downarrow}|\chi_i\rangle &= 0
\end{aligned}
$$

5.1.2 $N = 2$ electrons : $|\psi_i\rangle$

For $i = 1,2,3$, $|\psi_i\rangle = \alpha_{i,1}|\uparrow \quad \downarrow\rangle + \alpha_{i,2}|\downarrow \quad \uparrow\rangle + \alpha_{i,3}|\uparrow\downarrow \quad 0\rangle + \alpha_{i,4}|0 \quad \uparrow\downarrow\rangle$:

$$
\begin{aligned}
c^\dagger_{1\uparrow}|\psi_i\rangle &= \alpha_{i,2}|\uparrow\downarrow \quad \uparrow\rangle + \alpha_{i,4}|\uparrow \quad \uparrow\downarrow\rangle \\
c_{1\uparrow}|\psi_i\rangle &= -\alpha_{i,1}|0 \quad \downarrow\rangle - \alpha_{i,3}|\downarrow \quad 0\rangle \\
c^\dagger_{2\uparrow}|\psi_i\rangle &= -\alpha_{i,1}|\uparrow \quad \uparrow\downarrow\rangle + \alpha_{i,3}|\uparrow\downarrow \quad \uparrow\rangle \\
c_{2\uparrow}|\psi_i\rangle &= \alpha_{i,2}|\downarrow \quad 0\rangle - \alpha_{i,4}|0 \quad \downarrow\rangle \\
c^\dagger_{1\downarrow}|\psi_i\rangle &= -\alpha_{i,1}|\uparrow\downarrow \quad \downarrow\rangle + \alpha_{i,4}|\downarrow \quad \uparrow\downarrow\rangle \\
c_{1\downarrow}|\psi_i\rangle &= -\alpha_{i,2}|0 \quad \uparrow\rangle + \alpha_{i,3}|\uparrow \quad 0\rangle \\
c^\dagger_{2\downarrow}|\psi_i\rangle &= \alpha_{i,2}|\downarrow \quad \uparrow\downarrow\rangle + \alpha_{i,3}|\uparrow\downarrow \quad \downarrow\rangle \\
c_{2\downarrow}|\psi_i\rangle &= \alpha_{i,1}|\uparrow \quad 0\rangle + \alpha_{i,4}|0 \quad \uparrow\rangle
\end{aligned}
$$

Pour $|\psi_4\rangle = |\downarrow \quad \downarrow\rangle$:

$$
\begin{aligned}
c^\dagger_{1\uparrow}\,|\psi_4\rangle &= |\uparrow\downarrow \quad \downarrow\rangle\\
c_{1\uparrow}\,|\psi_4\rangle &= 0\\
c^\dagger_{2\uparrow}\,|\psi_4\rangle &= -|\downarrow \quad \uparrow\downarrow\rangle\\
c_{2\uparrow}\,|\psi_4\rangle &= 0\\
c^\dagger_{1\downarrow}\,|\psi_4\rangle &= 0\\
c_{1\downarrow}\,|\psi_4\rangle &= -|0 \quad \downarrow\rangle\\
c^\dagger_{2\downarrow}\,|\psi_4\rangle &= 0\\
c_{2\downarrow}\,|\psi_4\rangle &= |\downarrow \quad 0\rangle
\end{aligned}
$$

Pour $|\psi_5\rangle = |\uparrow \quad \uparrow\rangle$:

$$
\begin{aligned}
c^\dagger_{1\uparrow}\,|\psi_5\rangle &= 0\\
c_{1\uparrow}\,|\psi_5\rangle &= -|0 \quad \uparrow\rangle\\
c^\dagger_{2\uparrow}\,|\psi_5\rangle &= 0\\
c_{2\uparrow}\,|\psi_5\rangle &= |\uparrow \quad 0\rangle\\
c^\dagger_{1\downarrow}\,|\psi_5\rangle &= -|\uparrow\downarrow \quad \uparrow\rangle\\
c_{1\downarrow}\,|\psi_5\rangle &= 0\\
c^\dagger_{2\downarrow}\,|\psi_5\rangle &= |\uparrow \quad \uparrow\downarrow\rangle\\
c_{2\downarrow}\,|\psi_5\rangle &= 0
\end{aligned}
$$

Pour $|\psi_6\rangle = \frac{1}{\sqrt{2}}|\uparrow \quad \downarrow\rangle + \frac{1}{\sqrt{2}}|\downarrow \quad \uparrow\rangle$:

$$
\begin{aligned}
c^\dagger_{1\uparrow}\,|\psi_6\rangle &= \tfrac{1}{\sqrt{2}}|\uparrow\downarrow \quad \uparrow\rangle\\
c_{1\uparrow}\,|\psi_6\rangle &= -\tfrac{1}{\sqrt{2}}|0 \quad \downarrow\rangle\\
c^\dagger_{2\uparrow}\,|\psi_6\rangle &= -\tfrac{1}{\sqrt{2}}|\uparrow \quad \uparrow\downarrow\rangle\\
c_{2\uparrow}\,|\psi_6\rangle &= \tfrac{1}{\sqrt{2}}|\downarrow \quad 0\rangle\\
c^\dagger_{1\downarrow}\,|\psi_6\rangle &= -\tfrac{1}{\sqrt{2}}|\uparrow\downarrow \quad \downarrow\rangle\\
c_{1\downarrow}\,|\psi_6\rangle &= -\tfrac{1}{\sqrt{2}}|0 \quad \uparrow\rangle\\
c^\dagger_{2\downarrow}\,|\psi_6\rangle &= \tfrac{1}{\sqrt{2}}|\downarrow \quad \uparrow\downarrow\rangle\\
c_{2\downarrow}\,|\psi_6\rangle &= \tfrac{1}{\sqrt{2}}|\uparrow \quad 0\rangle
\end{aligned}
$$

5.1.3 $N = 3$ electrons : $|\phi_i\rangle$

For $i = 1,3$: $|\phi_i\rangle = \gamma_{i,2}|\downarrow \quad \uparrow\downarrow\rangle + \gamma_{i,4}|\uparrow\downarrow \quad \downarrow\rangle$:

$$
\begin{aligned}
c^\dagger_{1\uparrow}\,|\phi_i\rangle &= -\gamma_{i,2}|\uparrow\downarrow \quad \uparrow\downarrow\rangle\\
c_{1\uparrow}\,|\phi_i\rangle &= \gamma_{i,4}|\downarrow \quad \downarrow\rangle\\
c^\dagger_{2\uparrow}\,|\phi_i\rangle &= -\gamma_{i,4}|\uparrow\downarrow \quad \uparrow\downarrow\rangle\\
c_{2\uparrow}\,|\phi_i\rangle &= -\gamma_{i,2}|\downarrow \quad \downarrow\rangle\\
c^\dagger_{1\downarrow}\,|\phi_i\rangle &= 0\\
c_{1\downarrow}\,|\phi_i\rangle &= \gamma_{i,2}|0 \quad \uparrow\downarrow\rangle - \gamma_{i,4}|\uparrow \quad \downarrow\rangle\\
c^\dagger_{2\downarrow}\,|\phi_i\rangle &= 0\\
c_{2\downarrow}\,|\phi_i\rangle &= \gamma_{i,2}|\downarrow \quad \uparrow\rangle + \gamma_{i,4}|\uparrow\downarrow \quad 0\rangle
\end{aligned}
$$

For $i = 2, 4 : |\phi_i\rangle = \gamma_{i,1}|\uparrow \quad \uparrow\downarrow\rangle + \gamma_{i,3}|\uparrow\downarrow \quad \uparrow\rangle$:

$$\begin{aligned}
&c^\dagger_{1\uparrow}|\phi_i\rangle = 0\\
&c_{1\uparrow}|\phi_i\rangle = \gamma_{i,1}|0 \quad \uparrow\downarrow\rangle + \gamma_{i,3}|\downarrow \quad \uparrow\rangle\\
&c^\dagger_{2\uparrow}|\phi_i\rangle = 0\\
&c_{2\uparrow}|\phi_i\rangle = -\gamma_{i,1}|\uparrow \quad \downarrow\rangle + \gamma_{i,3}|\uparrow\downarrow \quad 0\rangle\\
&c^\dagger_{1\downarrow}|\phi_i\rangle = \gamma_{i,1}|\uparrow\downarrow \quad \uparrow\downarrow\rangle\\
&c_{1\downarrow}|\phi_i\rangle = -\gamma_{i,3}|\uparrow \quad \uparrow\rangle\\
&c^\dagger_{2\downarrow}|\phi_i\rangle = \gamma_{i,3}|\uparrow\downarrow \quad \uparrow\downarrow\rangle\\
&c_{2\downarrow}|\phi_i\rangle = \gamma_{i,1}|\uparrow \quad \uparrow\rangle
\end{aligned}$$

5.2 General case : scalar products

5.2.1 With $|\chi_0\rangle = \beta_{1,2}|\downarrow \quad 0\rangle + \beta_{1,4}|0 \quad \downarrow\rangle + \beta_{2,1}|\uparrow \quad 0\rangle + \beta_{2,3}|0 \quad \uparrow\rangle$

$$\begin{aligned}
\left\langle \chi_0 \left| c^\dagger_{1\uparrow} \right| 00 \right\rangle &= \left\langle 00 \left| c_{1\uparrow} \right| \chi_0 \right\rangle = \beta_{2,1} \\
\left\langle \chi_0 \left| c^\dagger_{2\uparrow} \right| 00 \right\rangle &= \left\langle 00 \left| c_{2\uparrow} \right| \chi_0 \right\rangle = \beta_{2,3} \\
\left\langle \chi_0 \left| c^\dagger_{1\downarrow} \right| 00 \right\rangle &= \left\langle 00 \left| c_{1\downarrow} \right| \chi_0 \right\rangle = \beta_{1,2} \\
\left\langle \chi_0 \left| c^\dagger_{2\downarrow} \right| 00 \right\rangle &= \left\langle 00 \left| c_{2\downarrow} \right| \chi_0 \right\rangle = \beta_{1,4}
\end{aligned}$$

$$\begin{aligned}
\left\langle \psi_i \left| c^\dagger_{1\uparrow} \right| \chi_0 \right\rangle &= \left\langle \chi_0 \left| c_{1\uparrow} \right| \psi_i \right\rangle = -\alpha_{i,1}\beta_{1,4} - \alpha_{i,3}\beta_{1,2} \\
\left\langle \psi_i \left| c^\dagger_{2\uparrow} \right| \chi_0 \right\rangle &= \left\langle \chi_0 \left| c_{2\uparrow} \right| \psi_i \right\rangle = \alpha_{i,2}\beta_{1,2} - \alpha_{i,4}\beta_{1,4} \\
\left\langle \psi_i \left| c^\dagger_{1\downarrow} \right| \chi_0 \right\rangle &= \left\langle \chi_0 \left| c_{1\downarrow} \right| \psi_i \right\rangle = -\alpha_{i,2}\beta_{2,3} + \alpha_{i,3}\beta_{2,1} \\
\left\langle \psi_i \left| c^\dagger_{2\downarrow} \right| \chi_0 \right\rangle &= \left\langle \chi_0 \left| c_{2\downarrow} \right| \psi_i \right\rangle = \alpha_{i,1}\beta_{2,1} + \alpha_{i,4}\beta_{2,3}
\end{aligned}$$

$$\begin{aligned}
\left\langle \psi_4 \left| c^\dagger_{1\uparrow} \right| \chi_0 \right\rangle &= \left\langle \chi_0 \left| c_{1\uparrow} \right| \psi_4 \right\rangle = 0 \\
\left\langle \psi_4 \left| c^\dagger_{2\uparrow} \right| \chi_0 \right\rangle &= \left\langle \chi_0 \left| c_{2\uparrow} \right| \psi_4 \right\rangle = 0 \\
\left\langle \psi_4 \left| c^\dagger_{1\downarrow} \right| \chi_0 \right\rangle &= \left\langle \chi_0 \left| c_{1\downarrow} \right| \psi_4 \right\rangle = -\beta_{1,4} \\
\left\langle \psi_4 \left| c^\dagger_{2\downarrow} \right| \chi_0 \right\rangle &= \left\langle \chi_0 \left| c_{2\downarrow} \right| \psi_4 \right\rangle = \beta_{1,2}
\end{aligned}$$

$$\begin{aligned}
\left\langle \psi_5 \left| c^\dagger_{1\uparrow} \right| \chi_0 \right\rangle &= \left\langle \chi_0 \left| c_{1\uparrow} \right| \psi_5 \right\rangle = -\beta_{2,3} \\
\left\langle \psi_5 \left| c^\dagger_{2\uparrow} \right| \chi_0 \right\rangle &= \left\langle \chi_0 \left| c_{2\uparrow} \right| \psi_5 \right\rangle = \beta_{2,1} \\
\left\langle \psi_5 \left| c^\dagger_{1\downarrow} \right| \chi_0 \right\rangle &= \left\langle \chi_0 \left| c_{1\downarrow} \right| \psi_5 \right\rangle = 0 \\
\left\langle \psi_5 \left| c^\dagger_{2\downarrow} \right| \chi_0 \right\rangle &= \left\langle \chi_0 \left| c_{2\downarrow} \right| \psi_5 \right\rangle = 0
\end{aligned}$$

$$\begin{aligned}
\left\langle \psi_6 \left| c^\dagger_{1\uparrow} \right| \chi_0 \right\rangle &= \left\langle \chi_0 \left| c_{1\uparrow} \right| \psi_6 \right\rangle = -\tfrac{\beta_{1,4}}{\sqrt{2}} \\
\left\langle \psi_6 \left| c^\dagger_{2\uparrow} \right| \chi_0 \right\rangle &= \left\langle \chi_0 \left| c_{2\uparrow} \right| \psi_6 \right\rangle = \tfrac{\beta_{1,2}}{\sqrt{2}} \\
\left\langle \psi_6 \left| c^\dagger_{1\downarrow} \right| \chi_0 \right\rangle &= \left\langle \chi_0 \left| c_{1\downarrow} \right| \psi_6 \right\rangle = -\tfrac{\beta_{2,3}}{\sqrt{2}} \\
\left\langle \psi_6 \left| c^\dagger_{2\downarrow} \right| \chi_0 \right\rangle &= \left\langle \chi_0 \left| c_{2\downarrow} \right| \psi_6 \right\rangle = \tfrac{\beta_{2,1}}{\sqrt{2}}
\end{aligned}$$

5.2.2 With $|\psi_0\rangle = \alpha_{0,1}|\uparrow \quad \downarrow\rangle + \alpha_{0,2}|\downarrow \quad \uparrow\rangle + \alpha_{0,3}|\uparrow\downarrow \quad 0\rangle + \alpha_{0,4}|0 \quad \uparrow\downarrow\rangle$

For $i = 1,3 : |\chi_i\rangle = \beta_{i,2}|\downarrow \quad 0\rangle + \beta_{i,4}|0 \quad \downarrow\rangle$:

$$\begin{aligned}
\left\langle \psi_0 \middle| c_{1\uparrow}^\dagger \middle| \chi_i \right\rangle &= \left\langle \chi_i \middle| c_{1\uparrow} \middle| \psi_0 \right\rangle = -\alpha_{0,3}\beta_{i,2} - \alpha_{0,1}\beta_{i,4} \\
\left\langle \psi_0 \middle| c_{2\uparrow}^\dagger \middle| \chi_i \right\rangle &= \left\langle \chi_i \middle| c_{2\uparrow} \middle| \psi_0 \right\rangle = \alpha_{0,2}\beta_{i,2} - \alpha_{0,4}\beta_{i,4} \\
\left\langle \psi_0 \middle| c_{1\downarrow}^\dagger \middle| \chi_i \right\rangle &= \left\langle \chi_i \middle| c_{1\downarrow} \middle| \psi_0 \right\rangle = 0 \\
\left\langle \psi_0 \middle| c_{2\downarrow}^\dagger \middle| \chi_i \right\rangle &= \left\langle \chi_i \middle| c_{2\downarrow} \middle| \psi_0 \right\rangle = 0
\end{aligned}$$

For $i = 2,4 : |\chi_i\rangle = \beta_{i,1}|\uparrow \quad 0\rangle + \beta_{i,3}|0 \quad \uparrow\rangle$:

$$\begin{aligned}
\left\langle \psi_0 \middle| c_{1\uparrow}^\dagger \middle| \chi_i \right\rangle &= \left\langle \chi_i \middle| c_{1\uparrow} \middle| \psi_0 \right\rangle = 0 \\
\left\langle \psi_0 \middle| c_{2\uparrow}^\dagger \middle| \chi_i \right\rangle &= \left\langle \chi_i \middle| c_{2\uparrow} \middle| \psi_0 \right\rangle = 0 \\
\left\langle \psi_0 \middle| c_{1\downarrow}^\dagger \middle| \chi_i \right\rangle &= \left\langle \chi_i \middle| c_{1\downarrow} \middle| \psi_0 \right\rangle = \alpha_{0,3}\beta_{i,1} - \alpha_{0,2}\beta_{i,3} \\
\left\langle \psi_0 \middle| c_{2\downarrow}^\dagger \middle| \chi_i \right\rangle &= \left\langle \chi_i \middle| c_{2\downarrow} \middle| \psi_0 \right\rangle = \alpha_{0,1}\beta_{i,1} + \alpha_{0,4}\beta_{i,3}
\end{aligned}$$

For $i = 1,3 : |\phi_i\rangle = \gamma_{i,2}|\downarrow \quad \uparrow\downarrow\rangle + \gamma_{i,4}|\uparrow\downarrow \quad \downarrow\rangle$:

$$\begin{aligned}
\left\langle \psi_0 \middle| c_{1\uparrow} \middle| \phi_i \right\rangle &= \left\langle \phi_i \middle| c_{1\uparrow}^\dagger \middle| \psi_0 \right\rangle = 0 \\
\left\langle \psi_0 \middle| c_{2\uparrow} \middle| \phi_i \right\rangle &= \left\langle \phi_i \middle| c_{2\uparrow}^\dagger \middle| \psi_0 \right\rangle = 0 \\
\left\langle \psi_0 \middle| c_{1\downarrow} \middle| \phi_i \right\rangle &= \left\langle \phi_i \middle| c_{1\downarrow}^\dagger \middle| \psi_0 \right\rangle = \gamma_{i,2}\alpha_{0,4} - \gamma_{i,4}\alpha_{0,1} \\
\left\langle \psi_0 \middle| c_{2\downarrow} \middle| \phi_i \right\rangle &= \left\langle \phi_i \middle| c_{2\downarrow}^\dagger \middle| \psi_0 \right\rangle = \gamma_{i,2}\alpha_{0,2} + \gamma_{i,4}\alpha_{0,3}
\end{aligned}$$

For $i = 2,4 : |\phi_i\rangle = \gamma_{i,1}|\uparrow \quad \uparrow\downarrow\rangle + \gamma_{i,3}|\uparrow\downarrow \quad \uparrow\rangle$:

$$\begin{aligned}
\left\langle \psi_0 \middle| c_{1\uparrow} \middle| \phi_i \right\rangle &= \left\langle \phi_i \middle| c_{1\uparrow}^\dagger \middle| \psi_0 \right\rangle = \gamma_{i,1}\alpha_{0,4} + \gamma_{i,3}\alpha_{0,2} \\
\left\langle \psi_0 \middle| c_{2\uparrow} \middle| \phi_i \right\rangle &= \left\langle \phi_i \middle| c_{2\uparrow}^\dagger \middle| \psi_0 \right\rangle = -\gamma_{i,1}\alpha_{0,1} + \gamma_{i,3}\alpha_{0,3} \\
\left\langle \psi_0 \middle| c_{1\downarrow} \middle| \phi_i \right\rangle &= \left\langle \phi_i \middle| c_{1\downarrow}^\dagger \middle| \psi_0 \right\rangle = 0 \\
\left\langle \psi_0 \middle| c_{2\downarrow} \middle| \phi_i \right\rangle &= \left\langle \phi_i \middle| c_{2\downarrow}^\dagger \middle| \psi_0 \right\rangle = 0
\end{aligned}$$

5.2.3 With $|\phi_0\rangle = \gamma_{2,1}|\uparrow \quad \uparrow\downarrow\rangle + \gamma_{1,2}|\downarrow \quad \uparrow\downarrow\rangle + \gamma_{2,3}|\uparrow\downarrow \quad \uparrow\rangle + \gamma_{1,4}|\uparrow\downarrow \quad \downarrow\rangle$

$$\begin{aligned}
\langle\uparrow\downarrow\uparrow\downarrow\left|c^\dagger_{1\uparrow}\right|\phi_0\rangle &= \langle\phi_0\left|c_{1\uparrow}\right|\uparrow\downarrow\uparrow\downarrow\rangle = -\gamma_{1,2}\\
\langle\uparrow\downarrow\uparrow\downarrow\left|c^\dagger_{2\uparrow}\right|\phi_0\rangle &= \langle\phi_0\left|c_{2\uparrow}\right|\uparrow\downarrow\uparrow\downarrow\rangle = -\gamma_{1,4}\\
\langle\uparrow\downarrow\uparrow\downarrow\left|c^\dagger_{1\downarrow}\right|\phi_0\rangle &= \langle\phi_0\left|c_{1\downarrow}\right|\uparrow\downarrow\uparrow\downarrow\rangle = \gamma_{2,1}\\
\langle\uparrow\downarrow\uparrow\downarrow\left|c^\dagger_{2\downarrow}\right|\phi_0\rangle &= \langle\phi_0\left|c_{2\downarrow}\right|\uparrow\downarrow\uparrow\downarrow\rangle = \gamma_{2,3}
\end{aligned}$$

$$\begin{aligned}
\langle\psi_i\left|c_{1\uparrow}\right|\phi_0\rangle &= \langle\phi_0\left|c^\dagger_{1\uparrow}\right|\psi_i\rangle = \alpha_{i,2}\gamma_{2,3} + \alpha_{i,4}\gamma_{2,1}\\
\langle\psi_i\left|c_{2\uparrow}\right|\phi_0\rangle &= \langle\phi_0\left|c^\dagger_{2\uparrow}\right|\psi_i\rangle = -\alpha_{i,1}\gamma_{2,1} + \alpha_{i,3}\gamma_{2,3}\\
\langle\psi_i\left|c_{1\downarrow}\right|\phi_0\rangle &= \langle\phi_0\left|c^\dagger_{1\downarrow}\right|\psi_i\rangle = -\alpha_{i,1}\gamma_{1,4} + \alpha_{i,4}\gamma_{1,2}\\
\langle\psi_i\left|c_{2\downarrow}\right|\phi_0\rangle &= \langle\phi_0\left|c^\dagger_{2\downarrow}\right|\psi_i\rangle = \alpha_{i,2}\gamma_{1,2} + \alpha_{i,3}\gamma_{1,4}
\end{aligned}$$

$$\begin{aligned}
\langle\psi_4\left|c_{1\uparrow}\right|\phi_0\rangle &= \langle\phi_0\left|c^\dagger_{1\uparrow}\right|\psi_4\rangle = \gamma_{1,4}\\
\langle\psi_4\left|c_{2\uparrow}\right|\phi_0\rangle &= \langle\phi_0\left|c^\dagger_{2\uparrow}\right|\psi_4\rangle = -\gamma_{1,2}\\
\langle\psi_4\left|c_{1\downarrow}\right|\phi_0\rangle &= \langle\phi_0\left|c^\dagger_{1\downarrow}\right|\psi_4\rangle = 0\\
\langle\psi_4\left|c_{2\downarrow}\right|\phi_0\rangle &= \langle\phi_0\left|c^\dagger_{2\downarrow}\right|\psi_4\rangle = 0
\end{aligned}$$

$$\begin{aligned}
\langle\psi_5\left|c_{1\uparrow}\right|\phi_0\rangle &= \langle\phi_0\left|c^\dagger_{1\uparrow}\right|\psi_5\rangle = 0\\
\langle\psi_5\left|c_{2\uparrow}\right|\phi_0\rangle &= \langle\phi_0\left|c^\dagger_{2\uparrow}\right|\psi_5\rangle = 0\\
\langle\psi_5\left|c_{1\downarrow}\right|\phi_0\rangle &= \langle\phi_0\left|c^\dagger_{1\downarrow}\right|\psi_5\rangle = -\gamma_{2,3}\\
\langle\psi_5\left|c_{2\downarrow}\right|\phi_0\rangle &= \langle\phi_0\left|c^\dagger_{2\downarrow}\right|\psi_5\rangle = \gamma_{2,1}
\end{aligned}$$

$$\begin{aligned}
\langle\psi_6\left|c_{1\uparrow}\right|\phi_0\rangle &= \langle\phi_0\left|c^\dagger_{1\uparrow}\right|\psi_6\rangle = \tfrac{\gamma_{2,3}}{\sqrt{2}}\\
\langle\psi_6\left|c_{2\uparrow}\right|\phi_0\rangle &= \langle\phi_0\left|c^\dagger_{2\uparrow}\right|\psi_6\rangle = -\tfrac{\gamma_{2,1}}{\sqrt{2}}\\
\langle\psi_6\left|c_{1\downarrow}\right|\phi_0\rangle &= \langle\phi_0\left|c^\dagger_{1\downarrow}\right|\psi_6\rangle = -\tfrac{\gamma_{1,4}}{\sqrt{2}}\\
\langle\psi_6\left|c_{2\downarrow}\right|\phi_0\rangle &= \langle\phi_0\left|c^\dagger_{2\downarrow}\right|\psi_6\rangle = \tfrac{\gamma_{1,2}}{\sqrt{2}}
\end{aligned}$$

5.3 General case : A and B expressions

5.3.1 N=1

$$\begin{aligned}
A^{N=1}_{11\uparrow} &= \beta^2_{2,1}\\
A^{N=1}_{22\uparrow} &= \beta^2_{2,3}\\
A^{N=1}_{12\uparrow} &= \beta_{2,1}\beta_{2,3}\\
A^{N=1}_{11\downarrow} &= \beta^2_{1,2}\\
A^{N=1}_{12\downarrow} &= \beta^2_{1,4}\\
A^{N=1}_{12\downarrow} &= \beta_{1,2}\beta_{1,4}
\end{aligned}$$

$$
\begin{aligned}
B^{N=1}_{1,11\uparrow} &= (\alpha_{0,1}\beta_{1,4} + \alpha_{0,3}\beta_{1,2})^2 \\
B^{N=1}_{1,22\uparrow} &= (\alpha_{0,2}\beta_{1,2} - \alpha_{0,4}\beta_{1,4})^2 \\
B^{N=1}_{1,12\uparrow} &= -(\alpha_{0,1}\beta_{1,4} + \alpha_{0,3}\beta_{1,2})(\alpha_{0,2}\beta_{1,2} - \alpha_{0,4}\beta_{1,4}) \\
B^{N=1}_{1,11\downarrow} &= (\alpha_{0,2}\beta_{2,3} - \alpha_{0,3}\beta_{2,1})^2 \\
B^{N=1}_{1,22\downarrow} &= (\alpha_{0,1}\beta_{2,1} + \alpha_{0,4}\beta_{2,3})^2 \\
B^{N=1}_{1,12\downarrow} &= -(\alpha_{0,2}\beta_{2,3} - \alpha_{0,3}\beta_{2,1})(\alpha_{0,1}\beta_{2,1} + \alpha_{0,4}\beta_{2,3})
\end{aligned}
$$

$$
\begin{aligned}
B^{N=1}_{2,11\uparrow} &= (\alpha_{1,1}\beta_{1,4} + \alpha_{1,3}\beta_{1,2})^2 \\
B^{N=1}_{2,22\uparrow} &= (\alpha_{1,2}\beta_{1,2} - \alpha_{1,4}\beta_{1,4})^2 \\
B^{N=1}_{2,12\uparrow} &= -(\alpha_{1,1}\beta_{1,4} + \alpha_{1,3}\beta_{1,2})(\alpha_{1,2}\beta_{1,2} - \alpha_{1,4}\beta_{1,4}) \\
B^{N=1}_{2,11\downarrow} &= (\alpha_{1,2}\beta_{2,3} - \alpha_{1,3}\beta_{2,1})^2 \\
B^{N=1}_{2,22\downarrow} &= (\alpha_{1,1}\beta_{2,1} + \alpha_{1,4}\beta_{2,3})^2 \\
B^{N=1}_{2,12\downarrow} &= -(\alpha_{1,2}\beta_{2,3} - \alpha_{1,3}\beta_{2,1})(\alpha_{1,1}\beta_{2,1} + \alpha_{1,4}\beta_{2,3})
\end{aligned}
$$

$$
\begin{aligned}
B^{N=1}_{3,11\uparrow} &= (\alpha_{2,1}\beta_{1,4} + \alpha_{2,3}\beta_{1,2})^2 \\
B^{N=1}_{3,22\uparrow} &= (\alpha_{2,2}\beta_{1,2} - \alpha_{2,4}\beta_{1,4})^2 \\
B^{N=1}_{3,12\uparrow} &= -(\alpha_{2,1}\beta_{1,4} + \alpha_{2,3}\beta_{1,2})(\alpha_{2,2}\beta_{1,2} - \alpha_{2,4}\beta_{1,4}) \\
B^{N=1}_{3,11\downarrow} &= (\alpha_{2,2}\beta_{2,3} - \alpha_{2,3}\beta_{2,1})^2 \\
B^{N=1}_{3,22\downarrow} &= (\alpha_{2,1}\beta_{2,1} + \alpha_{2,4}\beta_{2,3})^2 \\
B^{N=1}_{3,12\downarrow} &= -(\alpha_{2,2}\beta_{2,3} - \alpha_{2,3}\beta_{2,1})(\alpha_{2,1}\beta_{2,1} + \alpha_{2,4}\beta_{2,3})
\end{aligned}
$$

$$
\begin{aligned}
B^{N=1}_{4,11\uparrow} &= 0 \\
B^{N=1}_{4,22\uparrow} &= 0 \\
B^{N=1}_{4,12\uparrow} &= 0 \\
B^{N=1}_{4,11\downarrow} &= \beta^2_{1,4} \\
B^{N=1}_{4,22\downarrow} &= \beta^2_{1,2} \\
B^{N=1}_{4,12\downarrow} &= -\beta_{1,4}\beta_{1,2}
\end{aligned}
$$

$$
\begin{aligned}
B^{N=1}_{5,11\uparrow} &= \beta^2_{2,3} \\
B^{N=1}_{5,22\uparrow} &= \beta^2_{2,1} \\
B^{N=1}_{5,12\uparrow} &= -\beta_{2,3}\beta_{2,1} \\
B^{N=1}_{5,11\downarrow} &= 0 \\
B^{N=1}_{5,22\downarrow} &= 0 \\
B^{N=1}_{5,12\downarrow} &= 0
\end{aligned}
$$

$$
\begin{aligned}
B^{N=1}_{6,11\uparrow} &= \beta^2_{1,4}/2 \\
B^{N=1}_{6,22\uparrow} &= \beta^2_{1,2}/2 \\
B^{N=1}_{6,12\uparrow} &= -\beta_{1,4}\beta_{1,2}/2 \\
B^{N=1}_{6,11\downarrow} &= \beta^2_{2,3}/2 \\
B^{N=1}_{6,12\downarrow} &= \beta^2_{2,1}/2 \\
B^{N=1}_{6,12\downarrow} &= -\beta_{2,3}\beta_{2,1}/2
\end{aligned}
$$

5.3.2 N=2

$$
A^{N=2}_{m,ij\sigma} = \left\langle \psi_0 \left| c^{\dagger}_{i\sigma} \right| \chi_m \right\rangle \left\langle \chi_m \left| c_{j\sigma} \right| \psi_0 \right\rangle
$$

$$
B^{N=2}_{m,ij\sigma} = \left\langle \psi_0 \left| c_{i\sigma} \right| \phi_m \right\rangle \left\langle \phi_m \left| c^{\dagger}_{j\sigma} \right| \psi_0 \right\rangle
$$

$$
\begin{aligned}
A^{N=2}_{1,11\uparrow} &= (-\alpha_{0,3}\beta_{1,2} - \alpha_{0,1}\beta_{1,4})^2 \\
A^{N=2}_{1,22\uparrow} &= (\alpha_{0,2}\beta_{1,2} - \alpha_{0,4}\beta_{1,4})^2 \\
A^{N=2}_{1,12\uparrow} &= (-\alpha_{0,3}\beta_{1,2} - \alpha_{0,1}\beta_{1,4})(\alpha_{0,2}\beta_{1,2} - \alpha_{0,4}\beta_{1,4}) \\
A^{N=2}_{1,11\downarrow} &= 0 \\
A^{N=2}_{1,22\downarrow} &= 0 \\
A^{N=2}_{1,12\downarrow} &= 0
\end{aligned}
$$

$$
\begin{aligned}
A^{N=2}_{2,11\uparrow} &= 0 \\
A^{N=2}_{2,22\uparrow} &= 0 \\
A^{N=2}_{2,12\uparrow} &= 0 \\
A^{N=2}_{2,11\downarrow} &= (\alpha_{0,3}\beta_{2,1} - \alpha_{0,2}\beta_{2,3})^2 \\
A^{N=2}_{2,22\downarrow} &= (\alpha_{0,1}\beta_{2,1} + \alpha_{0,4}\beta_{2,3})^2 \\
A^{N=2}_{2,12\downarrow} &= (\alpha_{0,3}\beta_{2,1} - \alpha_{0,2}\beta_{2,3})(\alpha_{0,1}\beta_{2,1} + \alpha_{0,4}\beta_{2,3})
\end{aligned}
$$

$$
\begin{aligned}
A^{N=2}_{3,11\uparrow} &= (-\alpha_{0,3}\beta_{3,2} - \alpha_{0,1}\beta_{3,4})^2 \\
A^{N=2}_{3,22\uparrow} &= (\alpha_{0,2}\beta_{3,2} - \alpha_{0,4}\beta_{3,4})^2 \\
A^{N=2}_{3,12\uparrow} &= (-\alpha_{0,3}\beta_{3,2} - \alpha_{0,1}\beta_{3,4})(\alpha_{0,2}\beta_{3,2} - \alpha_{0,4}\beta_{3,4}) \\
A^{N=2}_{3,11\downarrow} &= 0 \\
A^{N=2}_{3,22\downarrow} &= 0 \\
A^{N=2}_{3,12\downarrow} &= 0
\end{aligned}
$$

$$
\begin{aligned}
A^{N=2}_{4,11\uparrow} &= 0 \\
A^{N=2}_{4,22\uparrow} &= 0 \\
A^{N=2}_{4,12\uparrow} &= 0 \\
A^{N=2}_{4,11\downarrow} &= (\alpha_{0,3}\beta_{4,1} - \alpha_{0,2}\beta_{4,3})^2 \\
A^{N=2}_{4,22\downarrow} &= (\alpha_{0,1}\beta_{4,1} + \alpha_{0,4}\beta_{4,3})^2 \\
A^{N=2}_{4,12\downarrow} &= (\alpha_{0,3}\beta_{4,1} - \alpha_{0,2}\beta_{4,3})(\alpha_{0,1}\beta_{4,1} + \alpha_{0,4}\beta_{4,3})
\end{aligned}
$$

$$
\begin{aligned}
B^{N=2}_{1,11\uparrow} &= 0 \\
B^{N=2}_{1,22\uparrow} &= 0 \\
B^{N=2}_{1,12\uparrow} &= 0 \\
B^{N=2}_{1,11\downarrow} &= (\alpha_{0,4}\gamma_{1,2} - \alpha_{0,1}\gamma_{1,4})^2 \\
B^{N=2}_{1,22\downarrow} &= (\alpha_{0,2}\gamma_{1,2} + \alpha_{0,3}\gamma_{1,4})^2 \\
B^{N=2}_{1,12\downarrow} &= (\alpha_{0,4}\gamma_{1,2} - \alpha_{0,1}\gamma_{1,4})(\alpha_{0,2}\gamma_{1,2} + \alpha_{0,3}\gamma_{1,4})
\end{aligned}
$$

$$
\begin{aligned}
B^{N=2}_{2,11\uparrow} &= (\alpha_{0,4}\gamma_{2,1} + \alpha_{0,2}\gamma_{2,3})^2 \\
B^{N=2}_{2,22\uparrow} &= (-\alpha_{0,1}\gamma_{2,1} + \alpha_{0,3}\gamma_{2,3})^2 \\
B^{N=2}_{2,12\uparrow} &= (\alpha_{0,4}\gamma_{2,1} + \alpha_{0,2}\gamma_{2,3})(-\alpha_{0,1}\gamma_{2,1} + \alpha_{0,3}\gamma_{2,3}) \\
B^{N=2}_{2,11\downarrow} &= 0 \\
B^{N=2}_{2,22\downarrow} &= 0 \\
B^{N=2}_{2,12\downarrow} &= 0
\end{aligned}
$$

$$
\begin{aligned}
B^{N=2}_{3,11\uparrow} &= 0 \\
B^{N=2}_{3,22\uparrow} &= 0 \\
B^{N=2}_{3,12\uparrow} &= 0 \\
B^{N=2}_{3,11\downarrow} &= (\alpha_{0,4}\gamma_{3,2} - \alpha_{0,1}\gamma_{3,4})^2 \\
B^{N=2}_{3,22\downarrow} &= (\alpha_{0,2}\gamma_{3,2} + \alpha_{0,3}\gamma_{3,4})^2 \\
B^{N=2}_{3,12\downarrow} &= (\alpha_{0,4}\gamma_{3,2} - \alpha_{0,1}\gamma_{3,4})(\alpha_{0,2}\gamma_{3,2} + \alpha_{0,3}\gamma_{3,4})
\end{aligned}
$$

$$B^{N=2}_{4,11\uparrow} = (\alpha_{0,4}\gamma_{4,1} + \alpha_{0,2}\gamma_{4,3})^2$$
$$B^{N=2}_{4,22\uparrow} = (-\alpha_{0,1}\gamma_{4,1} + \alpha_{0,3}\gamma_{4,3})^2$$
$$B^{N=2}_{4,12\uparrow} = (\alpha_{0,4}\gamma_{4,1} + \alpha_{0,2}\gamma_{4,3})(-\alpha_{0,1}\gamma_{4,1} + \alpha_{0,3}\gamma_{4,3})$$
$$B^{N=2}_{4,11\downarrow} = 0$$
$$B^{N=2}_{4,22\downarrow} = 0$$
$$B^{N=2}_{4,12\downarrow} = 0$$

5.3.3 N=3

$$A^{N=3}_{1,11\uparrow} =$$
$$A^{N=3}_{1,22\uparrow} =$$
$$A^{N=3}_{1,12\uparrow} =$$
$$A^{N=3}_{1,11\downarrow} =$$
$$A^{N=3}_{1,12\downarrow} =$$
$$A^{N=3}_{1,22\downarrow} =$$

$$A^{N=3}_{2,11\uparrow} =$$
$$A^{N=3}_{2,22\uparrow} =$$
$$A^{N=3}_{2,12\uparrow} =$$
$$A^{N=3}_{2,11\downarrow} =$$
$$A^{N=3}_{2,12\downarrow} =$$
$$A^{N=3}_{2,22\downarrow} =$$

$$A^{N=3}_{3,11\uparrow} =$$
$$A^{N=3}_{3,22\uparrow} =$$
$$A^{N=3}_{3,12\uparrow} =$$
$$A^{N=3}_{3,11\downarrow} =$$
$$A^{N=3}_{3,12\downarrow} =$$
$$A^{N=3}_{3,22\downarrow} =$$

$$A^{N=3}_{4,11\uparrow} =$$
$$A^{N=3}_{4,22\uparrow} =$$
$$A^{N=3}_{4,12\uparrow} =$$
$$A^{N=3}_{4,11\downarrow} =$$
$$A^{N=3}_{4,12\downarrow} =$$
$$A^{N=3}_{4,22\downarrow} =$$

$$A^{N=3}_{5,11\uparrow} =$$
$$A^{N=3}_{5,22\uparrow} =$$
$$A^{N=3}_{5,12\uparrow} =$$
$$A^{N=3}_{5,11\downarrow} =$$
$$A^{N=3}_{5,12\downarrow} =$$
$$A^{N=3}_{5,22\downarrow} =$$

$$A^{N=3}_{6,11\uparrow} =$$
$$A^{N=3}_{6,22\uparrow} =$$
$$A^{N=3}_{6,12\uparrow} =$$
$$A^{N=3}_{6,11\downarrow} =$$
$$A^{N=3}_{6,12\downarrow} =$$
$$A^{N=3}_{6,22\downarrow} =$$

$$B^{N=3}_{1,11\uparrow} =$$
$$B^{N=3}_{1,22\uparrow} =$$
$$B^{N=3}_{1,12\uparrow} =$$
$$B^{N=3}_{1,11\downarrow} =$$
$$B^{N=3}_{1,12\downarrow} =$$
$$B^{N=3}_{1,22\downarrow} =$$