The goal is to obtain the unitary transformation. In the half-filled subspace for the Hubbard dimer,

$$\mathcal{H} = \begin{array}{c} \begin{array}{cccc} |\uparrow,\downarrow\rangle & |\uparrow\downarrow,0\rangle & |\downarrow,\uparrow\rangle & |0,\uparrow\downarrow\rangle \end{array} \\ \begin{pmatrix} 0 & t & 0 & -t \\ t & U & -t & 0 \\ 0 & -t & 0 & t \\ -t & 0 & t & U \end{pmatrix} \end{array} \tag{1}$$

I have dropped the part of the Hamiltonian involving $|\uparrow,\uparrow\rangle$ and $|\downarrow,\downarrow\rangle$ because they are already decoupled and do not change under the RG. Notice that $\mathcal{H}$ can be written as

$$\mathcal{H} = \begin{array}{c} \begin{array}{cc} |n_{1\uparrow}=1\rangle & |n_{1\uparrow}=0\rangle \end{array} \\ \begin{pmatrix} a & b \\ b & a \end{pmatrix} \end{array} \tag{2}$$

Applying RG on this matrix,

$$H_e = H_h = a \tag{3}$$

$$T = b \tag{4}$$

$$\eta^\dagger = \frac{1}{E - H_e} c^\dagger_{1\uparrow} T = \frac{1}{E-a} c^\dagger_{1\uparrow} b \tag{5}$$

$$\implies \eta = b^\dagger c_{1\uparrow} \frac{1}{E-a} \tag{6}$$

From properties of η,

$$\hat{n}_{1\uparrow} = \eta^\dagger \eta = \frac{1}{E-a} c^\dagger_{1\uparrow} c_{1\uparrow} b b^\dagger \frac{1}{E-a} \tag{7}$$

$$\implies (E-a)^2 \hat{n}_{1\uparrow} = \hat{n}_{1\uparrow} b^2 \tag{8}$$

I used $b = -t\sigma_x \implies b^\dagger = b$. The two solutions for E are

$$E - a = \pm b \tag{9}$$

$$\implies E_\pm = a \pm b \tag{10}$$

$$\implies \mathcal{H}_{\text{rotated}} = \begin{array}{c} \begin{array}{cc} |n_{1\uparrow}=1\rangle & |n_{1\uparrow}=0\rangle \end{array} \\ \begin{pmatrix} a-b & 0 \\ 0 & a+b \end{pmatrix} \end{array} = \begin{pmatrix} 0 & 2t & 0 & 0 \\ 2t & U & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & U \end{pmatrix} \tag{11}$$

For this step, the unitary is

$$U_1 = \frac{1}{\sqrt{2}} \begin{array}{c} \begin{array}{cc} |n_{1\uparrow}=1\rangle & |n_{1\uparrow}=0\rangle \end{array} \\ \begin{pmatrix} -1 & 1 \\ 1 & 1 \end{pmatrix} \end{array} = \frac{1}{\sqrt{2}} \begin{pmatrix} -\mathbb{I}_{2\times 2} & \mathbb{I}_{2\times 2} \\ \mathbb{I}_{2\times 2} & \mathbb{I}_{2\times 2} \end{pmatrix} \tag{12}$$

Taking a look at $\mathcal{H}_{\text{rotated}}$, the lower block is diagonal. So, take the upper block as the new Hamiltonian,

$$\mathcal{H} = \begin{array}{c} \begin{matrix} |0,\downarrow\rangle & |\downarrow,0\rangle \end{matrix} \\ \begin{pmatrix} 0 & 2t \\ 2t & U \end{pmatrix} \end{array} \tag{13}$$

$$H_e = 0, H_h = U, T = 2t \tag{14}$$

$$\eta^\dagger = \frac{1}{E-H_e} c^\dagger_{1\downarrow} T = \frac{2t}{E} c^\dagger_{1\downarrow} \tag{15}$$

$$\eta = \frac{1}{E-H_h} T^\dagger c_{1\downarrow} = \frac{2t}{E-U} c_{1\downarrow} \tag{16}$$

$$\hat{n}_{1\downarrow} = \eta^\dagger \eta = \frac{4t^2}{E(E-U)} \hat{n}_{1\downarrow} \tag{17}$$

$$\implies E(E-U) = 4t^2 \implies E = \frac{U \pm \Delta}{2} \tag{18}$$

Therefore,

$$\mathcal{H}_{rotated} = \begin{pmatrix} \frac{U-\Delta}{2} & 0 \\ 0 & \frac{U+\Delta}{2} \end{pmatrix} \tag{19}$$

$$\mathcal{U} = \begin{pmatrix} \frac{4t}{U-\Delta} & \frac{4t}{U+\Delta} \\ 1 & 1 \end{pmatrix} \tag{20}$$

$N_\pm^2 = \Delta\left(\Delta \pm U\right)$. Since this unitary acts only on the upper block, the complete unitary for this stage is

$$U_2 = \begin{pmatrix} \mathcal{U} & 0_{2\times 2} \\ 0_{2\times 2} & \mathbb{I}_{2\times 2} \end{pmatrix} \tag{21}$$

The total unitary for the entire diagonalization process is

$$U = U_1 \times U_2 = \frac{1}{\sqrt{2}} \begin{pmatrix} -\mathcal{U} & 1 \\ \mathcal{U} & 1 \end{pmatrix} \tag{22}$$

To check whether these are correct, we can compute the eigenstates. The eigenstates of the unitarily rotated Hamiltonian are just the fermionic degrees of freedom $|n_{i\sigma}\rangle$. The eigenstates of the bare Hamiltonian are hence obtained by rotating these states:

$$\begin{aligned}
\overline{|\psi_1\rangle} = U|\uparrow,\downarrow\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} -\mathcal{U} & 1 \\ \mathcal{U} & 1 \end{pmatrix} \begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \end{bmatrix} &= \frac{1}{\sqrt{2}} \begin{bmatrix} -\frac{4t}{U-\Delta} \\ -1 \\ \frac{4t}{U-\Delta} \\ 1 \end{bmatrix} \sim \frac{1}{\sqrt{2}} \left\{ \frac{4t}{U-\Delta} \left(|\uparrow,\downarrow\rangle - |\downarrow,\uparrow\rangle\right) + \left(|\uparrow\downarrow,0\rangle - |0,\downarrow\uparrow\rangle\right) \right\} \\
\overline{|\psi_2\rangle} = U|\uparrow,\downarrow\rangle &= \frac{1}{\sqrt{2}} \begin{bmatrix} -\frac{4t}{U+\Delta} \\ -1 \\ \frac{4t}{U+\Delta} \\ 1 \end{bmatrix} \sim \frac{1}{\sqrt{2}} \left\{ \frac{4t}{U+\Delta} \left(|\uparrow,\downarrow\rangle - |\downarrow,\uparrow\rangle\right) + \left(|\uparrow\downarrow,0\rangle - |0,\downarrow\uparrow\rangle\right) \right\} \\
\overline{|\psi_3\rangle} = U|\uparrow,\downarrow\rangle &= \begin{bmatrix} 1 \\ 0 \\ 1 \\ 0 \end{bmatrix} \sim \frac{1}{\sqrt{2}} \left(|\uparrow,\downarrow\rangle + |\downarrow,\uparrow\rangle\right) \\
\overline{|\psi_4\rangle} = U|\uparrow,\downarrow\rangle &= \begin{bmatrix} 0 \\ 1 \\ 0 \\ 1 \end{bmatrix} \sim \frac{1}{\sqrt{2}} \left\{ |\uparrow\downarrow,0\rangle + |0,\uparrow\downarrow\rangle \right\}
\end{aligned} \tag{23}$$

Now that we have the unitary transformaiton, the contention is that the following is the correct effective Hamiltonian:

$$\overline{\mathcal{H}} = U\hat{n}_{2\uparrow}\hat{n}_{2\downarrow} + \frac{U-\Delta}{2}\hat{n}_{1\uparrow}\hat{n}_{2\downarrow} + \frac{U+\Delta}{2}\hat{n}_{1\uparrow}\hat{n}_{1\downarrow} \tag{24}$$

Matching eigenvalues

To check that this gives the correct eigenvalues, I operate this on the states which should be its eigenstates, that is, the decoupled degrees of freedom $|n_{i\sigma}\rangle$:

$$\begin{aligned}
\overline{\mathcal{H}}\,|\uparrow,\downarrow\rangle &= \begin{pmatrix} \frac{U-\Delta}{2} & 0 & 0 & 0 \\ 0 & \frac{U+\Delta}{2} & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & U \end{pmatrix} \begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \end{bmatrix} = \frac{U-\Delta}{2} \\
\overline{\mathcal{H}}\,|\uparrow\downarrow,0\rangle &= \begin{pmatrix} \frac{U-\Delta}{2} & 0 & 0 & 0 \\ 0 & \frac{U+\Delta}{2} & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & U \end{pmatrix} \begin{bmatrix} 0 \\ 1 \\ 0 \\ 0 \end{bmatrix} = \frac{U+\Delta}{2} \\
\overline{\mathcal{H}}\,|\downarrow,\uparrow\rangle &= \begin{pmatrix} \frac{U-\Delta}{2} & 0 & 0 & 0 \\ 0 & \frac{U+\Delta}{2} & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & U \end{pmatrix} \begin{bmatrix} 0 \\ 0 \\ 1 \\ 0 \end{bmatrix} = 0 \\
\overline{\mathcal{H}}\,|0,\uparrow\downarrow\rangle &= \begin{pmatrix} \frac{U-\Delta}{2} & 0 & 0 & 0 \\ 0 & \frac{U+\Delta}{2} & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & U \end{pmatrix} \begin{bmatrix} 0 \\ 0 \\ 0 \\ 1 \end{bmatrix} = U
\end{aligned} \tag{25}$$

Next is a proof that $\overline{\mathcal{H}}$ is unitarily linked with the bare Hamiltonian by the same unitary transformation:

$$U\overline{\mathcal{H}}U^{-1} = U \begin{pmatrix} \frac{U-\Delta}{2} & 0 & 0 & 0 \\ 0 & \frac{U+\Delta}{2} & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & U \end{pmatrix} U^{-1} = \begin{pmatrix} 0 & t & 0 & -t \\ t & U & -t & 0 \\ 0 & -t & 0 & t \\ -t & 0 & t & U \end{pmatrix} = \mathcal{H} \tag{26}$$

This proves that $\overline{\mathcal{H}}$ shares the symmetries of $\mathcal{H}$.

Rotated spin-inversion operator

The spin-inversion operator in the original basis is

$$T = \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & -1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix} = \begin{pmatrix} a & a+\mathbb{I} \\ a+\mathbb{I} & a \end{pmatrix} \tag{27}$$

where $a = \begin{pmatrix} 0 & 0 \\ 0 & -1 \end{pmatrix}$. To see the nature of the rotated spin-inversion operator,

$$\overline{T} = U^{-1}TU = \begin{pmatrix} -\mathbb{I} & 0 \\ 0 & \sigma_z \end{pmatrix} \tag{28}$$

To see that $\overline{T}$ commutes with $\overline{H}$,

$$\begin{aligned}
\bar{T}\bar{H} &= \begin{pmatrix} -\mathbb{I} & 0 \\ 0 & \sigma_z \end{pmatrix} \begin{pmatrix} \frac{U-\Delta}{2} & 0 & 0 & 0 \\ 0 & \frac{U+\Delta}{2} & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & U \end{pmatrix} = \begin{pmatrix} -\frac{U-\Delta}{2} & 0 & 0 & 0 \\ 0 & -\frac{U+\Delta}{2} & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -U \end{pmatrix} \\
\bar{H}\bar{T} &= \begin{pmatrix} \frac{U-\Delta}{2} & 0 & 0 & 0 \\ 0 & \frac{U+\Delta}{2} & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & U \end{pmatrix} \begin{pmatrix} -\mathbb{I} & 0 \\ 0 & \sigma_z \end{pmatrix} = \begin{pmatrix} -\frac{U-\Delta}{2} & 0 & 0 & 0 \\ 0 & -\frac{U+\Delta}{2} & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -U \end{pmatrix}
\end{aligned} \tag{29}$$

Entanglement

$$|GS\rangle = \frac{1}{\sqrt{2\left(1+\alpha^{-2}\right)}} \left[|\uparrow,\downarrow\rangle - |\downarrow,\uparrow\rangle + \alpha^{-1}\left(|0,\uparrow\downarrow\rangle - |\uparrow\downarrow,0\rangle\right)\right] \tag{30}$$

To determine the entanglement between the two states, I compute the von Neumann entropy of the reduced density matrix of the site 1 obtained by tracing out site 2.

$$\begin{aligned}
\rho &= |GS\rangle \langle GS| \\
\rho_1 &= \sum_{|x\rangle_2} \langle x| \rho |x\rangle
\end{aligned} \tag{31}$$

where the sum is over all the configurations of the second site: $\{|x\rangle\} = \{|0\rangle, |\uparrow\rangle, |\downarrow\rangle, |\uparrow\downarrow\rangle\}$

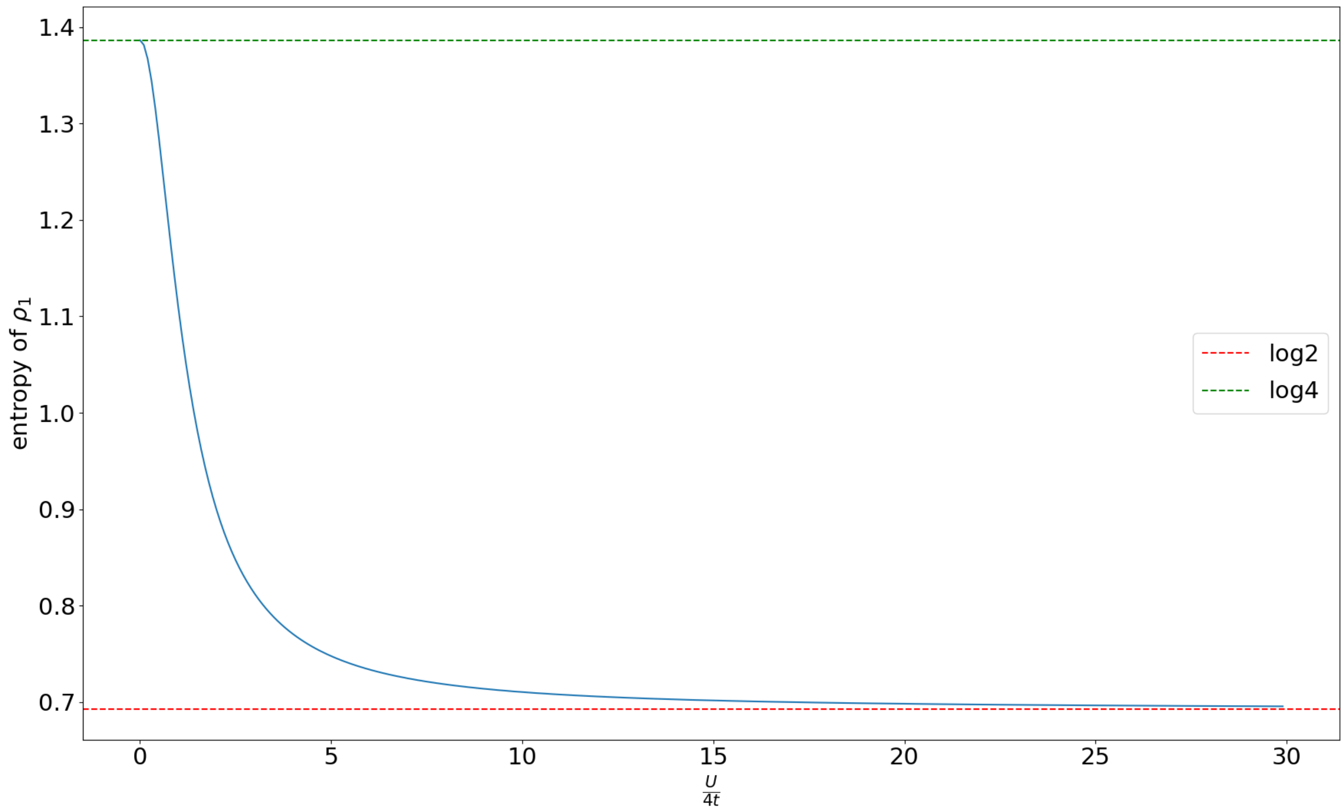
$$\begin{aligned}
\langle 0|_2 \rho |0\rangle_2 &= \frac{\alpha^{-2}}{2(1+\alpha^{-2})} |\uparrow\downarrow\rangle \langle\uparrow\downarrow| \\
\langle\uparrow|_2 \rho |\uparrow\rangle_2 &= \frac{1}{2(1+\alpha^{-2})} |\downarrow\rangle \langle\downarrow| \\
\langle\downarrow|_2 \rho |\downarrow\rangle_2 &= \frac{1}{2(1+\alpha^{-2})} |\uparrow\rangle \langle\uparrow| \\
\langle\uparrow\downarrow|_2 \rho |\uparrow\downarrow\rangle_2 &= \frac{\alpha^{-2}}{2(1+\alpha^{-2})} |0\rangle \langle 0|
\end{aligned} \tag{32}$$

Therefore,

$$\begin{aligned}
\rho_1 &= \frac{1}{2(1+\alpha^{-2})} \left[|\uparrow\rangle\langle\uparrow| + |\downarrow\rangle\langle\downarrow| + \alpha^{-2}\left(|\uparrow\downarrow\rangle\langle\uparrow\downarrow| + |0\rangle\langle 0|\right)\right] \\
&= \frac{1}{2(1+\alpha^{-2})} \begin{pmatrix} 1 & & & \\ & 1 & & \\ & & \alpha^{-2} & \\ & & & \alpha^{-2} \end{pmatrix}
\end{aligned} \tag{33}$$

The von Neumann entropy is given by $S_1 = -\sum_i \lambda_i \log \lambda_i$, where λ_i are the eigenvalues.

$$\begin{aligned}
S &= -\frac{1}{2(1+\alpha^{-2})} \times 2 \times \left[\ln \frac{1}{2(1+\alpha^{-2})} + \alpha^{-2} \ln \frac{\alpha^{-2}}{2(1+\alpha^{-2})}\right] \\
&= \frac{1}{(1+\alpha^{-2})} \left[\ln\left(2+2\alpha^{-2}\right) + \alpha^{-2} \ln\left(2+2\alpha^{2}\right)\right]
\end{aligned} \tag{34}$$



The entropy is maximum ($\log 4$) at $\frac{U}{4t} = 0$ and minimum ($\log 2$) at $\frac{U}{4t} \to \infty$. This is expected for the following reason: At $U = 0$, the ground state becomes an equal admixture of all four states. If a measurement is performed on site 2, site 1 ends up in any one of the four possible configurations ($|0\rangle, |\uparrow\rangle, |\downarrow\rangle, |\uparrow\downarrow\rangle$), with equal probability. The fact that the probabilities are equal means the resultant state will be maximally entangled, which leads to the entropy taking the form $\log N$, where N is the dimension of the reduced Hilbert space. Since site 1 can go into four possible states, the value of N is 4, and we get $S_1 = \log 4$.

For $U = \infty$, the ground state is just a singlet ($|\uparrow, \downarrow\rangle - |\downarrow, \uparrow\rangle$), that is, an equal admixture of two states. This means that on measuring site 2, site 1 now has only two options to choose from, $|\uparrow\rangle$ or $|\downarrow\rangle$, the doublon-holon states are out of the picture. This reduces the dimension of the available Hilbert space to 2, and we get $\log 2$.

To find the entanglement content of just the singlet part, I can project out the doublon-holon part from the density matrix.

$$\rho_{sg} = \frac{1}{2} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \tag{35}$$

The entropy will just be $\log 2$. Projecting out the singlet part and keeping the doublon-holon part will give the same entropy.