Hubbard Dimer Green's Function

1 Hubbard Model: Green's Function Calculation

To construct the one-electron Green's function for a two-site Hubbard model (Hubbard Dimer), we require the ground-state energies and wavefunctions for three scenarios:

1. $N-1$ electrons (the vacuum, $N=0$),
2. N electrons (one electron system, $N=1$),
3. $N+1$ electrons (two electrons system, $N=2$).

1.1 Hamiltonian

The Hubbard model Hamiltonian for two sites, with hopping t, on-site interaction U, and orbital energy ϵ, is given by:

$$\begin{aligned} \hat{H} = & -t \sum_{\sigma} (c_{1\sigma}^{\dagger} c_{2\sigma} + c_{2\sigma}^{\dagger} c_{1\sigma}) && (1) \\ & + U \sum_{i=1}^{2} n_{i\uparrow} n_{i\downarrow} + \epsilon \sum_{i\sigma} n_{i\sigma}. && (2) \end{aligned}$$

1.2 Energies and States

Vacuum State ($N=0$) The vacuum state $|0,0\rangle$ has energy:

$$E_{N-1} = 0. \tag{3}$$

One Electron System ($N=1$) The Hamiltonian matrix in the basis $\{|\uparrow,0\rangle, |0,\uparrow\rangle\}$ is:

$$H_{1e} = \begin{pmatrix} \epsilon & -t \\ -t & \epsilon \end{pmatrix}. \tag{4}$$

Two Electron System ($N=2$) The Hamiltonian matrix in the basis $\{|\uparrow\downarrow,0\rangle, |0,\uparrow\downarrow\rangle, |\uparrow,\downarrow\rangle, |\downarrow,\uparrow\rangle, |\uparrow,\uparrow\rangle, |\downarrow,\downarrow\rangle\}$ is:

$$H_{2e} = \begin{pmatrix} 2\epsilon & 0 & -t & -t & 0 & 0 \\ 0 & 2\epsilon & -t & -t & 0 & 0 \\ -t & -t & 2\epsilon + U & 0 & 0 & 0 \\ -t & -t & 0 & 2\epsilon + U & 0 & 0 \\ 0 & 0 & 0 & 0 & 2\epsilon & 0 \\ 0 & 0 & 0 & 0 & 0 & 2\epsilon \end{pmatrix}. \tag{5}$$

2 Analytical Solution of the Two-Site Hubbard Model

The two-site Hubbard model Hamiltonian in second quantization is characterized by parameters:

$$\epsilon \quad \text{(orbital energy)}, \quad t \quad \text{(hopping parameter)}, \quad U \quad \text{(onsite repulsion)}.$$

2.1 One-Electron Sector (N = 1)

The one-electron basis states are:

$$|\uparrow, 0\rangle, \quad |0, \uparrow\rangle$$

The Hamiltonian matrix in this basis is:

$$H_{1e} = \begin{pmatrix} \epsilon & -t \\ -t & \epsilon \end{pmatrix}$$

Diagonalizing this Hamiltonian, we obtain the eigenvalues:

$$E_1 = \epsilon - t, \quad E_2 = \epsilon + t$$

and corresponding eigenstates:

$$|\psi_1\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix}, \quad |\psi_2\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} -1 \\ 1 \end{pmatrix}.$$

The eigenvalues and eigenstates for the one-electron sector are summarized in Table 1.

Table 1: One-electron sector eigenvalues and eigenstates

Eigenvalue	Eigenstate	Description
$\epsilon - t$	$\frac{\lvert\uparrow,0\rangle + \lvert 0,\uparrow\rangle}{\sqrt{2}}$	Ground state (bonding)
$\epsilon + t$	$\frac{\lvert\uparrow,0\rangle - \lvert 0,\uparrow\rangle}{\sqrt{2}}$	Excited state (anti-bonding)

2.2 Two-Electron Sector (N+1 = 2)

In the two-electron sector, we choose the basis of six Slater determinants:

$$|\uparrow\downarrow, 0\rangle, |0, \uparrow\downarrow\rangle, |\uparrow, \uparrow\rangle, |\downarrow, \downarrow\rangle, |\uparrow, \downarrow\rangle, |\downarrow, \uparrow\rangle.$$

The Hamiltonian in this basis is:

$$H_{2e} = \begin{pmatrix} 2\epsilon + U & 0 & 0 & 0 & -t & -t \\ 0 & 2\epsilon + U & 0 & 0 & t & t \\ 0 & 0 & 2\epsilon & 0 & 0 & 0 \\ 0 & 0 & 0 & 2\epsilon & 0 & 0 \\ -t & t & 0 & 0 & 2\epsilon & 0 \\ -t & t & 0 & 0 & 0 & 2\epsilon \end{pmatrix}$$

Diagonalizing this Hamiltonian, we obtain the eigenvalues:

$$\begin{aligned}
E_1 &= 2\epsilon, \quad \text{(three-fold degeneracy)} \\
E_2 &= 2\epsilon + U \\
E_3 &= 2\epsilon + \frac{U}{2} - \frac{1}{2}\sqrt{U^2 + 16t^2} \\
E_4 &= 2\epsilon + \frac{U}{2} + \frac{1}{2}\sqrt{U^2 + 16t^2}
\end{aligned}$$

and corresponding eigenstates (unnormalized):

$$|\psi_{E=2\epsilon}\rangle : \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \\ 0 \\ 0 \end{pmatrix}, \quad \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \\ 0 \\ 0 \end{pmatrix}, \quad \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \\ -1 \\ 1 \end{pmatrix}$$

$$|\psi_{E=2\epsilon+U}\rangle : \begin{pmatrix} 1 \\ 1 \\ 0 \\ 0 \\ 0 \\ 0 \end{pmatrix}$$

$$|\psi_{E=2\epsilon+\frac{U}{2}-\frac{1}{2}\sqrt{U^2+16t^2}}\rangle : \begin{pmatrix} \frac{\epsilon}{t} - \frac{E_3}{2t} \\ -\frac{\epsilon}{t} + \frac{E_3}{2t} \\ 0 \\ 0 \\ 1 \\ 1 \end{pmatrix}, \quad |\psi_{E=2\epsilon+\frac{U}{2}+\frac{1}{2}\sqrt{U^2+16t^2}}\rangle : \begin{pmatrix} \frac{\epsilon}{t} - \frac{E_4}{2t} \\ -\frac{\epsilon}{t} + \frac{E_4}{2t} \\ 0 \\ 0 \\ 1 \\ 1 \end{pmatrix}$$

We already did this in class, but lets instead write these expressed in a basis where the singlet and triple sub-blocks are separated:

$$|\uparrow\downarrow, 0\rangle, \quad |0, \uparrow\downarrow\rangle, \quad \frac{|\uparrow,\downarrow\rangle - |\downarrow,\uparrow\rangle}{\sqrt{2}}, \quad \frac{|\uparrow,\downarrow\rangle + |\downarrow,\uparrow\rangle}{\sqrt{2}}, \quad |\uparrow,\uparrow\rangle, \quad |\downarrow,\downarrow\rangle$$

The eigenvalues and eigenstates for the two-electron sector are summarized in Table 2.

We define for convenience:

$$X = \frac{\frac{U}{2}}{t + \sqrt{\left(\frac{U}{2}\right)^2 + t^2}}$$

These analytical expressions allow explicit calculation of the exact Green's function via Lehmann's representation.

Table 2: Two-electron sector eigenvalues and eigenstates

Eigenvalue	Eigenstate	Description
$2\epsilon + \frac{U}{2} - \sqrt{\left(\frac{U}{2}\right)^2 + 4t^2}$	$\frac{\|\uparrow\downarrow,0\rangle + \|0,\uparrow\downarrow\rangle + X\frac{\|\uparrow,\downarrow\rangle - \|\downarrow,\uparrow\rangle}{\sqrt{2}}}{\sqrt{2+X^2}}$	Ground state (Singlet)
$2\epsilon + U$	$\frac{\|\uparrow\downarrow,0\rangle - \|0,\uparrow\downarrow\rangle}{\sqrt{2}}$	Singlet excited state
$2\epsilon + \frac{U}{2} + \sqrt{\left(\frac{U}{2}\right)^2 + 4t^2}$	$\frac{\|\uparrow\downarrow,0\rangle + \|0,\uparrow\downarrow\rangle - \frac{1}{X}\frac{\|\uparrow,\downarrow\rangle - \|\downarrow,\uparrow\rangle}{\sqrt{2}}}{\sqrt{2+1/X^2}}$	Singlet excited state
2ϵ	$\| \uparrow,\uparrow\rangle$	Triplet state ($S = 1, S_z = +1$)
2ϵ	$\| \downarrow,\downarrow\rangle$	Triplet state ($S = 1, S_z = -1$)
2ϵ	$\frac{\|\uparrow,\downarrow\rangle + \|\downarrow,\uparrow\rangle}{\sqrt{2}}$	Triplet state ($S = 1, S_z = 0$)

3 Exact Green's Function Using the Lehmann Representation

3.1 Lehmann Representation

The exact single-particle Green's function $G_{ij}(\omega)$ is given by the Lehmann representation as:

$$G_{ij\sigma}(\omega) = \sum_m \frac{\langle\psi_0^N|c_{i\sigma}|\psi_m^{N+1}\rangle\langle\psi_m^{N+1}|c_{j\sigma}^\dagger|\psi_0^N\rangle}{\omega - (E_m^{N+1} - E_0^N) + i\eta} + \sum_n \frac{\langle\psi_0^N|c_{j\sigma}^\dagger|\psi_n^{N-1}\rangle\langle\psi_n^{N-1}|c_{i\sigma}|\psi_0^N\rangle}{\omega - (E_0^N - E_n^{N-1}) - i\eta}.$$

Here:

- $|\psi_0^N\rangle$: Ground-state wavefunction of the N-electron system with energy E_0^N.
- $|\psi_m^{N+1}\rangle$: Eigenstates of the $(N+1)$-electron system with energies E_m^{N+1}.
- $|\psi_n^{N-1}\rangle$: Eigenstates of the $(N-1)$-electron system with energies E_n^{N-1}.
- $c_{i\sigma}^\dagger, c_{i\sigma}$: Spin resolved electron creation and annihilation operators at site i.
- η: Small positive number ensuring causality.

3.2 Two-Site Hubbard Model: N=1 Case

We illustrate this explicitly for the Hubbard model with one electron on two sites.

Action of Creation and Annihilation Operators on the One-Electron Ground State

We start with the one-electron ground state (with spin up):

$$|\psi_0^{N=1}\rangle = \frac{1}{\sqrt{2}}\left(|\uparrow,0\rangle + |0,\uparrow\rangle\right).$$

We need to evaluate the actions of creation and annihilation operators $c_{i\sigma}$ and $c_{i\sigma}^\dagger$ on this ground state.

Annihilation Operators: $c_{i\sigma}|\psi_0^{N=1}\rangle$ Annihilation of an electron on the single-electron states gives the vacuum state or zero:

$$c_{1\uparrow}|\uparrow,0\rangle = |0,0\rangle, \quad c_{2\uparrow}|0,\uparrow\rangle = |0,0\rangle,$$

and

$$c_{2\uparrow}|\uparrow,0\rangle = 0, \quad c_{1\uparrow}|0,\uparrow\rangle = 0.$$

Thus:

$$c_{1\uparrow}|\psi_0^{N=1}\rangle = \frac{|0,0\rangle}{\sqrt{2}}, \quad c_{2\uparrow}|\psi_0^{N=1}\rangle = \frac{|0,0\rangle}{\sqrt{2}}.$$

For spin down electrons (not initially present):

$$c_{1\downarrow}|\psi_0^{N=1}\rangle = 0, \quad c_{2\downarrow}|\psi_0^{N=1}\rangle = 0.$$

Creation Operators: $c_{i\sigma}^\dagger|\psi_0^{N=1}\rangle$ Creation of an electron from a one-electron state yields two-electron states:

For spin up:

$$c_{1\uparrow}^\dagger|\psi_0^{N=1}\rangle = c_{1\uparrow}^\dagger\frac{(|\uparrow,0\rangle + |0,\uparrow\rangle)}{\sqrt{2}} = \frac{c_{1\uparrow}^\dagger|\uparrow,0\rangle + c_{1\uparrow}^\dagger|0,\uparrow\rangle}{\sqrt{2}}.$$

Evaluate explicitly:

$$c_{1\uparrow}^\dagger|\uparrow,0\rangle = 0, \quad \text{(Pauli principle: double occupation with same spin at same site)}$$

$$c_{1\uparrow}^\dagger|0,\uparrow\rangle = -|\uparrow,\uparrow\rangle, \quad \text{(anticommutation rule: fermionic exchange gives negative sign)}$$

Thus we have clearly:

$$c_{1\uparrow}^\dagger|\psi_0^{N=1}\rangle = \frac{-|\uparrow,\uparrow\rangle}{\sqrt{2}}.$$

Similarly, for the second site:

$$c_{2\uparrow}^\dagger|\psi_0^{N=1}\rangle = \frac{c_{2\uparrow}^\dagger|\uparrow,0\rangle + c_{2\uparrow}^\dagger|0,\uparrow\rangle}{\sqrt{2}} = \frac{|\uparrow,\uparrow\rangle}{\sqrt{2}}.$$

For spin down:

$$c_{1\downarrow}^\dagger|\psi_0^{N=1}\rangle = \frac{|\uparrow\downarrow,0\rangle + |\downarrow,\uparrow\rangle}{\sqrt{2}}, \quad c_{2\downarrow}^\dagger|\psi_0^{N=1}\rangle = \frac{|\uparrow,\downarrow\rangle + |0,\uparrow\downarrow\rangle}{\sqrt{2}}.$$

Summary

$$\begin{aligned}
c_{1\uparrow}|\psi_0^{N=1}\rangle &= \frac{|0,0\rangle}{\sqrt{2}}, & c_{2\uparrow}|\psi_0^{N=1}\rangle &= \frac{|0,0\rangle}{\sqrt{2}}, \\
c_{1\downarrow}|\psi_0^{N=1}\rangle &= 0, & c_{2\downarrow}|\psi_0^{N=1}\rangle &= 0, \\
c_{1\uparrow}^\dagger|\psi_0^{N=1}\rangle &= -\frac{|\uparrow,\uparrow\rangle}{\sqrt{2}}, & c_{2\uparrow}^\dagger|\psi_0^{N=1}\rangle &= \frac{|\uparrow,\uparrow\rangle}{\sqrt{2}}, \\
c_{1\downarrow}^\dagger|\psi_0^{N=1}\rangle &= \frac{|\uparrow\downarrow,0\rangle + |\downarrow,\uparrow\rangle}{\sqrt{2}}, & c_{2\downarrow}^\dagger|\psi_0^{N=1}\rangle &= \frac{|\uparrow,\downarrow\rangle + |0,\uparrow\downarrow\rangle}{\sqrt{2}}.
\end{aligned}$$

4 Spin-Resolved Green's Functions for the Two-Site Hubbard Model

To explicitly derive the spin-resolved one-particle Green's function, we must separately consider spin-up and spin-down contributions.

The Green's function is given by the Lehmann representation as:

$$G_{ij,\sigma}(\omega) = G^{-}_{ij,\sigma}(\omega) + G^{+}_{ij,\sigma}(\omega),$$

with particle removal (hole) and particle addition parts defined as:

$$G^{-}_{ij,\sigma}(\omega) = \sum_n \frac{\langle \psi_0^{N=1} | c^\dagger_{i\sigma} | \psi_n^{N=0} \rangle \langle \psi_n^{N=0} | c_{j\sigma} | \psi_0^{N=1} \rangle}{\omega - (E_0^{N=1} - E_n^{N=0}) - i\eta},$$

and

$$G^{+}_{ij,\sigma}(\omega) = \sum_n \frac{\langle \psi_0^{N=1} | c_{i\sigma} | \psi_n^{N=2} \rangle \langle \psi_n^{N=2} | c^\dagger_{j\sigma} | \psi_0^{N=1} \rangle}{\omega - (E_n^{N=2} - E_0^{N=1}) + i\eta}.$$

4.1 Ground State for N=1 (One Electron)

The one-electron ground state is spin degenerate. Let us explicitly choose the spin-up ground state:

$$|\psi_0^{N=1}\rangle = \frac{1}{\sqrt{2}} \left(|\uparrow, 0\rangle + |0, \uparrow\rangle \right), \quad E_0^{N=1} = \epsilon - t.$$

4.2 Evaluation of Particle Removal (N=0)

The $N = 0$ vacuum state is $|0, 0\rangle$ with energy $E^{N=0} = 0$. Then, particle removal for spin-up is:

$$c_{1\uparrow} |\psi_0^{N=1}\rangle = \frac{1}{\sqrt{2}} |0, 0\rangle, \quad c_{2\uparrow} |\psi_0^{N=1}\rangle = \frac{1}{\sqrt{2}} |0, 0\rangle.$$

Thus,

$$G^{-}_{11,\uparrow}(\omega) = G^{-}_{22,\uparrow}(\omega) = \frac{\frac{1}{2}}{\omega - (\epsilon - t) - i\eta},$$

and similarly,

$$G^{-}_{12,\uparrow}(\omega) = G^{-}_{21,\uparrow}(\omega) = \frac{\frac{1}{2}}{\omega - (\epsilon - t) - i\eta}.$$

For spin-down, we have no occupancy; hence, there is no particle removal contribution:

$$G^{-}_{ij,\downarrow}(\omega) = 0.$$

4.3 Evaluation of Particle Addition (N=2)

Now we consider particle addition separately for spin-up and spin-down.

Spin-Up Particle Addition: The relevant two-electron state contributing to spin-up addition is the triplet state $|\uparrow,\uparrow\rangle$ with energy 2ϵ.

This is the only state that can result from a spin up electron addition to the one electron ground state

$$|\psi_0^{N=1}\rangle = \frac{1}{\sqrt{2}}\left(|\uparrow,0\rangle + |0,\uparrow\rangle\right).$$

as shown here:

$$c_{1\uparrow}^{\dagger}|\psi_0^{N=1}\rangle = -\frac{1}{\sqrt{2}}|\uparrow,\uparrow\rangle, \quad c_{2\uparrow}^{\dagger}|\psi_0^{N=1}\rangle = \frac{1}{\sqrt{2}}|\uparrow,\uparrow\rangle.$$

Hence,

$$G_{11,\uparrow}^{+}(\omega) = G_{22,\uparrow}^{+}(\omega) = \frac{\frac{1}{2}}{\omega - (\epsilon + t) + i\eta},$$

and cross terms are negative:

$$G_{12,\uparrow}^{+}(\omega) = G_{21,\uparrow}^{+}(\omega) = -\frac{\frac{1}{2}}{\omega - (\epsilon + t) + i\eta}.$$

Spin-Down particle addition$G_{ij,\downarrow}(\omega)$ The spin-down Green's function explicitly contains contributions from particle-addition terms only (as the particle removal term vanishes for spin-down). It is expressed as:

$$G_{ij,\downarrow}(\omega) = G_{ij,\downarrow}^{+}(\omega),$$

with the general form (Lehmann representation):

$$G_{ij,\downarrow}^{+}(\omega) = \sum_n \frac{\langle\psi_0^{N=1}|c_{i\downarrow}|\psi_n^{N=2}\rangle\langle\psi_n^{N=2}|c_{j\downarrow}^{\dagger}|\psi_0^{N=1}\rangle}{\omega - (E_n^{N=2} - E_0^{N=1}) + i\eta}.$$

For our two-site Hubbard model, the relevant two-electron eigenstates with nonzero overlap with the ground state of the one-electron sector $|\psi_0^{N=1}\rangle = \frac{|\uparrow,0\rangle + |0,\uparrow\rangle}{\sqrt{2}}$ are the three singlet states explicitly derived previously:

1. Eigenvalues and states (previously derived)

- **Ground singlet**:

$$|\psi_g^{N=2}\rangle = \frac{|d,0\rangle + |0,d\rangle + X\frac{|\uparrow,\downarrow\rangle - |\downarrow,\uparrow\rangle}{\sqrt{2}}}{\sqrt{2 + X^2}}, \quad E_g^{N=2} = 2\epsilon + \frac{U}{2} - \sqrt{\left(\frac{U}{2}\right)^2 + 4t^2}.$$

- **Singlet excited state 1**:

$$|\psi_{s,1}^{N=2}\rangle = \frac{|d,0\rangle - |0,d\rangle}{\sqrt{2}}, \quad E_{s,1}^{N=2} = 2\epsilon + U.$$

- **Singlet excited state 2**:

$$|\psi_{s,2}^{N=2}\rangle = \frac{|d,0\rangle + |0,d\rangle - \frac{1}{X}\frac{|\uparrow,\downarrow\rangle - |\downarrow,\uparrow\rangle}{\sqrt{2}}}{\sqrt{2 + 1/X^2}}, \quad E_{s,2}^{N=2} = 2\epsilon + \frac{U}{2} + \sqrt{\left(\frac{U}{2}\right)^2 + 4t^2}.$$

2. Explicit overlaps (Check!!):

- **Ground singlet** overlaps:

$$\langle \psi_g^{N=2} | c_{1\downarrow}^\dagger | \psi_0^{N=1} \rangle = \frac{1 - \frac{X}{\sqrt{2}}}{\sqrt{2(2+X^2)}}, \quad \langle \psi_g^{N=2} | c_{2\downarrow}^\dagger | \psi_0^{N=1} \rangle = \frac{1 + \frac{X}{\sqrt{2}}}{\sqrt{2(2+X^2)}}.$$

- **Excited singlet 1** overlaps:

$$\langle \psi_{s,1}^{N=2} | c_{1\downarrow}^\dagger | \psi_0^{N=1} \rangle = \frac{1}{2}, \quad \langle \psi_{s,1}^{N=2} | c_{2\downarrow}^\dagger | \psi_0^{N=1} \rangle = -\frac{1}{2}.$$

- **Excited singlet 2** overlaps:

$$\langle \psi_{s,2}^{N=2} | c_{1\downarrow}^\dagger | \psi_0^{N=1} \rangle = \frac{1 + \frac{1}{X\sqrt{2}}}{\sqrt{2(2+1/X^2)}}, \quad \langle \psi_{s,2}^{N=2} | c_{2\downarrow}^\dagger | \psi_0^{N=1} \rangle = \frac{1 - \frac{1}{X\sqrt{2}}}{\sqrt{2(2+1/X^2)}}.$$

3. Explicit final analytical result:
Thus, the explicit final result for the spin-down Green's function matrix is given by:

$$G_{ij,\downarrow}(\omega) = \frac{\langle \psi_0^{N=1} | c_{i\downarrow} | \psi_g^{N=2} \rangle \langle \psi_g^{N=2} | c_{j\downarrow}^\dagger | \psi_0^{N=1} \rangle}{\omega - \left(E_g^{N=2} - E_0^{N=1}\right) + i\eta} + \frac{\langle \psi_0^{N=1} | c_{i\downarrow} | \psi_{s,1}^{N=2} \rangle \langle \psi_{s,1}^{N=2} | c_{j\downarrow}^\dagger | \psi_0^{N=1} \rangle}{\omega - \left(E_{s,1}^{N=2} - E_0^{N=1}\right) + i\eta}$$

$$+ \frac{\langle \psi_0^{N=1} | c_{i\downarrow} | \psi_{s,2}^{N=2} \rangle \langle \psi_{s,2}^{N=2} | c_{j\downarrow}^\dagger | \psi_0^{N=1} \rangle}{\omega - \left(E_{s,2}^{N=2} - E_0^{N=1}\right) + i\eta},$$

where the denominators explicitly read:
- Ground singlet:

$$E_g^{N=2} - E_0^{N=1} = \epsilon + t + \frac{U}{2} - \sqrt{\left(\frac{U}{2}\right)^2 + 4t^2}$$

- Excited singlet 1:

$$E_{s,1}^{N=2} - E_0^{N=1} = \epsilon + t + U$$

- Excited singlet 2:

$$E_{s,2}^{N=2} - E_0^{N=1} = \epsilon + t + \frac{U}{2} + \sqrt{\left(\frac{U}{2}\right)^2 + 4t^2}$$

Thus, this is the fully explicit and correct analytical result for the spin-down Green's function $G_{ij,\downarrow}$.

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Summary of explicit final result in compact form:

$$\boxed{G_{ij,\downarrow}(\omega) = \sum_{n=g,s_1,s_2} \frac{\langle \psi_0^{N=1} | c_{i\downarrow} | \psi_n^{N=2} \rangle \langle \psi_n^{N=2} | c_{j\downarrow}^\dagger | \psi_0^{N=1} \rangle}{\omega - (E_n^{N=2} - E_0^{N=1}) + i\eta},}$$

5 Physical Interpretation of the Green's Function Poles and the Spectral Function

5.1 Interpretation of the Poles of the Green's Function

One can interpret the poles of the Green's function in terms of a simple molecular orbital picture. Consider the two-site Hubbard model, with single-particle orbital energies and hopping integrals defining two molecular orbitals: the *bonding* orbital at energy $\epsilon_0 - t$ and the *antibonding* orbital at energy $\epsilon_0 + t$. In the ground state for the one-electron case ($N = 1$), the single spin-up electron occupies the lower-energy bonding orbital.

For the non-interacting limit ($U = 0$), the possible electronic excitations correspond straightforwardly to either adding or removing electrons from these molecular orbitals:

- Removal of a spin-up electron from the occupied bonding orbital at $\omega = \epsilon_0 - t$.
- Addition of a spin-down electron to the bonding orbital at $\omega = \epsilon_0 - t$.
- Addition of spin-up or spin-down electrons to the unoccupied antibonding orbital at $\omega = \epsilon_0 + t$.

When the electron-electron interaction U is turned on, the single-particle picture changes significantly:

- The pole corresponding to the addition of a spin-down electron to the originally bonding orbital shifts to the energy

  $$\omega = \epsilon_0 + t + \frac{U - c}{2}, \quad c = \sqrt{U^2 + 16t^2}.$$

  This shift arises due to the electron-electron Coulomb repulsion U.
- The addition energy to the antibonding orbital splits into two distinct energies:

  $$\omega = \epsilon_0 + t \quad \text{and} \quad \omega = \epsilon_0 + t + U.$$

  The presence of interaction lifts the degeneracy seen at $U = 0$, reflecting distinct possible states of electron addition due to electron-electron repulsion.
- Furthermore, adding a spin-down electron may also excite the system into a higher-energy configuration, generating a satellite peak at:

  $$\omega = \epsilon_0 + t + \frac{U + c}{2}.$$

Thus, the electron-electron interaction not only shifts existing poles but also splits and introduces new satellite excitations, directly reflecting the correlated nature of the electron system.

5.2 Definition and Physical Meaning of the Spectral Function

The spectral function $A(\omega)$ is defined as:

$$A(\omega) = -\frac{1}{\pi} \mathrm{Im}\left[\mathrm{Tr}(G(\omega))\right].$$

Physically, the spectral function describes the probability of adding or removing an electron at a given energy. Peaks of $A(\omega)$ correspond directly to the excitation energies (poles of the Green's function) and can be measured experimentally through photoemission (electron removal) or inverse photoemission (electron addition) spectroscopy.

Connection to the Self-energy The Green's function $G(\omega)$ is related to the non-interacting Green's function $G_0(\omega)$ and the self-energy $\Sigma(\omega)$ through Dyson's equation:

$$G(\omega) = \left[G_0^{-1}(\omega) - \Sigma(\omega)\right]^{-1}.$$

Hence, the spectral function explicitly depends on the self-energy via:

$$A(\omega) = -\frac{1}{\pi}\mathrm{Im}\left[\mathrm{Tr}\left(\left[G_0^{-1}(\omega) - \Sigma(\omega)\right]^{-1}\right)\right].$$

5.3 Results in our numerical model $\epsilon = 0$ and $t = 1$ and $U = 2$

For the two-site Hubbard model, the non-interacting (one-electron) Hamiltonian is given by:

$$H^{(1)} = \begin{pmatrix} \epsilon & -t \\ -t & \epsilon \end{pmatrix},$$

with eigenvalues corresponding to bonding and antibonding molecular orbitals:

$$E_{\pm}^{(1)} = \epsilon \pm t.$$

Choosing the parameters $\epsilon = 0$ and $t = 1$, we have the molecular orbital energies:

$$E_{+}^{(1)} = 1, \quad E_{-}^{(1)} = -1.$$

For a system with a single electron ($N = 1$), the ground-state energy is thus:

$$E_0^{N=1} = -1,$$

with the electron occupying the lower-energy bonding orbital.

Two-electron energies ($N = 2$ sector) For the two-electron Hubbard dimer, the relevant eigenvalues (with parameters $\epsilon = 0$, $t = 1$, $U = 2$) are:

- Ground-state singlet:

$$E_g^{N=2} = \frac{U}{2} - \sqrt{\left(\frac{U}{2}\right)^2 + 4t^2} \approx -1.236$$

- Trivial singlet/triplet states (no hopping due to symmetry):

$$E_{\text{trivial}}^{N=2} = 2\epsilon = 0$$

- Double-occupation state:

$$E_{\text{double}}^{N=2} = 2\epsilon + U = 2$$

- Excited singlet:

$$E_{\text{excited}}^{N=2} = \frac{U}{2} + \sqrt{\left(\frac{U}{2}\right)^2 + 4t^2} \approx 3.236$$

Thus, the two-electron energy spectrum is:

$$-1.236, \quad 0, \quad 2, \quad 3.236.$$

Poles of the interacting Green's function The poles of the particle-addition Green's function are given by the excitation energies:

$$\omega = E_n^{N=2} - E_0^{N=1}.$$

Evaluating explicitly:

- **Spin-up electron addition** (initial state with one spin-up electron):
  - Triplet state (spin-aligned electrons): $E_n^{N=2} = 0$, pole at:
  $$0 - (-1) = 1$$
  - Double occupation (localized two electrons on one site): $E_n^{N=2} = 2$, pole at:
  $$2 - (-1) = 3$$
- **Spin-down electron addition** (initially one spin-up electron):
  - Ground-state singlet: $E_n^{N=2} \approx -1.236$, pole at:
  $$-1.236 - (-1) = -0.236$$
  - Trivial singlet state: $E_n^{N=2} = 0$, pole at:
  $$0 - (-1) = 1$$
  - Excited singlet state: $E_n^{N=2} \approx 3.236$, pole at:
  $$3.236 - (-1) = 4.236$$

5.4 Identification of Spectral Peaks in Numerical Calculations

Using the provided numerical code to compute $A(\omega)$ based on the self-energy derived from the analytical Green's function, one explicitly identifies peaks at the predicted excitation energies. Specifically, the spectral function exhibits peaks at the energies:

$$\omega = -0.236, \quad 1, \quad 3, \quad 4.236,$$

consistent with the analytical Lehmann representation results derived above.

6 Evaluation of the GW approximation: N=1

6.1 Polarizability

We start with the definition of the polarization $P_{ij}(\omega)$ within the Random Phase Approximation (RPA):

$$P_{ij}(\omega) = -i \int \frac{d\omega'}{2\pi} \sum_{\sigma,\sigma'} G_{i\sigma,j\sigma'}(\omega + \omega')\, G_{j\sigma',i\sigma}(\omega')$$

At quarter filling (N=1) in the Hubbard dimer, the non-interacting Green's function is given explicitly by the equations derived above for the spin-up block ($G_{ij}^{0\uparrow}(\omega)$). Note that the polarization function $P(\omega)$ is constructed from products of single-particle Green's functions $G(\omega)$. Each Green's function $G_{i\sigma,j\sigma'}(\omega)$ describes the propagation of an electron from state $j\sigma'$ to state $i\sigma$.

Now, the polarization at this level of approximation (RPA, or Random Phase Approximation) involves transitions where electrons do not flip their spins** during the excitation process, because the the Coulomb interaction here

$$U\sum_i n_{i\uparrow}n_{i\downarrow},$$

does not couple different spins directly given that is diagonal in spin. As our N=1 electron is spin up (our choice) the spin-down polarization is identically zero.

$$G^{0\uparrow}_{ij}(\omega) = \frac{(-1)^{i-j}}{2}\left(\frac{1}{\omega-(\varepsilon_0+t)+i\eta}+\frac{(-1)^{i-j}}{\omega-(\varepsilon_0-t)-i\eta}\right)$$

Let's first simplify and clearly rewrite this Green's function in a simpler form:

$$G^{0\uparrow}_{ij}(\omega) = \frac{1}{2}\left[\frac{(-1)^{i-j}}{\omega-(\varepsilon_0+t)+i\eta}+\frac{1}{\omega-(\varepsilon_0-t)-i\eta}\right]$$

$$P^{\uparrow}_{ij}(\omega) = -i\int\frac{d\omega'}{2\pi}G^{0\uparrow}_{ij}(\omega+\omega')G^{0\uparrow}_{ji}(\omega')$$

Considering explicitly the diagonal elements (for simplicity we start with $i=j=1$):

$$P^{\uparrow}_{11}(\omega) = -i\int\frac{d\omega'}{2\pi}G^{0\uparrow}_{11}(\omega+\omega')G^{0\uparrow}_{11}(\omega')$$

Expanding explicitly these Green's functions:

$$P^{\uparrow}_{11}(\omega) = -i\int\frac{d\omega'}{2\pi}\frac{1}{4}\left[\frac{1}{\omega+\omega'-\varepsilon_0-t+i\eta}+\frac{1}{\omega+\omega'-\varepsilon_0+t-i\eta}\right]\left[\frac{1}{\omega'-\varepsilon_0-t+i\eta}+\frac{1}{\omega'-\varepsilon_0+t-i\eta}\right]$$

Multiplying these terms gives us four integrals, each of the type:

$$I_{ab}(\omega) = -\frac{i}{4}\int\frac{d\omega'}{2\pi}\frac{1}{\omega+\omega'-E_a+i\eta}\frac{1}{\omega'-E_b+i\eta'},$$

with E_a, E_b being either ε_0+t or ε_0-t, and $\eta,\eta'\to 0^+$ infinitesimal positive numbers.

These integrals can be solved explicitly by contour integration (closing the contour in the upper or lower half-plane depending on the signs of the infinitesimal imaginary parts). Each integral picks up a pole contribution from one of the Green's functions.

For example, one of these integrals explicitly is:

$$I(\omega) = -\frac{i}{4}\int\frac{d\omega'}{2\pi}\frac{1}{(\omega+\omega')-(\varepsilon_0+t)+i\eta}\frac{1}{\omega'-(\varepsilon_0-t)+i\eta}$$

To evaluate this integral, we perform a contour integration in the complex ω' plane, closing the contour in the upper half-plane. This picks the pole at $\omega'=\varepsilon_0-t$:

$$I(\omega) = -\frac{i}{4}\left[2\pi i\frac{1}{(\omega+(\varepsilon_0-t))-(\varepsilon_0+t)+i\eta}\right]\frac{1}{2\pi} = -\frac{1}{4}\frac{1}{\omega-2t+i\eta}$$

Doing similar evaluations for all four terms, after careful algebra (note the cancellations between symmetric terms), we end up with the very simple form:

$$P_{11}^{\uparrow}(\omega) = \frac{1}{4}\left(\frac{1}{\omega - 2t + i\eta} - \frac{1}{\omega + 2t - i\eta}\right)$$

In a similar way, one finds that the off-diagonal terms ($i \neq j$) have opposite sign due to the factors $(-1)^{i-j}$. Thus, one obtains:

$$P_{ij}^{\uparrow}(\omega) = \frac{(-1)^{i-j}}{4}\left(\frac{1}{\omega - 2t + i\eta} - \frac{1}{\omega + 2t - i\eta}\right)$$

Final derived result:

$$\boxed{P_{ij}^{\uparrow}(\omega) = \frac{(-1)^{i-j}}{4}\left(\frac{1}{\omega - 2t + i\eta} - \frac{1}{\omega + 2t - i\eta}\right)}$$

6.2 Screened Coulomb Interaction W

The screened Coulomb interaction $W(\omega)$ in terms of the bare Coulomb interaction v_c and the polarizability $P(\omega)$ is obtained through the Dyson equation for W:

$$W_{ij,\uparrow}(\omega) = v_{ij} + \sum_{kl} v_{ik} P_{kl,\uparrow}(\omega) W_{lj,\uparrow}(\omega),$$

where for the two-site Hubbard dimer model, the Coulomb interaction is given by:

$$v_{ij} = U\delta_{ij}.$$

Thus, explicitly, the Dyson-like equation for the screened interaction $W(\omega)$ becomes:

$$W_{ij,\uparrow}(\omega) = U\delta_{ij} + U\sum_{k} P_{ik,\uparrow}(\omega) W_{kj,\uparrow}(\omega).$$

For two sites (1,2), explicitly writing this in matrix form:

$$\begin{pmatrix} W_{11,\uparrow}(\omega) & W_{12,\uparrow}(\omega) \\ W_{21,\uparrow}(\omega) & W_{22,\uparrow}(\omega) \end{pmatrix} = U\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} + U\begin{pmatrix} P_{11,\uparrow}(\omega) & P_{12,\uparrow}(\omega) \\ P_{21,\uparrow}(\omega) & P_{22,\uparrow}(\omega) \end{pmatrix}\begin{pmatrix} W_{11,\uparrow}(\omega) & W_{12,\uparrow}(\omega) \\ W_{21,\uparrow}(\omega) & W_{22,\uparrow}(\omega) \end{pmatrix}.$$

This can be rearranged as:

$$\left[\mathbb{I} - U\mathbf{P}_{\uparrow}(\omega)\right]\mathbf{W}_{\uparrow}(\omega) = U\mathbb{I},$$

where the identity $\mathbb{I}$ is the 2×2 identity matrix and $\mathbf{P}_{\uparrow}(\omega)$ and $\mathbf{W}_{\uparrow}(\omega)$ are the 2×2 polarization and screened interaction matrices, respectively.

Solving for $\mathbf{W}_{\uparrow}(\omega)$:

$$\mathbf{W}_{\uparrow}(\omega) = U\left[\mathbb{I} - U\mathbf{P}_{\uparrow}(\omega)\right]^{-1}.$$

Using the derived polarization function $P_{ij,\uparrow}(\omega)$

$$P_{ij,\uparrow}(\omega) = \frac{(-1)^{i-j}}{2}\left(\frac{1}{\omega - 2t + i\eta} - \frac{1}{\omega + 2t + i\eta}\right).$$

Thus, the polarization matrix is explicitly given by:

$$\mathbf{P}_{\uparrow}(\omega) = \frac{1}{2}\left(\frac{1}{\omega - 2t + i\eta} - \frac{1}{\omega + 2t + i\eta}\right)\begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix}.$$

Define the scalar polarizability factor clearly:

$$P(\omega) = \frac{1}{2}\left(\frac{1}{\omega - 2t + i\eta} - \frac{1}{\omega + 2t + i\eta}\right).$$

Then,

$$\mathbf{P}_{\uparrow}(\omega) = P(\omega)\begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix}.$$

Thus, clearly:

$$\mathbf{W}_{\uparrow}(\omega) = U\left[\mathbb{I} - UP(\omega)\begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix}\right]^{-1}.$$

We explicitly evaluate the inverse of the 2×2 matrix:

$$\left[\mathbb{I} - UP(\omega)\begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix}\right] = \begin{pmatrix} 1 - UP(\omega) & UP(\omega) \\ UP(\omega) & 1 - UP(\omega) \end{pmatrix}.$$

The inverse of a general 2×2 matrix $\begin{pmatrix} a & b \\ c & d \end{pmatrix}$ is:

$$\frac{1}{ad - bc}\begin{pmatrix} d & -b \\ -c & a \end{pmatrix}.$$

Applying this explicitly, the determinant is:

$$(1 - UP(\omega))^2 - (UP(\omega))^2 = 1 - 2UP(\omega).$$

Thus, explicitly:

$$\left[\mathbb{I} - UP(\omega)\begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix}\right]^{-1} = \frac{1}{1 - 2UP(\omega)}\begin{pmatrix} 1 - UP(\omega) & -UP(\omega) \\ -UP(\omega) & 1 - UP(\omega) \end{pmatrix}.$$

Therefore, the diagonal element $W_{11,\uparrow}(\omega)$ is explicitly:

$$W_{11,\uparrow}(\omega) = U\frac{1 - UP(\omega)}{1 - 2UP(\omega)}.$$

Substituting the explicit form of $P(\omega)$
Recall explicitly that we have:

$$P(\omega) = \frac{1}{2}\left(\frac{1}{\omega - 2t + i\eta} - \frac{1}{\omega + 2t + i\eta}\right) = \frac{2t}{(\omega + i\eta)^2 - (2t)^2}.$$

Therefore, for example the explicit form for the screened Coulomb interaction $W_{11,\uparrow}(\omega)$ becomes:

$$\boxed{W_{11,\uparrow}(\omega) = U\frac{1 - \frac{2tU}{(\omega+i\eta)^2 - (2t)^2}}{1 - \frac{4tU}{(\omega+i\eta)^2 - (2t)^2}}}.$$

Note that this expression is different from the one in the paper (J. Chem. Phys. 131, 154111 (2009)). The reason for it is that this result is the exact RPA result,

$$W(\omega) = \frac{U}{1 - UP(\omega)}$$

while in the paper they compute the second-order truncation of the series expansion:.

$$\frac{1}{1 - UP(\omega)} = 1 + UP(\omega) + U^2 P(\omega)^2 + U^3 P(\omega)^3 + \dots$$

6.3 Self energy Σ

We will use the screened Coulomb interaction $W_{ij}(\omega)$, as given by the paper (second order expansion)

$$W_{ij}(\omega) = U\delta_{ij} + (-1)^{i-j} \frac{U^2 t}{\omega^2 - h^2},$$

where:

$$h = \sqrt{(\epsilon_0 + t)^2 + 4tU}.$$

The GW approximation for the self-energy is defined explicitly as (for spin-resolved case):

$$\Sigma_{ij\sigma}(\omega) = i \int \frac{d\omega'}{2\pi} G_{ij\sigma}(\omega + \omega') W_{ji}(\omega'),$$

with $G = G_0$ (non-interacting Green's function) which is obtained from our previous calculation of the full G setting U=0.

Substituting explicitly and performing the integral via contour integration (closing the integration path in the complex plane and using the residue theorem), one finds:

$$\Sigma_{ij\uparrow}(\omega) = \frac{U^2 t}{4h} \left[\frac{1}{\omega - (\epsilon_0 + t + h) + i\eta} + \frac{(-1)^{i-j}}{\omega - (\epsilon_0 - t - h) - i\eta} \right].$$

For spin-down electrons, the explicit calculation is different, as the spin-down Green's function describes particle addition to a spin-up occupied system, thus including different poles.

Performing again the frequency integral explicitly, we derive equation (24) from the provided paper:

$$\Sigma_{ij\downarrow}(\omega) = \frac{U}{2}\delta_{ij} + \frac{U^2 t}{4h} \left[\frac{1}{\omega - (\epsilon_0 + t + h) + i\eta} + \frac{(-1)^{i-j}}{\omega - (\epsilon_0 - t + h) + i\eta} \right].$$

The first term ($U/2$) is the static Hartree contribution to the self-energy, arising due to the static Coulomb interaction with the spin-up electron already occupying one orbital.

7 Behavior of the GW Approximation in Two Limiting Cases

7.1 Non-Interacting Limit ($U \to 0$)

When the on-site interaction U vanishes, the Hubbard model becomes a system of non-interacting electrons. In this regime, the fully interacting Green's function derived within GW reduces to the same poles and weights as the non-interacting (mean-field) theory. Concretely, some of the poles in the GW solution coalesce exactly onto the usual bonding and antibonding energies,

$$\omega = \epsilon_0 \mp t,$$

reflecting that the self-energy corrections fade away as $U \to 0$.

However, the GW scheme also generates a small number of additional poles $(\omega_-^1, \omega_+^2, \omega_+^4)$, which move to energies such as $\epsilon_0 \pm 3t$.

Why? In the GW approximation, the Green's function is given by the Dyson equation:

$$G_{\mathrm{GW}}(\omega) = [G_0^{-1}(\omega) - \Sigma_{\mathrm{GW}}(\omega)]^{-1}.$$

Here, the self-energy Σ_{GW} depends on the screened Coulomb interaction W, which itself includes many-body effects encoded through the polarization P.

Because of this additional complexity, the GW self-energy introduces extra frequency dependence, creating additional poles in the Green's function besides the simple non-interacting ones.

- The poles originally associated with many-body effects do not vanish immediately. Instead, as $U \to 0$, most poles collapse nicely onto the non-interacting solutions $(\epsilon_0 \pm t)$.

- However, certain additional poles generated by GW $(\omega_-^1, \omega_+^2, \omega_+^4)$ do not converge exactly to $\epsilon_0 \pm t$. Instead, these special poles move towards:

$$\omega = \epsilon_0 \pm 3t$$

These particular poles do not match the non-interacting energies. These poles are shifted by exactly $\pm 2t$ away from the usual non-interacting bonding and antibonding energies $(\epsilon_0 \pm t)$. This offset of $2t$ is significant because:

- In the two-site Hubbard dimer, the polarization function $P(\omega)$ (which determines the screening) has poles precisely at energy $2t$.

- Physically, the polarization $P(\omega)$ describes electron-hole pair excitations. Thus, these additional poles appearing at $\epsilon_0 \pm 3t$ can be viewed as **satellites**: they're poles created by the electron-hole excitations that GW treats explicitly via $P(\omega)$.

In other words, these extra GW poles are not simple single-particle excitations. Instead, they correspond to the interaction of a single-particle excitation with an electron-hole pair excitation (collective excitation). — What about the intensity (or weight) of these poles?

As $U \to 0$:

- These satellite poles at $\epsilon_0 \pm 3t$ lose spectral weight and become infinitely weaker. This means their intensity (amplitude) diminishes and eventually goes to zero.

- Hence, even though these poles mathematically remain present, they have zero measurable impact on the physical single-particle spectrum.

The poles remain formally present because the GW approximation inherently includes screening and polarization effects. Even if the strength of this effect (controlled by U) disappears, the structure that GW creates (the mathematical form of the equations) remains. Thus, these poles persist mathematically at those shifted positions but carry no physical weight.

This is a subtle artifact of the mathematical structure of the GW equations: a remnant of many-body physics that vanishes as the interaction disappears.

7.2 Atomic Limit ($t \to 0$)

A very different picture emerges when the hopping amplitude t is driven to zero, so each site becomes isolated. In principle, the exact atomic-limit solution for the spin-down channel should exhibit peaks at ϵ_0 and $\epsilon_0 + U$ with equal spectral weight (since the added electron can find an empty or occupied site). However, the GW approximation effectively treats the density as a classical half-filling on each site for small t. Consequently, one finds that each spin-up pole converges onto a single value $\omega = \epsilon_0$ (giving the correct location but missing certain dynamical details). For the spin-down poles, GW merges only two of them near ϵ_0 with *zero* amplitude, while the other two move around $\epsilon_0 + \frac{U}{2}$ with *unequal* weights. As a result, the characteristic splitting into ϵ_0 and $\epsilon_0 + U$ (each with $\frac{1}{4}$ weight) is *not* reproduced within standard GW in the limit $t \to 0$.

This shortcoming can be seen by noting that, in the atomic limit, the GW self-energy for the spin-down block becomes effectively static (just $\frac{U}{2}$ as a Hartree shift), missing the frequency-dependent part that would produce an additional pole at $\epsilon_0 + U$. In contrast, the exact self-energy in this limit contains a resolvent-like term that yields a genuine second peak. Thus, one concludes that GW breaks down for strongly localized electrons: it does not generate a separate "empty-site vs. occupied-site" splitting. Additional vertex corrections beyond the standard GW (ones that introduce real frequency dependence in the self-energy) are needed to fix this atomic-limit problem.