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,

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

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

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

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

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

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

Therefore,

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

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

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

$$U_2 = \begin{pmatrix} \frac{\mathcal{U}}{\sqrt{2}} & 0_{2\times2} \\ 0_{2\times2} & \mathbb{I}_{2\times2} \end{pmatrix} \tag{21}$$

The total unitary for the entire diagonalization process is

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

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:

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

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

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

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 $|n_{i\sigma}\rangle$:

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

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

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

This proves that $\overline{\mathcal{H}}$ shares the symmetries of $\mathcal{H}$. To see the nature of the rotated spin-inversion operator,

$$T = S_1^x \otimes S_2^x = \begin{pmatrix} \sigma_x & 0 \\ 0 & \sigma_x \end{pmatrix} \tag{27}$$

$$\overline{T} = UTU^T = \frac{1}{2}\begin{pmatrix} -\frac{\mathcal{U}}{\sqrt{2}} & 1 \\ \frac{\mathcal{U}}{\sqrt{2}} & 1 \end{pmatrix}\begin{pmatrix} \sigma_x & 0 \\ 0 & \sigma_x \end{pmatrix}\begin{pmatrix} -\frac{\mathcal{U}^T}{\sqrt{2}} & \frac{\mathcal{U}^T}{\sqrt{2}} \\ 1 & 1 \end{pmatrix} = \frac{1}{2}\begin{pmatrix} \frac{\mathcal{U}\sigma_x\mathcal{U}^T}{2} + \sigma_x & -\frac{\mathcal{U}\sigma_x\mathcal{U}^T}{2} + \sigma_x \\ -\frac{\mathcal{U}\sigma_x\mathcal{U}^T}{2} + \sigma_x & \frac{\mathcal{U}\sigma_x\mathcal{U}^T}{2} + \sigma_x \end{pmatrix} \tag{28}$$

Some calculation yields

$$\frac{\mathcal{U}\sigma_x\mathcal{U}^T}{2} = \frac{1}{2N_+N_-}\begin{pmatrix} 32t^2 & 8Ut \\ 8Ut & -32t^2 \end{pmatrix} = \frac{1}{\Delta}\left(4t^2\sigma_z + U\sigma_x\right) \tag{29}$$

So,

$$\begin{aligned} \overline{T} = UTU^T &= \frac{1}{2\Delta}\begin{pmatrix} 4t^2\sigma_z + (U+\Delta)\,\sigma_x & -4t^2\sigma_z - (U-\Delta)\,\sigma_x \\ -4t^2\sigma_z - (U-\Delta)\,\sigma_x & 4t^2\sigma_z + (U+\Delta)\,\sigma_x \end{pmatrix} \\ &= \frac{1}{2}\left(1 + \frac{U}{\Delta}\right)T + \frac{2t^2}{\Delta}\sigma_z \otimes \mathbb{I} - \frac{1}{\Delta}\left\{2t^2\sigma_z + \frac{U-\Delta}{2}\sigma_x\right\} \otimes \sigma_x \end{aligned} \tag{30}$$