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

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

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

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

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

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

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

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

For this step, the unitary is

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

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

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

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

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

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

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

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

Therefore,

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

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

$\mathcal{N}^2$. 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

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

To check whether these are correct, we can compute an eigenstate.

$$U\left|\uparrow,\downarrow\right\rangle = \begin{pmatrix} -\mathcal{U} & 1 \\ & \\ \mathcal{U} & 1 \end{pmatrix} \begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \end{bmatrix} = \begin{bmatrix} -4t \\ -U + \Delta \\ 4t \\ U - \Delta \end{bmatrix} \sim 4t\left(\left|\uparrow,\downarrow\right\rangle - \left|\downarrow,\uparrow\right\rangle\right) + (U - \Delta)\left(\left|\uparrow\downarrow,0\right\rangle - \left|0,\downarrow\uparrow\right\rangle\right) \tag{23}$$

This is a correct eigenstate. Now that we have the unitary transformaiton, the contention is that the following is the correct effective Hamiltonian:

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

This can be proved by showing that it is unitarily linked with the bare Hamiltonian by the same unitary transformation:

$$U\overline{\mathcal{H}}U^T = \begin{pmatrix} -\mathcal{U} & 1 \\ \mathcal{U} & 1 \end{pmatrix} \begin{pmatrix} \frac{U-\Delta}{2} & 0 & 0 & 0 \\ 0 & \frac{U-\Delta}{2} & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & U \end{pmatrix} \begin{pmatrix} -\mathcal{U} & \mathcal{U} \\ 1 & 1 \end{pmatrix} = \begin{pmatrix} 0 & t & 0 & -t \\ t & U & -t & 0 \\ 0 & -t & 0 & t \\ -t & 0 & t & U \end{pmatrix} = \mathcal{H} \tag{25}$$

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