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:

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

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

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

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:

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

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.