# Hubbard dimer: exact solutions

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# 1 Introduction

Conventions:

$$|\uparrow\downarrow\rangle \uparrow\downarrow\rangle = c_{2\downarrow}^{\dagger} c_{2\uparrow}^{\dagger} c_{1\downarrow}^{\dagger} c_{2\uparrow}^{\dagger} |0 \quad 0\rangle$$

$$c_{i}^{\dagger} |\dots, n_{i}, \dots\rangle_{a} = (1 - n_{i}) \cdot (-1)^{\sum_{j>i} n_{j}} |\dots, n_{i} + 1, \dots\rangle_{a}$$

$$c_{i} |\dots, n_{i}, \dots\rangle_{a} = n_{i} \cdot (-1)^{\sum_{j>i} n_{j}} |\dots, n_{i} - 1, \dots\rangle_{a}$$

$$\hat{n}_{i\sigma} = c_{i\sigma}^{\dagger} c_{i\sigma}$$

$$\hat{n}_{i\sigma} |\dots, n_{i\sigma}, \dots\rangle_{a} = n_{i\sigma} |\dots, n_{i\sigma}, \dots\rangle_{a}$$

Hamiltonian:

$$H = -t \sum_{\substack{i,j=1,2\\i\neq j}} \sum_{\sigma} c_{i\sigma}^{\dagger} c_{j\sigma} + \frac{U}{2} \sum_{i=1,2} \sum_{\sigma\sigma'} c_{i\sigma}^{\dagger} c_{i\sigma'}^{\dagger} c_{i\sigma'} c_{i\sigma} + \epsilon_0 \sum_{\sigma,i=1,2} n_{i\sigma}$$

Useful relations:

$$\left\{c_{i\sigma}, c_{j\sigma'}^{\dagger}\right\} = \delta_{\sigma\sigma'}\delta_{ij} \quad \left\{c_{i\sigma}, c_{j\sigma'}\right\} = 0 \quad \left\{c_{i\sigma}^{\dagger}, c_{j\sigma'}^{\dagger}\right\} = 0$$
$$<\alpha|c_{i}|\beta> = <\beta|c_{i}^{\dagger}|\alpha>$$

# 2 General case : $U_1 \neq U_2$ and $\epsilon_1 \neq \epsilon_2$

## 2.1 Hamiltonian solutions

#### 2.1.1 one electron solution

$$H = \begin{pmatrix} \epsilon_1 & 0 & -t & 0 \\ 0 & \epsilon_1 & 0 & -t \\ -t & 0 & \epsilon_2 & 0 \\ 0 & -t & 0 & \epsilon_2 \end{pmatrix}$$

$$\begin{array}{|c|c|c|c|c|} \hline E_i & | \uparrow 0 \rangle & | \downarrow 0 \rangle & | 0 \uparrow \rangle & | 0 \downarrow \rangle \\ \hline (\epsilon_1 + \epsilon_2)/2 - d & 0 & -(\epsilon_1 - \epsilon_2 - 2d)/e & 0 & 2t/e \\ (\epsilon_1 + \epsilon_2)/2 - d & -(\epsilon_1 - \epsilon_2 - 2d)/e & 0 & 2t/e & 0 \\ (\epsilon_1 + \epsilon_2)/2 + d & 0 & -(\epsilon_1 - \epsilon_2 + 2d)/f & 0 & 2t/f \\ \hline (\epsilon_1 + \epsilon_2)/2 + d & -(\epsilon_1 - \epsilon_2 + 2d)/f & 0 & 2t/f & 0 \\ \hline \end{array}$$

with 
$$d = \sqrt{(\epsilon_1 - \epsilon_2)^2 + 4t^2}/2$$
,  $e = \sqrt{(\epsilon_1 - \epsilon_2 - 2d)^2 + 4t^2}$ , and  $f = \sqrt{(\epsilon_1 - \epsilon_2 + 2d)^2 + 4t^2}$ .

### 2.1.2 two electrons solution

$$H = \begin{pmatrix} \epsilon_1 + \epsilon_2 & 0 & 0 & 0 & -t & -t \\ 0 & \epsilon_1 + \epsilon_2 & 0 & 0 & t & t \\ 0 & 0 & \epsilon_1 + \epsilon_2 & 0 & 0 & 0 \\ 0 & 0 & 0 & \epsilon_1 + \epsilon_2 & 0 & 0 \\ -t & t & 0 & 0 & 2\epsilon_1 + U_1 & 0 \\ -t & t & 0 & 0 & 0 & 2\epsilon_2 + U_2 \end{pmatrix}$$

$$A = (18t^{2} + 3U_{1}U_{2} - 9(\epsilon_{1} - \epsilon_{2})(\epsilon_{1} - \epsilon_{2} + U_{1} - U_{2}))(U_{1} + U_{2}) - 2(U_{1}^{3} + 2U_{2}^{3})$$

$$B = -3(\epsilon_{1} - \epsilon_{2})^{2} - 3(U_{1} - U_{2})(\epsilon_{1} - \epsilon_{2}) - U_{1}^{2} - U_{2}^{2} + U_{1}U_{2} - 12t^{2}$$

$$D = (A + \sqrt{4B^{3} + A^{2}})^{\frac{1}{3}}$$

$$K_{0} = \frac{U_{1} + U_{2}}{3} + \frac{2^{\frac{1}{3}B}}{3D} - \frac{D}{3 \times 2^{\frac{1}{3}}}$$

$$K_{+} = \frac{U_{1} + U_{2}}{3} - \frac{(1 + i\sqrt{3})B}{3 \times 2^{\frac{2}{3}}D} + \frac{(1 - i\sqrt{3})D}{6 \times 2^{\frac{1}{3}}}$$

$$K_{-} = \frac{U_{1} + U_{2}}{3} - \frac{(1 - i\sqrt{3})B}{3 \times 2^{\frac{2}{3}}D} + \frac{(1 + i\sqrt{3})D}{6 \times 2^{\frac{1}{3}}}$$

Despite  $K_i$  have imaginary parts, especially with D which is an imaginary number, all these quantites are real when evaluated numerically!

$E_i$	$ \uparrow \downarrow \rangle$	$ \downarrow \uparrow \rangle$	$ \uparrow \uparrow \rangle$	$ \downarrow\downarrow\downarrow\rangle$	$ \uparrow\downarrow 0\rangle$	$ 0\uparrow\downarrow\rangle$
$\epsilon_1 + \epsilon_2 + K_0$	$-\frac{1}{C_0} \frac{t(U_1 + U_2 - 2K_0)}{K_0(\epsilon_1 - \epsilon_2 + U_1 - K_0)}$	$\frac{1}{C_0} \frac{t(U_1 + U_2 - 2K_0)}{K_0(\epsilon_1 - \epsilon_2 + U_1 - K_0)}$	0	0	$\frac{1}{C_0} \frac{\epsilon_2 - \epsilon_1 + U_2 - K_0}{\epsilon_1 - \epsilon_2 + U_1 - K_0}$	$\frac{1}{C_0}$
$\epsilon_1 + \epsilon_2 + K_+$	$ -\frac{1}{C_{+}} \frac{t(U_{1}+U_{2}-2K_{+})}{K_{+}(\epsilon_{1}-\epsilon_{2}+U_{1}-K_{+})} $	$\frac{1}{C_{+}} \frac{t(U_{1} + U_{2} - 2K_{+})}{K_{+}(\epsilon_{1} - \epsilon_{2} + U_{1} - K_{+})}$	0	0	$\frac{1}{C_{+}} \frac{\epsilon_{2} - \epsilon_{1} + U_{2} - K_{+}}{\epsilon_{1} - \epsilon_{2} + U_{1} - K_{+}}$	$\frac{1}{C_{+}}$
$\epsilon_1 + \epsilon_2 + K$	$ -\frac{1}{C_{-}} \frac{t(U_{1}+U_{2}-2K_{-})}{K_{-}(\epsilon_{1}-\epsilon_{2}+U_{1}-K_{-})} $	$\frac{1}{C_{-}} \frac{t(U_{1} + U_{2} - 2K_{-})}{K_{-}(\epsilon_{1} - \epsilon_{2} + U_{1} - K_{-})}$	0	0	$\frac{1}{C_{-}} \frac{\epsilon_2 - \epsilon_1 + U_2 - K_{-}}{\epsilon_1 - \epsilon_2 + U_1 - K_{-}}$	$\frac{1}{C_{-}}$
$\epsilon_1 + \epsilon_2$	0	0	0	1	0	0
$\epsilon_1 + \epsilon_2$	0	0	1	0	0	0
$\epsilon_1 + \epsilon_2$	$1/\sqrt{2}$	$1/\sqrt{2}$	0	0	0	0

By normalizing the vectors:

$$C_{i} = \sqrt{\left| -\frac{t(U_{1} + U_{2} - 2K_{i})}{K_{i}(\epsilon_{1} - \epsilon_{2} + U_{1} - K_{i})} \right|^{2} + \left| \frac{t(U_{1} + U_{2} - 2K_{i})}{K_{i}(\epsilon_{1} - \epsilon_{2} + U_{1} - K_{i})} \right|^{2} + \left| \frac{\epsilon_{2} - \epsilon_{1} + U_{2} - K_{i}}{\epsilon_{1} - \epsilon_{2} + U_{1} - K_{i}} \right|^{2} + 1}$$

Numerically, we have these solution converging to the basic case solution!

### 2.1.3 three electrons solution

$$H = \begin{pmatrix} \epsilon_1 + 2\epsilon_2 + U_2 & 0 & -t & 0\\ 0 & \epsilon_1 + 2\epsilon_2 + U_2 & 0 & -t\\ -t & 0 & 2\epsilon_1 + \epsilon_2 + U_1 & 0\\ 0 & -t & 0 & 2\epsilon_1 + \epsilon_2 + U_1 \end{pmatrix}$$

with 
$$g = \sqrt{((\epsilon_1 - \epsilon_2) + (U_1 - U_2))^2 + 4t^2}$$
,  $m_+ = \frac{\epsilon_1 - \epsilon_2 + U_1 - U_2 + g}{2t}$ ,  $m_- = \frac{\epsilon_1 - \epsilon_2 + U_1 - U_2 - g}{2t}$ 

#### 2.1.4 other solutions

$$H|0 \quad 0\rangle = 0|0 \quad 0\rangle$$

$$H|\uparrow\downarrow \quad \uparrow\downarrow\rangle = (2\epsilon_1 + 2\epsilon_2 + U_1 + U_2)|\uparrow\downarrow \quad \uparrow\downarrow\rangle$$

## 2.2 One particle Green's function and density matrix

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.

#### **2.2.1** N = 1 electron

$$G_{11\uparrow}(\omega) = \frac{(\alpha_{0,1}\beta_{1,4} + \alpha_{0,3}\beta_{1,2})^2}{\omega - (E_{\psi_0} - E_0) + i\eta} + \frac{(\alpha_{1,1}\beta_{1,4} + \alpha_{1,3}\beta_{1,2})^2}{\omega - (E_{\psi_1} - E_0) + i\eta} + \frac{(\alpha_{2,1}\beta_{1,4} + \alpha_{2,3}\beta_{1,2})^2}{\omega - (E_{\psi_2} - E_0) + i\eta} + \frac{\beta_{2,3}^2}{\omega - (E_{\psi_4} - E_0) + i\eta} + \frac{\beta_{2,1}^2}{\omega - (E_{\psi_5} - E_0) - i\eta} + \frac{\beta_{2,1}^2}{\omega - E_0 - i\eta}$$

$$G_{22\uparrow}(\omega) = \frac{(\alpha_{0,2}\beta_{1,2} - \alpha_{0,4}\beta_{1,4})^2}{\omega - (E_{\psi_0} - E_0) + i\eta} + \frac{(\alpha_{1,2}\beta_{1,2} - \alpha_{1,4}\beta_{1,4})^2}{\omega - (E_{\psi_1} - E_0) + i\eta} + \frac{(\alpha_{2,2}\beta_{1,2} - \alpha_{2,4}\beta_{1,4})^2}{\omega - (E_{\psi_2} - E_0) + i\eta} + \frac{\beta_{2,1}^2}{\omega - (E_{\psi_4} - E_0) + i\eta} + \frac{\beta_{2,3}^2}{\omega - (E_{\psi_5} - E_0) - i\eta} + \frac{\beta_{2,3}^2}{\omega - E_0 - i\eta}$$

$$G_{12\uparrow}(\omega) = -\frac{(\alpha_{0,1}\beta_{1,4} + \alpha_{0,3}\beta_{1,2})(\alpha_{0,2}\beta_{1,2} - \alpha_{0,4}\beta_{1,4})}{\omega - (E_{\psi_0} - E_0) + i\eta} - \frac{(\alpha_{1,1}\beta_{1,4} + \alpha_{1,3}\beta_{1,2})(\alpha_{1,2}\beta_{1,2} - \alpha_{1,4}\beta_{1,4})}{\omega - (E_{\psi_1} - E_0) + i\eta} - \frac{(\alpha_{2,1}\beta_{1,4} + \alpha_{2,3}\beta_{1,2})(\alpha_{2,2}\beta_{1,2} - \alpha_{2,4}\beta_{1,4})}{\omega - (E_{\psi_2} - E_0) + i\eta} - \frac{\beta_{2,3}\beta_{2,1}}{\omega - (E_{\psi_4} - E_0) + i\eta} - \frac{\beta_{1,4}\beta_{1,2}/2}{\omega - (E_{\psi_5} - E_0) - i\eta} + \frac{\beta_{2,1}\beta_{2,3}}{\omega - E_0 - i\eta}$$

$$G_{11\downarrow}(\omega) = \frac{(\alpha_{0,2}\beta_{2,3} - \alpha_{0,3}\beta_{2,1})^2}{\omega - (E_{\psi_0} - E_0) + i\eta} + \frac{(\alpha_{1,2}\beta_{2,3} - \alpha_{1,3}\beta_{2,1})^2}{\omega - (E_{\psi_1} - E_0) + i\eta} + \frac{(\alpha_{2,2}\beta_{2,3} - \alpha_{2,3}\beta_{2,1})^2}{\omega - (E_{\psi_2} - E_0) + i\eta} + \frac{\beta_{1,2}^2}{\omega - (E_{\psi_3} - E_0) + i\eta} + \frac{\beta_{1,2}^2}{\omega - (E_{\psi_3} - E_0) - i\eta}$$

$$G_{22\downarrow}(\omega) = \frac{(\alpha_{0,1}\beta_{2,1} + \alpha_{0,4}\beta_{2,3})^2}{\omega - (E_{\psi_0} - E_0) + i\eta} + \frac{(\alpha_{1,1}\beta_{2,1} + \alpha_{1,4}\beta_{2,3})^2}{\omega - (E_{\psi_1} - E_0) + i\eta} + \frac{(\alpha_{2,1}\beta_{2,1} + \alpha_{2,4}\beta_{2,3})^2}{\omega - (E_{\psi_2} - E_0) + i\eta} + \frac{\beta_{1,2}^2}{\omega - (E_{\psi_3} - E_0) + i\eta} + \frac{\beta_{2,1}^2/2}{\omega - (E_{\psi_5} - E_0) - i\eta} + \frac{\beta_{1,4}^2}{\omega - E_0 - i\eta}$$

$$G_{12\downarrow}(\omega) = -\frac{(\alpha_{0,2}\beta_{2,3} - \alpha_{0,3}\beta_{2,1})(\alpha_{0,1}\beta_{2,1} + \alpha_{0,4}\beta_{2,3})}{\omega - (E_{\psi_0} - E_0) + i\eta} - \frac{(\alpha_{1,2}\beta_{2,3} - \alpha_{1,3}\beta_{2,1})(\alpha_{1,1}\beta_{2,1} + \alpha_{1,4}\beta_{2,3})}{\omega - (E_{\psi_1} - E_0) + i\eta} - \frac{(\alpha_{2,2}\beta_{2,3} - \alpha_{2,3}\beta_{2,1})(\alpha_{2,1}\beta_{2,1} + \alpha_{2,4}\beta_{2,3})}{\omega - (E_{\psi_2} - E_0) + i\eta} - \frac{\beta_{1,4}\beta_{1,2}}{\omega - (E_{\psi_3} - E_0) + i\eta} - \frac{\beta_{2,3}\beta_{2,1}/2}{\omega - (E_{\psi_5} - E_0) - i\eta} + \frac{\beta_{1,2}\beta_{1,4}}{\omega - E_0 - i\eta}$$

#### **2.2.2** N = 2 electrons

$$G_{11\uparrow}(\omega) = \frac{(-\alpha_{0,3}\beta_{1,2} - \alpha_{0,1}\beta_{1,4})^2}{\omega + (E_{\chi_1} - E_0) - i\eta} + \frac{(\alpha_{0,4}\gamma_{2,1} + \alpha_{0,2}\gamma_{2,3})^2}{\omega - (E_{\phi_2} - E_0) + i\eta}$$

$$+ \frac{(\alpha_{0,3}\beta_{3,2} + \alpha_{0,1}\beta_{3,4})^2}{\omega + (E_{\chi_3} - E_0) - i\eta} + \frac{(\alpha_{0,4}\gamma_{4,1} + \alpha_{0,2}\gamma_{4,3})^2}{\omega - (E_{\phi_4} - E_0) + i\eta}$$

$$G_{22\uparrow}(\omega) = \frac{(\alpha_{0,2}\beta_{1,2} - \alpha_{0,4}\beta_{1,4})^2}{\omega + (E_{\chi_1} - E_0) - i\eta} + \frac{(-\alpha_{0,1}\gamma_{2,1} + \alpha_{0,3}\gamma_{2,3})^2}{\omega - (E_{\phi_2} - E_0) + i\eta}$$

$$+ \frac{(\alpha_{0,2}\beta_{3,2} - \alpha_{0,4}\beta_{3,4})^2}{\omega + (E_{\chi_3} - E_0) - i\eta} + \frac{(-\alpha_{0,1}\gamma_{4,1} + \alpha_{0,3}\gamma_{4,3})^2}{\omega - (E_{\phi_4} - E_0) + i\eta}$$

$$G_{12\uparrow}(\omega) = \frac{(-\alpha_{0,3}\beta_{1,2} - \alpha_{0,1}\beta_{1,4})(\alpha_{0,2}\beta_{1,2} - \alpha_{0,4}\beta_{1,4})}{\omega + (E_{\chi_1} - E_0) - i\eta} + \frac{(\alpha_{0,4}\gamma_{2,1} + \alpha_{0,2}\gamma_{2,3})(-\alpha_{0,1}\gamma_{2,1} + \alpha_{0,3}\gamma_{2,3})}{\omega - (E_{\phi_2} - E_0) + i\eta}$$

$$+ \frac{(\alpha_{0,3}\beta_{3,2} + \alpha_{0,1}\beta_{3,4})(\alpha_{0,2}\beta_{3,2} - \alpha_{0,4}\beta_{3,4})}{\omega + (E_{\chi_3} - E_0) - i\eta} + \frac{(\alpha_{0,4}\gamma_{4,1} + \alpha_{0,2}\gamma_{4,3})(-\alpha_{0,1}\gamma_{4,1} + \alpha_{0,3}\gamma_{4,3})}{\omega - (E_{\phi_4} - E_0) + i\eta}$$

$$G_{11\downarrow}(\omega) = \frac{(\alpha_{0,4}\gamma_{1,2} - \alpha_{0,1}\gamma_{1,4})^2}{\omega - (E_{\phi_3} - E_0) + i\eta} + \frac{(\alpha_{0,3}\beta_{2,1} - \alpha_{0,2}\beta_{2,3})^2}{\omega + (E_{\chi_2} - E_0) - i\eta}$$

$$+ \frac{(\alpha_{0,4}\gamma_{3,2} - \alpha_{0,1}\gamma_{3,4})^2}{\omega - (E_{\phi_3} - E_0) + i\eta} + \frac{(\alpha_{0,3}\beta_{4,1} - \alpha_{0,2}\beta_{4,3})^2}{\omega + (E_{\chi_2} - E_0) - i\eta}$$

$$+ \frac{(\alpha_{0,2}\gamma_{3,2} + \alpha_{0,3}\gamma_{3,4})^2}{\omega - (E_{\phi_3} - E_0) + i\eta} + \frac{(\alpha_{0,1}\beta_{2,1} + \alpha_{0,4}\beta_{2,3})^2}{\omega + (E_{\chi_2} - E_0) - i\eta}$$

$$+ \frac{(\alpha_{0,4}\gamma_{1,2} - \alpha_{0,1}\gamma_{1,4})(\alpha_{0,2}\gamma_{1,2} + \alpha_{0,3}\gamma_{1,4})}{\omega - (E_{\phi_3} - E_0) + i\eta} + \frac{(\alpha_{0,3}\beta_{4,1} - \alpha_{0,2}\beta_{2,3})(\alpha_{0,1}\beta_{2,1} + \alpha_{0,4}\beta_{2,3})}{\omega + (E_{\chi_2} - E_0) - i\eta}$$

$$+ \frac{(\alpha_{0,4}\gamma_{3,2} - \alpha_{0,1}\gamma_{3,4})(\alpha_{0,2}\gamma_{3,2} + \alpha_{0,3}\gamma_{3,4})}{\omega - (E_{\phi_3} - E_0) + i\eta} + \frac{(\alpha_{0,3}\beta_{4,1} - \alpha_{0,2}\beta_{3,3})(\alpha_{0,1}\beta_{2,1} + \alpha_{0,4}\beta_{2,3})}{\omega + (E_{\chi_2} - E_0) - i\eta}$$

$$+ \frac{(\alpha_{0,4}\gamma_{3,2} - \alpha_{0,1}\gamma_{3,4})(\alpha_{0,2}\gamma_{3,2} + \alpha_{0,3}\gamma_{3,4})}{\omega - (E_{\phi_3} - E_0) + i\eta} + \frac{(\alpha_{0,3}\beta_{4,1} - \alpha_{0,2}\beta_{3,3})(\alpha_{0,1}\beta_{2,1} + \alpha_{0,4}\beta_{2,3})}{\omega + (E_{\chi_2} - E_0) - i\eta}$$

$$+ \frac{(\alpha_{0,4}\gamma_{3,2} - \alpha_{0,1}\gamma_{3,4})(\alpha_{0,2}\gamma_{3,2}$$

$$\gamma_{22\uparrow}(\omega) = (\alpha_{0,2}\beta_{1,2} - \alpha_{0,4}\beta_{1,4})^2 + (\alpha_{0,2}\beta_{3,2} - \alpha_{0,4}\beta_{3,4})^2$$

$$\gamma_{12\uparrow}(\omega) = (-\alpha_{0,3}\beta_{1,2} - \alpha_{0,1}\beta_{1,4})(\alpha_{0,2}\beta_{1,2} - \alpha_{0,4}\beta_{1,4}) + (\alpha_{0,3}\beta_{3,2} + \alpha_{0,1}\beta_{3,4})(\alpha_{0,2}\beta_{3,2} - \alpha_{0,4}\beta_{3,4})$$

$$\gamma_{11\downarrow}(\omega) = (\alpha_{0,3}\beta_{2,1} - \alpha_{0,2}\beta_{2,3})^2 + (\alpha_{0,3}\beta_{4,1} - \alpha_{0,2}\beta_{4,3})^2$$

$$\gamma_{22\downarrow}(\omega) = (\alpha_{0,1}\beta_{2,1} + \alpha_{0,4}\beta_{2,3})^2 + (\alpha_{0,1}\beta_{4,1} + \alpha_{0,4}\beta_{4,3})^2$$

$$\gamma_{12\downarrow}(\omega) = (\alpha_{0,3}\beta_{2,1} - \alpha_{0,2}\beta_{2,3})(\alpha_{0,1}\beta_{2,1} + \alpha_{0,4}\beta_{2,3}) + (\alpha_{0,3}\beta_{4,1} - \alpha_{0,2}\beta_{4,3})(\alpha_{0,1}\beta_{4,1} + \alpha_{0,4}\beta_{4,3})$$

### **2.2.3** N = 3 electrons

$$\begin{split} G_{11\uparrow}(\omega) &= \frac{\gamma_{1,2}^2}{\omega - (E_{\uparrow\downarrow\uparrow\downarrow} - E_0) + i\eta} + \frac{(\alpha_{0,2}\gamma_{2,3} + \alpha_{0,4}\gamma_{2,1})^2}{\omega + (E_{\psi_0} - E_0) - i\eta} + \frac{(\alpha_{1,2}\gamma_{2,3} + \alpha_{1,4}\gamma_{2,1})^2}{\omega + (E_{\psi_1} - E_0) - i\eta} \\ &+ \frac{(\alpha_{2,2}\gamma_{2,3} + \alpha_{2,4}\gamma_{2,1})^2}{\omega + (E_{\psi_2} - E_0) - i\eta} + \frac{\gamma_{1,4}^2}{\omega + (E_{\psi_3} - E_0) - i\eta} + \frac{\gamma_{2,3}^2/2}{\omega + (E_{\psi_5} - E_0) - i\eta} \end{split}$$

$$G_{22\uparrow}(\omega) = \frac{\gamma_{1,4}^2}{\omega - (E_{\uparrow\downarrow\uparrow\downarrow} - E_0) + i\eta} + \frac{(\alpha_{0,3}\gamma_{2,3} - \alpha_{0,1}\gamma_{2,1})^2}{\omega + (E_{\psi_0} - E_0) - i\eta} + \frac{(\alpha_{1,3}\gamma_{2,3} - \alpha_{1,1}\gamma_{2,1})^2}{\omega + (E_{\psi_1} - E_0) - i\eta} + \frac{(\alpha_{2,3}\gamma_{2,3} - \alpha_{2,1}\gamma_{2,1})^2}{\omega + (E_{\psi_2} - E_0) - i\eta} + \frac{\gamma_{1,2}^2}{\omega + (E_{\psi_3} - E_0) - i\eta} + \frac{\gamma_{2,1}^2/2}{\omega + (E_{\psi_5} - E_0) - i\eta}$$

$$G_{12\uparrow}(\omega) = \frac{\gamma_{1,2}\gamma_{1,4}}{\omega - (E_{\uparrow\downarrow\uparrow\downarrow} - E_0) + i\eta} + \frac{(\alpha_{0,2}\gamma_{2,3} + \alpha_{0,4}\gamma_{2,1})(\alpha_{0,3}\gamma_{2,3} - \alpha_{0,1}\gamma_{2,1})}{\omega + (E_{\psi_0} - E_0) - i\eta}$$

$$+ \frac{(\alpha_{1,2}\gamma_{2,3} + \alpha_{1,4}\gamma_{2,1})(\alpha_{1,3}\gamma_{2,3} - \alpha_{1,1}\gamma_{2,1})}{\omega + (E_{\psi_1} - E_0) - i\eta} + \frac{(\alpha_{2,2}\gamma_{2,3} + \alpha_{2,4}\gamma_{2,1})(\alpha_{2,3}\gamma_{2,3} - \alpha_{2,1}\gamma_{2,1})}{\omega + (E_{\psi_2} - E_0) - i\eta}$$

$$- \frac{\gamma_{1,4}\gamma_{1,2}}{\omega + (E_{\psi_3} - E_0) - i\eta} - \frac{\gamma_{2,3}\gamma_{2,1}/2}{\omega + (E_{\psi_5} - E_0) - i\eta}$$

$$\begin{split} G_{11\downarrow}(\omega) &= \frac{\gamma_{2,1}^2}{\omega - (E_{\uparrow\downarrow\uparrow\downarrow} - E_0) + i\eta} + \frac{(\alpha_{0,4}\gamma_{1,2} - \alpha_{0,1}\gamma_{1,4})^2}{\omega + (E_{\psi_0} - E_0) - i\eta} + \frac{(\alpha_{1,4}\gamma_{1,2} - \alpha_{1,1}\gamma_{1,4})^2}{\omega + (E_{\psi_1} - E_0) - i\eta} \\ &+ \frac{(\alpha_{2,4}\gamma_{1,2} - \alpha_{2,1}\gamma_{1,4})^2}{\omega + (E_{\psi_2} - E_0) - i\eta} + \frac{\gamma_{2,3}^2}{\omega + (E_{\psi_3} - E_0) - i\eta} + \frac{\gamma_{1,4}^2/2}{\omega + (E_{\psi_5} - E_0) - i\eta} \end{split}$$

$$G_{22\downarrow}(\omega) = \frac{\gamma_{2,3}^2}{\omega - (E_{\uparrow\downarrow\uparrow\downarrow} - E_0) + i\eta} + \frac{(\alpha_{0,2}\gamma_{1,2} + \alpha_{0,3}\gamma_{1,4})^2}{\omega + (E_{\psi_0} - E_0) - i\eta} + \frac{(\alpha_{1,2}\gamma_{1,2} + \alpha_{1,3}\gamma_{1,4})^2}{\omega + (E_{\psi_1} - E_0) - i\eta} + \frac{(\alpha_{2,2}\gamma_{1,2} + \alpha_{2,3}\gamma_{1,4})^2}{\omega + (E_{\psi_2} - E_0) - i\eta} + \frac{\gamma_{2,1}^2}{\omega + (E_{\psi_2} - E_0) - i\eta}$$

$$G_{12\downarrow}(\omega) = \frac{\gamma_{2,1}\gamma_{2,3}}{\omega - (E_{\uparrow\downarrow\uparrow\downarrow} - E_0) + i\eta} + \frac{(\alpha_{0,4}\gamma_{1,2} - \alpha_{0,1}\gamma_{1,4})(\alpha_{0,2}\gamma_{1,2} + \alpha_{0,3}\gamma_{1,4})}{\omega + (E_{\psi_0} - E_0) - i\eta}$$

$$+ \frac{(\alpha_{1,4}\gamma_{1,2} - \alpha_{1,1}\gamma_{1,4})(\alpha_{1,2}\gamma_{1,2} + \alpha_{1,3}\gamma_{1,4})}{\omega + (E_{\psi_1} - E_0) - i\eta} + \frac{(\alpha_{2,4}\gamma_{1,2} - \alpha_{2,1}\gamma_{1,4})(\alpha_{2,2}\gamma_{1,2} + \alpha_{2,3}\gamma_{1,4})}{\omega + (E_{\psi_2} - E_0) - i\eta}$$

$$- \frac{\gamma_{2,3}\gamma_{2,1}}{\omega + (E_{\psi_4} - E_0) - i\eta} - \frac{\gamma_{1,4}\gamma_{1,2}/2}{\omega + (E_{\psi_5} - E_0) - i\eta}$$

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

# 3.1 Hamiltonian solutions

#### 3.1.1 one electron solution

$$H = \begin{pmatrix} \epsilon_0 & 0 & -t & 0 \\ 0 & \epsilon_0 & 0 & -t \\ -t & 0 & \epsilon_0 & 0 \\ 0 & -t & 0 & \epsilon_0 \end{pmatrix}$$

	$E_i$	$ \uparrow 0\rangle$	$ \downarrow 0\rangle$	$ 0\uparrow\rangle$	$ 0\downarrow\rangle$
ſ	$\epsilon_0 - t$	0	$1/\sqrt{2}$	0	$1/\sqrt{2}$
	$\epsilon_0 - t$	$1/\sqrt{2}$	0	$1/\sqrt{2}$	0
		0		0	$-1/\sqrt{2}$
	$\epsilon_0 + t$	$1/\sqrt{2}$	0	$-1/\sqrt{2}$	0

#### 3.1.2 two electrons solution

$$H = \begin{pmatrix} 2\epsilon_0 & 0 & 0 & 0 & -t & -t \\ 0 & 2\epsilon_0 & 0 & 0 & t & t \\ 0 & 0 & 2\epsilon_0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 2\epsilon_0 & 0 & 0 \\ -t & t & 0 & 0 & 2\epsilon_0 + U & 0 \\ -t & t & 0 & 0 & 0 & 2\epsilon_0 + U \end{pmatrix}$$

$E_i$		$ \downarrow\uparrow\rangle$	↑↑	$ \downarrow\downarrow\rangle$	$ \uparrow\downarrow0\rangle$	$ 0\uparrow\downarrow\rangle$
$2\epsilon_0 + (U-c)/2$	$\frac{4t}{a(c-U)}$	$-\frac{4t}{a(c-U)}$	0	0	1/a	1/a
$2\epsilon_0 + (U+c)/2$	$-\frac{4t}{b(c+U)}$	$\frac{4t}{b(c+U)}$	0	0	1/b	1/b
$2\epsilon_0 + U$	0	0	0	0	$-1/\sqrt{2}$	$1/\sqrt{2}$
$2\epsilon_0$	0	0	0	1	0	0
$2\epsilon_0$	0	0	1	0	0	0
$2\epsilon_0$	$1/\sqrt{2}$	$1/\sqrt{2}$	0	0	0	0

With 
$$a = \frac{\sqrt{2}}{(c-U)}\sqrt{16t^2 + (c-U)^2}$$
,  $b = \frac{\sqrt{2}}{(c+U)}\sqrt{16t^2 + (c+U)^2}$ ,  $c = \sqrt{16t^2 + U^2}$ .

#### 3.1.3 three electrons solution

$$H = \begin{pmatrix} 3\epsilon_0 + \mathbf{U} & 0 & -t & 0\\ 0 & 3\epsilon_0 + \mathbf{U} & 0 & -t\\ -t & 0 & 3\epsilon_0 + \mathbf{U} & 0\\ 0 & -t & 0 & 3\epsilon_0 + \mathbf{U} \end{pmatrix}$$

$E_i$	$ \uparrow\uparrow\downarrow\rangle$	$ \downarrow\uparrow\downarrow\rangle$	$ \uparrow\downarrow\uparrow\rangle$	$ \uparrow\downarrow\downarrow\rangle$
$3\epsilon_0 + U - t$	0	$1/\sqrt{2}$	0	$1/\sqrt{2}$
$3\epsilon_0 + U - t$	$1/\sqrt{2}$	0	$1/\sqrt{2}$	0
$3\epsilon_0 + U + t$	0	$-1/\sqrt{2}$	0	$1/\sqrt{2}$
$3\epsilon_0 + U + t$	$-1/\sqrt{2}$	0	$1/\sqrt{2}$	0

# 3.2 One particle Green's function and density matrix

#### **3.2.1** N = 1 electron

$$G_{ij\uparrow}(\omega) = \frac{(-1)^{(i-j)}}{2} \left[ \frac{1}{\omega - (\epsilon_0 + t) + i\eta} + \frac{(-1)^{(i-j)}}{\omega - (\epsilon_0 - t) - i\eta} \right]$$

$$G_{ij\downarrow}(\omega) = \frac{(-1)^{(i-j)}}{4} \left[ \frac{1}{\omega - (\epsilon_0 + t) + i\eta} + \frac{1}{\omega - (\epsilon_0 + t + U) + i\eta} \right]$$

$$+ \frac{1}{2} \left[ \frac{\frac{1}{a^2} \left( 1 + \frac{4t}{(c-U)} \right)^2}{\omega - (\epsilon_0 + t - (c - U)/2) + i\eta} + \frac{\frac{1}{b^2} \left( 1 - \frac{4t}{(c+U)} \right)^2}{\omega - (\epsilon_0 + t + (c + U)/2) + i\eta} \right]$$

#### **3.2.2** N = 2 electrons

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

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

$$G_{a}(\omega) = -\frac{1}{2a^{2}} \left[ \frac{\left(1 + \frac{4t}{(c-U)}\right)^{2}}{\omega - (\epsilon_{0} - t + (c+U)/2) + i\eta} - \frac{\left(1 - \frac{4t}{(c-U)}\right)^{2}}{\omega - (\epsilon_{0} + t + (c+U)/2) + i\eta} \right]$$

$$+ \frac{1}{2a^{2}} \left[ \frac{\left(1 + \frac{4t}{(c-U)}\right)^{2}}{\omega - (\epsilon_{0} + t - (c-U)/2) - i\eta} - \frac{\left(1 - \frac{4t}{(c-U)}\right)^{2}}{\omega - (\epsilon_{0} - t - (c-U)/2) - i\eta} \right]$$

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

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

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

### **3.2.3** N = 3 electrons

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

# 4 Annexes

# 4.1 General case: calculus on eigenvectors

## **4.1.1** N = 1 electron : $|\chi_i\rangle$

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

$$c^{\dagger}_{1\uparrow}|\chi_i\rangle = -\beta_{i,2}|\uparrow\downarrow 0\rangle - \beta_{i,4}|\uparrow\downarrow\rangle$$

$$c_{1\uparrow}|\chi_i\rangle = 0$$

$$c^{\dagger}_{2\uparrow}|\chi_i\rangle = \beta_{i,2}|\downarrow\uparrow\rangle - \beta_{i,4}|0\uparrow\downarrow\rangle$$

$$c_{2\uparrow}|\chi_i\rangle = 0$$

$$c^{\dagger}_{1\downarrow}|\chi_i\rangle = -\beta_{i,4}|\downarrow\downarrow\rangle$$

$$c_{1\downarrow}|\chi_i\rangle = \beta_{i,2}|0\downarrow\downarrow\rangle$$

$$c_{2\downarrow}|\chi_i\rangle = \beta_{i,2}|\downarrow\downarrow\rangle$$

$$c_{2\downarrow}|\chi_i\rangle = \beta_{i,4}|0\downarrow\rangle$$

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

$$c_{1\uparrow}^{\dagger} | \chi_{i} \rangle = -\beta_{i,3} | \uparrow \uparrow \rangle$$

$$c_{1\uparrow} | \chi_{i} \rangle = \beta_{i,1} | 0 \quad 0 \rangle$$

$$c_{2\uparrow}^{\dagger} | \chi_{i} \rangle = \beta_{i,1} | \uparrow \uparrow \rangle$$

$$c_{2\uparrow} | \chi_{i} \rangle = \beta_{i,3} | 0 \quad 0 \rangle$$

$$c_{1\downarrow}^{\dagger} | \chi_{i} \rangle = \beta_{i,1} | \uparrow \downarrow 0 \rangle - \beta_{i,3} | \downarrow \uparrow \rangle$$

$$c_{1\downarrow} | \chi_{i} \rangle = 0$$

$$c_{2\downarrow}^{\dagger} | \chi_{i} \rangle = \beta_{i,1} | \uparrow \downarrow \rangle + \beta_{i,3} | 0 \quad \uparrow \downarrow \rangle$$

$$c_{2\downarrow} | \chi_{i} \rangle = 0$$

## **4.1.2** N=2 electrons : $|\psi_i\rangle$

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

$$\begin{array}{l} c_{1\uparrow}^{\dagger} \left| \psi_{i} \right\rangle = \alpha_{i,2} \right| \uparrow \downarrow \quad \uparrow \rangle + \alpha_{i,4} \right| \uparrow \quad \uparrow \downarrow \rangle \\ c_{1\uparrow} \left| \psi_{i} \right\rangle = -\alpha_{i,1} \middle| 0 \quad \downarrow \rangle - \alpha_{i,3} \middle| \downarrow \quad 0 \rangle \\ c_{2\uparrow}^{\dagger} \left| \psi_{i} \right\rangle = -\alpha_{i,1} \middle| \uparrow \quad \uparrow \downarrow \rangle + \alpha_{i,3} \middle| \uparrow \downarrow \quad \uparrow \rangle \\ c_{2\uparrow} \left| \psi_{i} \right\rangle = \alpha_{i,2} \middle| \downarrow \quad 0 \rangle - \alpha_{i,4} \middle| 0 \quad \downarrow \rangle \\ c_{1\downarrow}^{\dagger} \left| \psi_{i} \right\rangle = -\alpha_{i,1} \middle| \uparrow \downarrow \quad \downarrow \rangle + \alpha_{i,4} \middle| \downarrow \quad \uparrow \downarrow \rangle \\ c_{1\downarrow} \left| \psi_{i} \right\rangle = -\alpha_{i,2} \middle| 0 \quad \uparrow \rangle + \alpha_{i,3} \middle| \uparrow \quad 0 \rangle \\ c_{2\downarrow}^{\dagger} \left| \psi_{i} \right\rangle = \alpha_{i,2} \middle| \downarrow \quad \uparrow \downarrow \rangle + \alpha_{i,3} \middle| \uparrow \downarrow \quad \downarrow \rangle \\ c_{2\downarrow} \left| \psi_{i} \right\rangle = \alpha_{i,1} \middle| \uparrow \quad 0 \rangle + \alpha_{i,4} \middle| 0 \quad \uparrow \rangle \end{array}$$

Pour 
$$|\psi_3\rangle=|\downarrow\downarrow\downarrow\rangle$$
: 
$$c^{\dagger}_{1\uparrow}|\psi_3\rangle=|\uparrow\downarrow\downarrow\downarrow\rangle$$
 
$$c_{1\uparrow}|\psi_3\rangle=0$$

$$c_{1\uparrow} | \psi_3 \rangle = 0$$

$$c_{2\uparrow}^{\dagger} | \psi_3 \rangle = - | \downarrow \uparrow \downarrow \rangle$$

$$c_{2\uparrow} | \psi_3 \rangle = 0$$

$$c_{1\downarrow}^{\dagger} |\psi_3\rangle = 0$$

$$c_{1\downarrow} |\psi_3\rangle = -|0 \downarrow\rangle$$

$$c_{2\downarrow}^{\dagger} \left| \psi_3 \right\rangle = 0$$

$$c_{2\downarrow} |\psi_3\rangle = |\downarrow 0\rangle$$

Pour 
$$|\psi_4\rangle = |\uparrow \uparrow\rangle$$
:

$$c_{1\uparrow}^{\dagger} |\psi_4\rangle = 0$$

$$c_{1\uparrow}^{\dagger} |\psi_4\rangle = -|0 \uparrow\rangle$$

$$c_{2\uparrow}^{\dagger} |\psi_4\rangle = 0$$

$$c_{2\uparrow} |\psi_4\rangle = |\uparrow \quad 0\rangle$$

$$c_{1\downarrow}^{\uparrow} | \psi_4 \rangle = -| \uparrow \downarrow \uparrow \uparrow \rangle$$

$$c_{1\downarrow}^{\downarrow} | \psi_4 \rangle = 0$$

$$c_{1\downarrow}^{-1}|\psi_4\rangle=0$$

$$c_{2\downarrow}^{\dagger} |\psi_4\rangle = |\uparrow \uparrow \downarrow\rangle$$

$$c_{2\downarrow} |\psi_4\rangle = 0$$

$$c_{2\downarrow} |\psi_4\rangle = 0$$

Pour 
$$|\psi_5\rangle = \frac{1}{\sqrt{2}}|\uparrow \downarrow \rangle + \frac{1}{\sqrt{2}}|\downarrow \uparrow \rangle$$
:

$$c_{1\uparrow}^{\dagger} |\psi_5\rangle = \frac{1}{\sqrt{2}} |\uparrow\downarrow\rangle$$

$$c_{1\uparrow} |\psi_5\rangle = -\frac{1}{\sqrt{2}} |0\rangle$$

$$c_{2\uparrow}^{\dagger} |\psi_5\rangle = -\frac{1}{\sqrt{2}} |\uparrow \uparrow \downarrow \rangle$$

$$c_{2\uparrow} |\psi_5\rangle = \frac{1}{\sqrt{2}} |\downarrow\rangle$$
 0

$$\begin{array}{c} c_{1\uparrow}^{\dagger} \left| \psi_{5} \right\rangle = \frac{1}{\sqrt{2}} \right| \uparrow \downarrow \quad \uparrow \rangle \\ c_{1\uparrow} \left| \psi_{5} \right\rangle = -\frac{1}{\sqrt{2}} \middle| 0 \quad \downarrow \rangle \\ c_{2\uparrow}^{\dagger} \left| \psi_{5} \right\rangle = -\frac{1}{\sqrt{2}} \middle| \uparrow \quad \uparrow \downarrow \rangle \\ c_{2\uparrow} \left| \psi_{5} \right\rangle = \frac{1}{\sqrt{2}} \middle| \downarrow \quad 0 \rangle \\ c_{1\downarrow}^{\dagger} \left| \psi_{5} \right\rangle = -\frac{1}{\sqrt{2}} \middle| \uparrow \downarrow \quad \downarrow \rangle \\ c_{1\downarrow} \left| \psi_{5} \right\rangle = -\frac{1}{\sqrt{2}} \middle| 0 \quad \uparrow \rangle \\ c_{2\downarrow}^{\dagger} \left| \psi_{5} \right\rangle = \frac{1}{\sqrt{2}} \middle| \downarrow \quad \uparrow \downarrow \rangle \\ c_{2\downarrow} \left| \psi_{5} \right\rangle = \frac{1}{\sqrt{2}} \middle| \uparrow \quad 0 \rangle \end{array}$$

$$c_{1\downarrow}|\psi_5\rangle = -\frac{1}{\sqrt{2}}|0 \uparrow\rangle$$

$$c_{2\downarrow}^{\dagger} |\psi_5\rangle = \frac{1}{\sqrt{2}} |\downarrow \uparrow \downarrow \rangle$$

$$c_{2\downarrow} |\psi_5\rangle = \frac{1}{\sqrt{2}} |\uparrow \rangle$$

## 4.1.3 N=3 electrons : $|\phi_i\rangle$

For 
$$i=1,3: |\phi_i\rangle = \gamma_{i,2}|\downarrow \uparrow\downarrow\rangle + \gamma_{i,4}|\uparrow\downarrow\downarrow\rangle$$
:
$$c^{\dagger}_{1\uparrow}|\phi_i\rangle = -\gamma_{i,2}|\uparrow\downarrow\uparrow\downarrow\rangle$$

$$c_{1\uparrow}|\phi_i\rangle = \gamma_{i,4}|\downarrow\downarrow\downarrow\rangle$$

$$c^{\dagger}_{2\uparrow}|\phi_i\rangle = -\gamma_{i,4}|\uparrow\downarrow\uparrow\downarrow\rangle$$

$$c_{2\uparrow}|\phi_i\rangle = -\gamma_{i,2}|\downarrow\downarrow\downarrow\rangle$$

$$c^{\dagger}_{1\downarrow}|\phi_i\rangle = 0$$

$$c_{1\downarrow}|\phi_i\rangle = \gamma_{i,2}|0 \uparrow\downarrow\rangle - \gamma_{i,4}|\uparrow\downarrow\rangle$$

$$c^{\dagger}_{2\downarrow}|\phi_i\rangle = 0$$

$$c_{2\downarrow}|\phi_i\rangle = \gamma_{i,2}|\downarrow\uparrow\uparrow\rangle + \gamma_{i,4}|\uparrow\downarrow\downarrow\rangle$$

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

$$\begin{array}{l} c_{1\uparrow}^{\dagger} \left| \phi_{i} \right\rangle = 0 \\ c_{1\uparrow} \left| \phi_{i} \right\rangle = \gamma_{i,1} \middle| 0 \quad \uparrow \downarrow \right\rangle + \gamma_{i,3} \middle| \downarrow \quad \uparrow \right\rangle \\ c_{2\uparrow}^{\dagger} \left| \phi_{i} \right\rangle = 0 \\ c_{2\uparrow} \left| \phi_{i} \right\rangle = -\gamma_{i,1} \middle| \uparrow \quad \downarrow \right\rangle + \gamma_{i,3} \middle| \uparrow \downarrow \quad 0 \right\rangle \\ c_{1\downarrow}^{\dagger} \left| \phi_{i} \right\rangle = \gamma_{i,1} \middle| \uparrow \downarrow \quad \uparrow \downarrow \right\rangle \\ c_{1\downarrow} \left| \phi_{i} \right\rangle = -\gamma_{i,3} \middle| \uparrow \quad \uparrow \right\rangle \\ c_{2\downarrow}^{\dagger} \left| \phi_{i} \right\rangle = \gamma_{i,3} \middle| \uparrow \downarrow \quad \uparrow \downarrow \right\rangle \\ c_{2\downarrow} \left| \phi_{i} \right\rangle = \gamma_{i,1} \middle| \uparrow \quad \uparrow \right\rangle \end{array}$$

# 4.2 General case : scalar products

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

$$\langle \chi_0 \mid c_{1\uparrow}^{\dagger} \mid 00 \rangle = \langle 00 \mid c_{1\uparrow} \mid \chi_0 \rangle = \beta_{2,1}$$

$$\langle \chi_0 \mid c_{1\downarrow}^{\dagger} \mid 00 \rangle = \langle 00 \mid c_{2\uparrow} \mid \chi_0 \rangle = \beta_{2,3}$$

$$\langle \chi_0 \mid c_{1\downarrow}^{\dagger} \mid 00 \rangle = \langle 00 \mid c_{1\downarrow} \mid \chi_0 \rangle = \beta_{1,2}$$

$$\langle \chi_0 \mid c_{2\downarrow}^{\dagger} \mid 00 \rangle = \langle 00 \mid c_{2\downarrow} \mid \chi_0 \rangle = \beta_{1,4}$$

$$\langle \psi_i \mid c_{1\uparrow}^{\dagger} \mid \chi_0 \rangle = \langle \chi_0 \mid c_{1\uparrow} \mid \psi_i \rangle = -\alpha_{i,1}\beta_{1,4} - \alpha_{i,3}\beta_{1,2}$$

$$\langle \psi_i \mid c_{1\downarrow}^{\dagger} \mid \chi_0 \rangle = \langle \chi_0 \mid c_{2\uparrow} \mid \psi_i \rangle = \alpha_{i,2}\beta_{1,2} - \alpha_{i,4}\beta_{1,4}$$

$$\langle \psi_i \mid c_{1\downarrow}^{\dagger} \mid \chi_0 \rangle = \langle \chi_0 \mid c_{1\downarrow} \mid \psi_i \rangle = -\alpha_{i,2}\beta_{2,3} + \alpha_{i,3}\beta_{2,1}$$

$$\langle \psi_i \mid c_{1\downarrow}^{\dagger} \mid \chi_0 \rangle = \langle \chi_0 \mid c_{1\downarrow} \mid \psi_i \rangle = \alpha_{i,1}\beta_{2,1} + \alpha_{i,4}\beta_{2,3}$$

$$\langle \psi_3 \mid c_{1\uparrow}^{\dagger} \mid \chi_0 \rangle = \langle \chi_0 \mid c_{2\downarrow} \mid \psi_i \rangle = \alpha_{i,1}\beta_{2,1} + \alpha_{i,4}\beta_{2,3}$$

$$\langle \psi_3 \mid c_{1\uparrow}^{\dagger} \mid \chi_0 \rangle = \langle \chi_0 \mid c_{1\downarrow} \mid \psi_3 \rangle = 0$$

$$\langle \psi_3 \mid c_{1\downarrow}^{\dagger} \mid \chi_0 \rangle = \langle \chi_0 \mid c_{1\downarrow} \mid \psi_3 \rangle = 0$$

$$\langle \psi_3 \mid c_{1\downarrow}^{\dagger} \mid \chi_0 \rangle = \langle \chi_0 \mid c_{1\downarrow} \mid \psi_3 \rangle = -\beta_{1,4}$$

$$\langle \psi_3 \mid c_{1\downarrow}^{\dagger} \mid \chi_0 \rangle = \langle \chi_0 \mid c_{1\downarrow} \mid \psi_4 \rangle = -\beta_{2,3}$$

$$\langle \psi_4 \mid c_{1\uparrow}^{\dagger} \mid \chi_0 \rangle = \langle \chi_0 \mid c_{1\uparrow} \mid \psi_4 \rangle = -\beta_{2,3}$$

$$\langle \psi_4 \mid c_{1\downarrow}^{\dagger} \mid \chi_0 \rangle = \langle \chi_0 \mid c_{1\downarrow} \mid \psi_4 \rangle = 0$$

$$\langle \psi_4 \mid c_{1\downarrow}^{\dagger} \mid \chi_0 \rangle = \langle \chi_0 \mid c_{1\downarrow} \mid \psi_4 \rangle = 0$$

$$\langle \psi_4 \mid c_{1\downarrow}^{\dagger} \mid \chi_0 \rangle = \langle \chi_0 \mid c_{1\downarrow} \mid \psi_4 \rangle = 0$$

$$\langle \psi_4 \mid c_{1\downarrow}^{\dagger} \mid \chi_0 \rangle = \langle \chi_0 \mid c_{1\downarrow} \mid \psi_4 \rangle = 0$$

$$\langle \psi_4 \mid c_{1\downarrow}^{\dagger} \mid \chi_0 \rangle = \langle \chi_0 \mid c_{1\downarrow} \mid \psi_5 \rangle = -\frac{\beta_{1,4}}{\sqrt{2}}$$

$$\langle \psi_5 \mid c_{1\downarrow}^{\dagger} \mid \chi_0 \rangle = \langle \chi_0 \mid c_{1\uparrow} \mid \psi_5 \rangle = -\frac{\beta_{1,2}}{\sqrt{2}}$$

$$\langle \psi_5 \mid c_{1\downarrow}^{\dagger} \mid \chi_0 \rangle = \langle \chi_0 \mid c_{1\downarrow} \mid \psi_5 \rangle = \frac{\beta_{1,2}}{\sqrt{2}}$$

$$\langle \psi_5 \mid c_{1\downarrow}^{\dagger} \mid \chi_0 \rangle = \langle \chi_0 \mid c_{1\downarrow} \mid \psi_5 \rangle = \frac{\beta_{2,1}}{\sqrt{2}}$$

$$\langle \psi_5 \mid c_{1\downarrow}^{\dagger} \mid \chi_0 \rangle = \langle \chi_0 \mid c_{1\downarrow} \mid \psi_5 \rangle = \frac{\beta_{2,1}}{\sqrt{2}}$$

$$\langle \psi_5 \mid c_{1\downarrow}^{\dagger} \mid \chi_0 \rangle = \langle \chi_0 \mid c_{2\downarrow} \mid \psi_5 \rangle = \frac{\beta_{2,1}}{\sqrt{2}}$$

$$\langle \psi_5 \mid c_{1\downarrow}^{\dagger} \mid \chi_0 \rangle = \langle \chi_0 \mid c_{2\downarrow} \mid \psi_5 \rangle = \frac{\beta_{2,1}}{\sqrt{2}}$$

$$\langle \psi_5 \mid c_{1\downarrow}^{\dagger} \mid \chi_0 \rangle = \langle \chi_0 \mid c_{2\downarrow} \mid \psi_5 \rangle = \frac{\beta_{2,1}}{\sqrt{2}}$$

$$\langle \psi_5 \mid c_{1\downarrow}^{\dagger} \mid \chi_0 \rangle = \langle \chi_0 \mid c_{2\downarrow} \mid \psi_5 \rangle = \frac{\beta_{2,1}}{\sqrt{2}}$$

$$\langle \psi_5 \mid c_{1\downarrow}^{\dagger} \mid \chi_0 \rangle = \langle \chi_0 \mid c_{2\downarrow} \mid \psi_5 \rangle = \frac{\beta_{2,1}}{\sqrt{2}}$$

$$\langle \psi_5 \mid c_{1\downarrow}^{\dagger} \mid \chi$$

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

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

$$\langle \psi_0 \begin{vmatrix} c_{1\uparrow}^{\dagger} | \chi_i \rangle = \langle \chi_i | c_{1\uparrow} | \psi_0 \rangle = -\alpha_{0,3}\beta_{i,2} - \alpha_{0,1}\beta_{i,4}$$

$$\langle \psi_0 | c_{2\uparrow}^{\dagger} | \chi_i \rangle = \langle \chi_i | c_{2\uparrow} | \psi_0 \rangle = \alpha_{0,2}\beta_{i,2} - \alpha_{0,4}\beta_{i,4}$$

$$\langle \psi_0 | c_{1\downarrow}^{\dagger} | \chi_i \rangle = \langle \chi_i | c_{1\downarrow} | \psi_0 \rangle = 0$$

$$\langle \psi_0 | c_{2\downarrow}^{\dagger} | \chi_i \rangle = \langle \chi_i | c_{2\downarrow} | \psi_0 \rangle = 0$$

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

$$\langle \psi_0 \begin{vmatrix} c_{1\uparrow}^{\dagger} & \chi_i \rangle = \langle \chi_i | c_{1\uparrow} | \psi_0 \rangle = 0$$

$$\langle \psi_0 | c_{2\uparrow}^{\dagger} & \chi_i \rangle = \langle \chi_i | c_{2\uparrow} | \psi_0 \rangle = 0$$

$$\langle \psi_0 | c_{1\downarrow}^{\dagger} & \chi_i \rangle = \langle \chi_i | c_{1\downarrow} | \psi_0 \rangle = \alpha_{0,3} \beta_{i,1} - \alpha_{0,2} \beta_{i,3}$$

$$\langle \psi_0 | c_{2\downarrow}^{\dagger} & \chi_i \rangle = \langle \chi_i | c_{2\downarrow} | \psi_0 \rangle = \alpha_{0,1} \beta_{i,1} + \alpha_{0,4} \beta_{i,3}$$

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

$$\langle \psi_0 | c_{1\uparrow} | \phi_i \rangle = \langle \phi_i | c_{1\uparrow}^{\dagger} | \psi_0 \rangle = 0$$

$$\langle \psi_0 | c_{2\uparrow} | \phi_i \rangle = \langle \phi_i | c_{2\uparrow}^{\dagger} | \psi_0 \rangle = 0$$

$$\langle \psi_0 | c_{1\downarrow} | \phi_i \rangle = \langle \phi_i | c_{1\downarrow}^{\dagger} | \psi_0 \rangle = \gamma_{i,2} \alpha_{0,4} - \gamma_{i,4} \alpha_{0,1}$$

$$\langle \psi_0 | c_{2\downarrow} | \phi_i \rangle = \langle \phi_i | c_{2\downarrow}^{\dagger} | \psi_0 \rangle = \gamma_{i,2} \alpha_{0,2} + \gamma_{i,4} \alpha_{0,3}$$

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

$$\langle \psi_0 | c_{1\uparrow} | \phi_i \rangle = \langle \phi_i | c_{1\uparrow}^{\dagger} | \psi_0 \rangle = \gamma_{i,1} \alpha_{0,4} + \gamma_{i,3} \alpha_{0,2}$$

$$\langle \psi_0 | c_{2\uparrow} | \phi_i \rangle = \langle \phi_i | c_{2\uparrow}^{\dagger} | \psi_0 \rangle = -\gamma_{i,1} \alpha_{0,1} + \gamma_{i,3} \alpha_{0,3}$$

$$\langle \psi_0 | c_{1\downarrow} | \phi_i \rangle = \langle \phi_i | c_{1\downarrow}^{\dagger} | \psi_0 \rangle = 0$$

$$\langle \psi_0 | c_{2\downarrow} | \phi_i \rangle = \langle \phi_i | c_{2\downarrow}^{\dagger} | \psi_0 \rangle = 0$$

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

$$\langle \uparrow\downarrow\uparrow\downarrow | c_{1\uparrow}^{\dagger}| \phi_0\rangle = \langle \phi_0 | c_{1\uparrow}| \uparrow\downarrow\uparrow\downarrow \rangle = -\gamma_{1,2}$$

$$\langle \uparrow\downarrow\uparrow\downarrow | c_{1\downarrow}^{\dagger}| \phi_0\rangle = \langle \phi_0 | c_{2\downarrow}| \uparrow\downarrow\uparrow\downarrow \rangle = -\gamma_{1,4}$$

$$\langle \uparrow\downarrow\uparrow\downarrow | c_{1\downarrow}^{\dagger}| \phi_0\rangle = \langle \phi_0 | c_{1\downarrow}| \uparrow\downarrow\uparrow\downarrow \rangle = \gamma_{2,1}$$

$$\langle \uparrow\downarrow\uparrow\downarrow | c_{2\downarrow}^{\dagger}| \phi_0\rangle = \langle \phi_0 | c_{2\downarrow}| \uparrow\downarrow\uparrow\downarrow \rangle = \gamma_{2,3}$$

$$\langle \psi_i | c_{1\uparrow}| \phi_0\rangle = \langle \phi_0 | c_{1\uparrow}^{\dagger}| \psi_i\rangle = \alpha_{i,2}\gamma_{2,3} + \alpha_{i,4}\gamma_{2,1}$$

$$\langle \psi_i | c_{2\uparrow}| \phi_0\rangle = \langle \phi_0 | c_{1\uparrow}^{\dagger}| \psi_i\rangle = -\alpha_{i,1}\gamma_{2,1} + \alpha_{i,3}\gamma_{2,3}$$

$$\langle \psi_i | c_{1\downarrow}| \phi_0\rangle = \langle \phi_0 | c_{1\downarrow}^{\dagger}| \psi_i\rangle = -\alpha_{i,1}\gamma_{1,4} + \alpha_{i,4}\gamma_{1,2}$$

$$\langle \psi_i | c_{2\downarrow}| \phi_0\rangle = \langle \phi_0 | c_{2\downarrow}^{\dagger}| \psi_i\rangle = \alpha_{i,2}\gamma_{1,2} + \alpha_{i,3}\gamma_{1,4}$$

$$\langle \psi_3 | c_{1\uparrow}| \phi_0\rangle = \langle \phi_0 | c_{1\downarrow}^{\dagger}| \psi_i\rangle = \alpha_{i,2}\gamma_{1,2} + \alpha_{i,3}\gamma_{1,4}$$

$$\langle \psi_3 | c_{2\uparrow}| \phi_0\rangle = \langle \phi_0 | c_{1\downarrow}^{\dagger}| \psi_3\rangle = \gamma_{1,2}$$

$$\langle \psi_3 | c_{1\downarrow}| \phi_0\rangle = \langle \phi_0 | c_{1\downarrow}^{\dagger}| \psi_3\rangle = 0$$

$$\langle \psi_3 | c_{2\downarrow}| \phi_0\rangle = \langle \phi_0 | c_{1\downarrow}^{\dagger}| \psi_3\rangle = 0$$

$$\langle \psi_4 | c_{1\uparrow}| \phi_0\rangle = \langle \phi_0 | c_{1\downarrow}^{\dagger}| \psi_4\rangle = 0$$

$$\langle \psi_4 | c_{1\downarrow}| \phi_0\rangle = \langle \phi_0 | c_{1\downarrow}^{\dagger}| \psi_4\rangle = 0$$

$$\langle \psi_4 | c_{1\downarrow}| \phi_0\rangle = \langle \phi_0 | c_{1\downarrow}^{\dagger}| \psi_4\rangle = -\gamma_{2,3}$$

$$\langle \psi_4 | c_{2\downarrow}| \phi_0\rangle = \langle \phi_0 | c_{2\downarrow}^{\dagger}| \psi_4\rangle = \gamma_{2,1}$$

 $\langle \psi_5 | c_{1\uparrow} | \phi_0 \rangle = \langle \phi_0 | c_{1\uparrow}^{\dagger} | \psi_5 \rangle = \frac{\gamma_{2,3}}{\sqrt{2}}$ 

 $\langle \psi_5 | c_{2\uparrow} | \phi_0 \rangle = \langle \phi_0 | c_{2\uparrow}^{\dagger} | \psi_5 \rangle = -\frac{\gamma_{2,1}}{\sqrt{2}}$ 

 $\langle \psi_5 | c_{1\downarrow} | \phi_0 \rangle = \langle \phi_0 | c_{1\downarrow}^{\dagger} | \psi_5 \rangle = -\frac{\gamma_{1,4}}{\sqrt{2}}$  $\langle \psi_5 | c_{2\downarrow} | \phi_0 \rangle = \langle \phi_0 | c_{2\downarrow}^{\dagger} | \psi_5 \rangle = \frac{\gamma_{1,2}}{\sqrt{2}}$ 

## 4.3 General case : one particle Green's function

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

## **4.3.1** N = 1 electron

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

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

$$G_{11\uparrow}(\omega) = \frac{(\alpha_{0,1}\beta_{1,4} + \alpha_{0,3}\beta_{1,2})^2}{\omega - (E_{\psi_0} - E_0) + i\eta} + \frac{(\alpha_{1,1}\beta_{1,4} + \alpha_{1,3}\beta_{1,2})^2}{\omega - (E_{\psi_1} - E_0) + i\eta} + \frac{(\alpha_{2,1}\beta_{1,4} + \alpha_{2,3}\beta_{1,2})^2}{\omega - (E_{\psi_2} - E_0) + i\eta} + \frac{\beta_{2,3}^2}{\omega - (E_{\psi_4} - E_0) + i\eta} + \frac{\beta_{2,1}^2}{\omega - (E_{\psi_5} - E_0) - i\eta} + \frac{\beta_{2,1}^2}{\omega - E_0 - i\eta}$$

$$\begin{split} G_{22\uparrow}(\omega) &= \frac{(\alpha_{0,2}\beta_{1,2} - \alpha_{0,4}\beta_{1,4})^2}{\omega - (E_{\psi_0} - E_0) + i\eta} + \frac{(\alpha_{1,2}\beta_{1,2} - \alpha_{1,4}\beta_{1,4})^2}{\omega - (E_{\psi_1} - E_0) + i\eta} + \frac{(\alpha_{2,2}\beta_{1,2} - \alpha_{2,4}\beta_{1,4})^2}{\omega - (E_{\psi_2} - E_0) + i\eta} \\ &+ \frac{\beta_{2,1}^2}{\omega - (E_{\psi_4} - E_0) + i\eta} + \frac{\beta_{1,2}^2/2}{\omega - (E_{\psi_5} - E_0) - i\eta} + \frac{\beta_{2,3}^2}{\omega - E_0 - i\eta} \end{split}$$

$$G_{12\uparrow}(\omega) = -\frac{(\alpha_{0,1}\beta_{1,4} + \alpha_{0,3}\beta_{1,2})(\alpha_{0,2}\beta_{1,2} - \alpha_{0,4}\beta_{1,4})}{\omega - (E_{\psi_0} - E_0) + i\eta} - \frac{(\alpha_{1,1}\beta_{1,4} + \alpha_{1,3}\beta_{1,2})(\alpha_{1,2}\beta_{1,2} - \alpha_{1,4}\beta_{1,4})}{\omega - (E_{\psi_1} - E_0) + i\eta} - \frac{(\alpha_{2,1}\beta_{1,4} + \alpha_{2,3}\beta_{1,2})(\alpha_{2,2}\beta_{1,2} - \alpha_{2,4}\beta_{1,4})}{\omega - (E_{\psi_2} - E_0) + i\eta} - \frac{\beta_{2,3}\beta_{2,1}}{\omega - (E_{\psi_4} - E_0) + i\eta} - \frac{\beta_{1,4}\beta_{1,2}/2}{\omega - (E_{\psi_4} - E_0) - i\eta} + \frac{\beta_{2,1}\beta_{2,3}}{\omega - (E_{\psi_4} - E_0) - i\eta}$$

$$G_{11\downarrow}(\omega) = \frac{(\alpha_{0,2}\beta_{2,3} - \alpha_{0,3}\beta_{2,1})^2}{\omega - (E_{\psi_0} - E_0) + i\eta} + \frac{(\alpha_{1,2}\beta_{2,3} - \alpha_{1,3}\beta_{2,1})^2}{\omega - (E_{\psi_1} - E_0) + i\eta} + \frac{(\alpha_{2,2}\beta_{2,3} - \alpha_{2,3}\beta_{2,1})^2}{\omega - (E_{\psi_2} - E_0) + i\eta} + \frac{\beta_{1,2}^2}{\omega - (E_{\psi_3} - E_0) + i\eta} + \frac{\beta_{1,2}^2}{\omega - (E_{\psi_3} - E_0) - i\eta}$$

$$G_{22\downarrow}(\omega) = \frac{(\alpha_{0,1}\beta_{2,1} + \alpha_{0,4}\beta_{2,3})^2}{\omega - (E_{\psi_0} - E_0) + i\eta} + \frac{(\alpha_{1,1}\beta_{2,1} + \alpha_{1,4}\beta_{2,3})^2}{\omega - (E_{\psi_1} - E_0) + i\eta} + \frac{(\alpha_{2,1}\beta_{2,1} + \alpha_{2,4}\beta_{2,3})^2}{\omega - (E_{\psi_2} - E_0) + i\eta} + \frac{\beta_{1,2}^2}{\omega - (E_{\psi_3} - E_0) + i\eta} + \frac{\beta_{2,1}^2/2}{\omega - (E_{\psi_5} - E_0) - i\eta} + \frac{\beta_{1,4}^2}{\omega - E_0 - i\eta}$$

$$G_{12\downarrow}(\omega) = -\frac{(\alpha_{0,2}\beta_{2,3} - \alpha_{0,3}\beta_{2,1})(\alpha_{0,1}\beta_{2,1} + \alpha_{0,4}\beta_{2,3})}{\omega - (E_{\psi_0} - E_0) + i\eta} - \frac{(\alpha_{1,2}\beta_{2,3} - \alpha_{1,3}\beta_{2,1})(\alpha_{1,1}\beta_{2,1} + \alpha_{1,4}\beta_{2,3})}{\omega - (E_{\psi_1} - E_0) + i\eta} - \frac{(\alpha_{2,2}\beta_{2,3} - \alpha_{2,3}\beta_{2,1})(\alpha_{2,1}\beta_{2,1} + \alpha_{2,4}\beta_{2,3})}{\omega - (E_{\psi_2} - E_0) + i\eta} - \frac{\beta_{1,4}\beta_{1,2}}{\omega - (E_{\psi_3} - E_0) - i\eta} + \frac{\beta_{1,2}\beta_{1,4}}{\omega - E_0 - i\eta}$$

### **4.3.2** N = 2 electrons

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

$$G_{11\uparrow}(\omega) = \frac{(-\alpha_{0,3}\beta_{1,2} - \alpha_{0,1}\beta_{1,4})^{2}}{\omega + (E_{\chi_{1}} - E_{0}) - i\eta} + \frac{(\alpha_{0,4}\gamma_{2,1} + \alpha_{0,2}\gamma_{2,3})^{2}}{\omega - (E_{\phi_{2}} - E_{0}) + i\eta}$$

$$+ \frac{(\alpha_{0,3}\beta_{3,2} + \alpha_{0,1}\beta_{3,4})^{2}}{\omega + (E_{\chi_{3}} - E_{0}) - i\eta} + \frac{(\alpha_{0,4}\gamma_{4,1} + \alpha_{0,2}\gamma_{4,3})^{2}}{\omega - (E_{\phi_{4}} - E_{0}) + i\eta}$$

$$G_{22\uparrow}(\omega) = \frac{(\alpha_{0,2}\beta_{1,2} - \alpha_{0,4}\beta_{1,4})^{2}}{\omega + (E_{\chi_{1}} - E_{0}) - i\eta} + \frac{(-\alpha_{0,1}\gamma_{2,1} + \alpha_{0,3}\gamma_{2,3})^{2}}{\omega - (E_{\phi_{2}} - E_{0}) + i\eta}$$

$$+ \frac{(\alpha_{0,2}\beta_{3,2} - \alpha_{0,4}\beta_{3,4})^{2}}{\omega + (E_{\chi_{3}} - E_{0}) - i\eta} + \frac{(-\alpha_{0,1}\gamma_{4,1} + \alpha_{0,3}\gamma_{4,3})^{2}}{\omega - (E_{\phi_{4}} - E_{0}) + i\eta}$$

$$G_{12\uparrow}(\omega) = \frac{(-\alpha_{0,3}\beta_{1,2} - \alpha_{0,1}\beta_{1,4})(\alpha_{0,2}\beta_{1,2} - \alpha_{0,4}\beta_{1,4})}{\omega + (E_{\chi_{1}} - E_{0}) - i\eta} + \frac{(\alpha_{0,4}\gamma_{2,1} + \alpha_{0,2}\gamma_{2,3})(-\alpha_{0,1}\gamma_{2,1} + \alpha_{0,3}\gamma_{2,3})}{\omega - (E_{\phi_{2}} - E_{0}) + i\eta}$$

$$+ \frac{(\alpha_{0,3}\beta_{3,2} + \alpha_{0,1}\beta_{3,4})(\alpha_{0,2}\beta_{3,2} - \alpha_{0,4}\beta_{3,4})}{\omega + (E_{\chi_{3}} - E_{0}) - i\eta} + \frac{(\alpha_{0,4}\gamma_{1,2} - \alpha_{0,1}\gamma_{1,4})^{2}}{\omega - (E_{\phi_{1}} - E_{0}) + i\eta} + \frac{(\alpha_{0,4}\gamma_{4,1} + \alpha_{0,2}\gamma_{4,3})(-\alpha_{0,1}\gamma_{4,1} + \alpha_{0,3}\gamma_{4,3})}{\omega - (E_{\phi_{4}} - E_{0}) + i\eta}$$

$$G_{11\downarrow}(\omega) = \frac{(\alpha_{0,4}\gamma_{1,2} - \alpha_{0,1}\gamma_{1,4})^{2}}{\omega - (E_{\phi_{1}} - E_{0}) + i\eta} + \frac{(\alpha_{0,3}\beta_{2,1} - \alpha_{0,2}\beta_{2,3})^{2}}{\omega + (E_{\chi_{2}} - E_{0}) - i\eta}$$

$$+ \frac{(\alpha_{0,4}\gamma_{3,2} - \alpha_{0,1}\gamma_{3,4})^{2}}{\omega - (E_{\phi_{3}} - E_{0}) + i\eta} + \frac{(\alpha_{0,3}\beta_{4,1} - \alpha_{0,2}\beta_{4,3})^{2}}{\omega + (E_{\chi_{4}} - E_{0}) - i\eta}$$

$$+ \frac{(\alpha_{0,2}\gamma_{3,2} + \alpha_{0,3}\gamma_{1,4})^{2}}{\omega - (E_{\phi_{3}} - E_{0}) + i\eta} + \frac{(\alpha_{0,1}\beta_{2,1} + \alpha_{0,4}\beta_{2,3})^{2}}{\omega + (E_{\chi_{4}} - E_{0}) - i\eta}$$

$$+ \frac{(\alpha_{0,2}\gamma_{3,2} + \alpha_{0,3}\gamma_{3,4})^{2}}{\omega - (E_{\phi_{3}} - E_{0}) + i\eta} + \frac{(\alpha_{0,1}\beta_{4,1} + \alpha_{0,4}\beta_{4,3})^{2}}{\omega + (E_{\chi_{4}} - E_{0}) - i\eta}$$

$$+ \frac{(\alpha_{0,2}\gamma_{3,2} + \alpha_{0,3}\gamma_{3,4})^{2}}{\omega - (E_{\phi_{3}} - E_{0}) + i\eta} + \frac{(\alpha_{0,1}\beta_{4,1} + \alpha_{0,4}\beta_{4,3})^{2}}{\omega + (E_{\chi$$

$$G_{12\downarrow}(\omega) = \frac{(\alpha_{0,4}\gamma_{1,2} - \alpha_{0,1}\gamma_{1,4})(\alpha_{0,2}\gamma_{1,2} + \alpha_{0,3}\gamma_{1,4})}{\omega - (E_{\phi_1} - E_0) + i\eta} + \frac{(\alpha_{0,3}\beta_{2,1} - \alpha_{0,2}\beta_{2,3})(\alpha_{0,1}\beta_{2,1} + \alpha_{0,4}\beta_{2,3})}{\omega + (E_{\chi_2} - E_0) - i\eta} + \frac{(\alpha_{0,4}\gamma_{3,2} - \alpha_{0,1}\gamma_{3,4})(\alpha_{0,2}\gamma_{3,2} + \alpha_{0,3}\gamma_{3,4})}{\omega - (E_{\phi_3} - E_0) + i\eta} + \frac{(\alpha_{0,3}\beta_{4,1} - \alpha_{0,2}\beta_{4,3})(\alpha_{0,1}\beta_{4,1} + \alpha_{0,4}\beta_{4,3})}{\omega + (E_{\chi_4} - E_0) - i\eta}$$

## **4.3.3** N = 3 electrons

$$G_{ij\sigma}(\omega) = \frac{\left\langle \uparrow \downarrow \uparrow \downarrow \middle| c_{i\sigma}^{\dagger} \middle| \phi_{0} \right\rangle \left\langle \phi_{0} \middle| c_{j\sigma} \middle| \uparrow \downarrow \uparrow \downarrow \right\rangle}{\omega - (E_{\uparrow \downarrow \uparrow \downarrow} - E_{0}) + i\eta} + \sum_{\psi} \frac{\left\langle \psi \middle| c_{i\sigma} \middle| \phi_{0} \right\rangle \left\langle \phi_{0} \middle| c_{j\sigma}^{\dagger} \middle| \psi \right\rangle}{\omega + (E_{\psi} - E_{0}) - i\eta}$$
With  $E_{0} = \frac{1}{2} (3\epsilon_{1} + 3\epsilon_{2} + U_{1} + U_{2} - g)$  and  $E_{\uparrow \downarrow \uparrow \downarrow} = (2\epsilon_{1} + 2\epsilon_{2} + U_{1} + U_{2})$ 

$$G_{11\uparrow}(\omega) = \frac{\gamma_{1,2}^{2}}{\omega - (E_{\uparrow \downarrow \uparrow \downarrow} - E_{0}) + i\eta} + \frac{(\alpha_{0,2}\gamma_{2,3} + \alpha_{0,4}\gamma_{2,1})^{2}}{\omega + (E_{\psi_{0}} - E_{0}) - i\eta} + \frac{(\alpha_{1,2}\gamma_{2,3} + \alpha_{1,4}\gamma_{2,1})^{2}}{\omega + (E_{\psi_{1}} - E_{0}) - i\eta} + \frac{\gamma_{1,4}^{2}}{\omega + (E_{\psi_{2}} - E_{0}) - i\eta} + \frac{\gamma_{2,3}^{2}/2}{\omega + (E_{\psi_{5}} - E_{0}) - i\eta}$$

$$G_{22\uparrow}(\omega) = \frac{\gamma_{1,4}^{2}}{\omega - (E_{\uparrow \downarrow \uparrow \downarrow} - E_{0}) + i\eta} + \frac{(\alpha_{0,3}\gamma_{2,3} - \alpha_{0,1}\gamma_{2,1})^{2}}{\omega + (E_{\psi_{0}} - E_{0}) - i\eta} + \frac{(\alpha_{1,3}\gamma_{2,3} - \alpha_{1,1}\gamma_{2,1})^{2}}{\omega + (E_{\psi_{1}} - E_{0}) - i\eta} + \frac{\gamma_{1,2}^{2}}{\omega + (E_{\psi_{1}} - E_{0}) - i\eta}$$

$$G_{12\uparrow}(\omega) = \frac{\gamma_{1,2}\gamma_{1,4}}{\omega - (E_{\uparrow \downarrow \uparrow \downarrow} - E_{0}) + i\eta} + \frac{(\alpha_{0,2}\gamma_{2,3} + \alpha_{0,4}\gamma_{2,1})(\alpha_{0,3}\gamma_{2,3} - \alpha_{0,1}\gamma_{2,1})}{\omega + (E_{\psi_{0}} - E_{0}) - i\eta}$$

$$G_{12\uparrow}(\omega) = \frac{\gamma_{1,2}\gamma_{1,4}}{\omega - (E_{\uparrow \downarrow \uparrow \downarrow} - E_{0}) + i\eta} + \frac{(\alpha_{0,2}\gamma_{2,3} + \alpha_{0,4}\gamma_{2,1})(\alpha_{0,3}\gamma_{2,3} - \alpha_{0,1}\gamma_{2,1})}{\omega + (E_{\psi_{2}} - E_{0}) - i\eta}$$

$$G_{12\uparrow}(\omega) = \frac{\gamma_{1,4}\gamma_{1,2}}{\omega - (E_{\uparrow \downarrow \uparrow \downarrow} - E_{0}) + i\eta} - \frac{\gamma_{2,3}\gamma_{2,1}/2}{\omega + (E_{\psi_{0}} - E_{0}) - i\eta}$$

$$G_{11\downarrow}(\omega) = \frac{\gamma_{2,1}}{\omega - (E_{\uparrow \downarrow \uparrow \downarrow} - E_{0}) + i\eta} + \frac{(\alpha_{0,4}\gamma_{1,2} - \alpha_{0,1}\gamma_{1,4})^{2}}{\omega + (E_{\psi_{0}} - E_{0}) - i\eta} + \frac{(\alpha_{1,4}\gamma_{1,2} - \alpha_{1,1}\gamma_{1,4})^{2}}{\omega + (E_{\psi_{0}} - E_{0}) - i\eta}$$

$$G_{11\downarrow}(\omega) = \frac{\gamma_{2,1}^{2}}{\omega - (E_{\uparrow \downarrow \uparrow \downarrow} - E_{0}) + i\eta} + \frac{(\alpha_{0,4}\gamma_{1,2} - \alpha_{0,1}\gamma_{1,4})^{2}}{\omega + (E_{\psi_{0}} - E_{0}) - i\eta} + \frac{\gamma_{1,4}^{2}/2}{\omega + (E_{\psi_{0}} - E_{0}) - i\eta}$$

 $+\frac{(\alpha_{2,2}\gamma_{1,2}+\alpha_{2,3}\gamma_{1,4})^2}{\omega+(F_{ch}-F_0)-in}+\frac{\gamma_{2,1}^2}{\omega+(F_{ch}-F_0)-in}+\frac{\gamma_{1,2}^2/2}{\omega+(F_{ch}-F_0)-in}$ 

 $G_{22\downarrow}(\omega) = \frac{\gamma_{2,3}^2}{\omega - (E_{\uparrow\downarrow\uparrow} - E_0) + i\eta} + \frac{(\alpha_{0,2}\gamma_{1,2} + \alpha_{0,3}\gamma_{1,4})^2}{\omega + (E_{\jmath\downarrow_0} - E_0) - i\eta} + \frac{(\alpha_{1,2}\gamma_{1,2} + \alpha_{1,3}\gamma_{1,4})^2}{\omega + (E_{\jmath\downarrow_0} - E_0) - i\eta}$ 

$$G_{12\downarrow}(\omega) = \frac{\gamma_{2,1}\gamma_{2,3}}{\omega - (E_{\uparrow\downarrow\uparrow\downarrow} - E_0) + i\eta} + \frac{(\alpha_{0,4}\gamma_{1,2} - \alpha_{0,1}\gamma_{1,4})(\alpha_{0,2}\gamma_{1,2} + \alpha_{0,3}\gamma_{1,4})}{\omega + (E_{\psi_0} - E_0) - i\eta}$$

$$+ \frac{(\alpha_{1,4}\gamma_{1,2} - \alpha_{1,1}\gamma_{1,4})(\alpha_{1,2}\gamma_{1,2} + \alpha_{1,3}\gamma_{1,4})}{\omega + (E_{\psi_1} - E_0) - i\eta} + \frac{(\alpha_{2,4}\gamma_{1,2} - \alpha_{2,1}\gamma_{1,4})(\alpha_{2,2}\gamma_{1,2} + \alpha_{2,3}\gamma_{1,4})}{\omega + (E_{\psi_2} - E_0) - i\eta}$$

$$- \frac{\gamma_{2,3}\gamma_{2,1}}{\omega + (E_{\psi_4} - E_0) - i\eta} - \frac{\gamma_{1,4}\gamma_{1,2}/2}{\omega + (E_{\psi_5} - E_0) - i\eta}$$