Unitary Renormalization Group Approach to the Hubbard Dimer and Anderson Molecule

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Overview

- **Exact diagonalization of the models**

- **Formalism of the unitary renormalization group**

- **Applying the URG to the models**

- **Comparison with Schrieffer-Wolff transformation**

$$\mathcal{H} = \underbrace{-t \sum_{\sigma} \left(c_{1\sigma}^{\dagger} c_{2\sigma} + c_{2\sigma}^{\dagger} c_{1\sigma} \right)}_{\text{hopping term}} + \overbrace{U \sum_{i} \hat{n}_{i\uparrow} \hat{n}_{i\downarrow}}^{\text{Hubbard term}}$$

Symmetries of the problem

- Total number of particles

- Total magnetization

- Site parity: $\hat{P} : \Psi(i,j) \to \Psi(j,i)$

Some easy eigenstates using the commuting operators

Similarly for $N = 3$

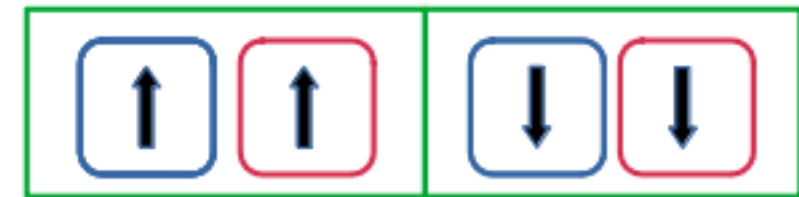# Exact diagonalization of Hubbard dimer

$N = 2$ requires a bit more work

magnetization $= \pm 1$ is easy

Exact diagonalization of Anderson molecule

$$\mathcal{H} = \overbrace{\epsilon_s \sum_\sigma \hat{n}_{2\sigma}}^{\text{conduction band (CB)}} + \overbrace{\epsilon_d \sum_\sigma \hat{n}_{1\sigma}}^{\text{impurity site(IS)}} \underbrace{- t \sum_\sigma \left(c^\dagger_{1\sigma} c_{2\sigma} + c^\dagger_{2\sigma} c_{1\sigma} \right)}_{\text{hopping b/w CB and IS}} + \overbrace{U \hat{n}_{1\uparrow} \hat{n}_{1\downarrow}}^{\text{IS repulsion}}$$

This also proceeds very similarly using the symmetries.

Given $\longrightarrow$ some **non-diagonal** Hamiltonian $\longrightarrow$

$$\begin{array}{|c|c|} \hline A & B \\ \hline C & D \\ \hline \end{array}$$

Goal $\longrightarrow$ a **block-diagonal** Hamiltonian $\longrightarrow$

$$\begin{array}{|c|c|} \hline E & \\ \hline & \v{E} \\ \hline \end{array}$$

Important: We are talking about *block*-diagonalization

The resolution of the Hamiltonian is in the occupied and vacant states of some degree of freedom $\hat{n}$.

$$\mathcal{H}_{2n \times 2n} = \begin{pmatrix} |\hat{n}=1\rangle & |\hat{n}=0\rangle \\ (\hat{H}_e)_{n \times n} & (\hat{T})_{n \times n} \\ \\ (\hat{T}^\dagger)_{n \times n} & (\hat{H}_h)_{n \times n} \end{pmatrix}$$

$\hat{H}_e \longrightarrow$ **occupied part**

$\hat{H}_h \longrightarrow$ **unoccupied part**

$\hat{T}, \hat{T}^\dagger \longrightarrow$ **transitions between**

$\hat{A}$ & $\hat{B}$

So how do we determine this block-diagonal form?

Consider a new operator: $\mathcal{P} = U^{\dagger} \hat{n} U$

What does this do? $\mathcal{P} \mathcal{H} \mathcal{P} = \begin{pmatrix} E & 0 \\ 0 & 0 \end{pmatrix}$

$\mathcal{P}$ **rotates** the Hamiltonian into block-diagonal form and **projects** out the upper block.

$$\mathcal{P} : \begin{pmatrix} H_e & T \\ T^{\dagger} & H_h \end{pmatrix} \xrightarrow{rotation} \begin{pmatrix} E & 0 \\ 0 & E' \end{pmatrix} \xrightarrow{projection} \begin{pmatrix} E & 0 \\ 0 & 0 \end{pmatrix}$$

Since the projection operator mixes the components of the Hamiltonian, we take the following form:

$$\mathcal{P} \sim 1 + \eta + \eta^\dagger$$

η takes an occupied state to an unoccupied state

$$\eta : |1\rangle \otimes |\Psi_n\rangle \rightarrow |0\rangle \otimes |\Phi_n\rangle$$

$$\begin{pmatrix} \Psi_n \\ 0 \end{pmatrix} \rightarrow \begin{pmatrix} 0 \\ \Phi_n \end{pmatrix}$$

Use $\longrightarrow$

Properties of $\eta, \eta^{\dagger}$
Projection property of $\mathcal{P}$
Some linear algebra

$\xrightarrow{\text{to get}}$

$$\eta^{\dagger}\eta = \hat{n}, \eta\eta^{\dagger} = 1 - \hat{n}$$

$$\eta^{\dagger} = \left(\hat{E} - \hat{H}_e\right)^{-1} c^{\dagger}T$$

$$\eta = \left(\hat{E} - \hat{H}_h\right)^{-1} T^{\dagger}c$$

First determine the working equation

- **Choose $1\uparrow$ as the degree of freedom to disentangle.**

- **Calculate $\hat{H}_e, \hat{H}_h$ and $\hat{T}$**

$$H_e = Tr\left[\mathcal{H}\,\hat{n}_{1\uparrow}\right]$$

$$H_h = Tr\left[\mathcal{H}\left(1 - \hat{n}_{1\uparrow}\right)\right]$$

$$T = Tr\left[\mathcal{H}\,c_{1\uparrow}\right]$$
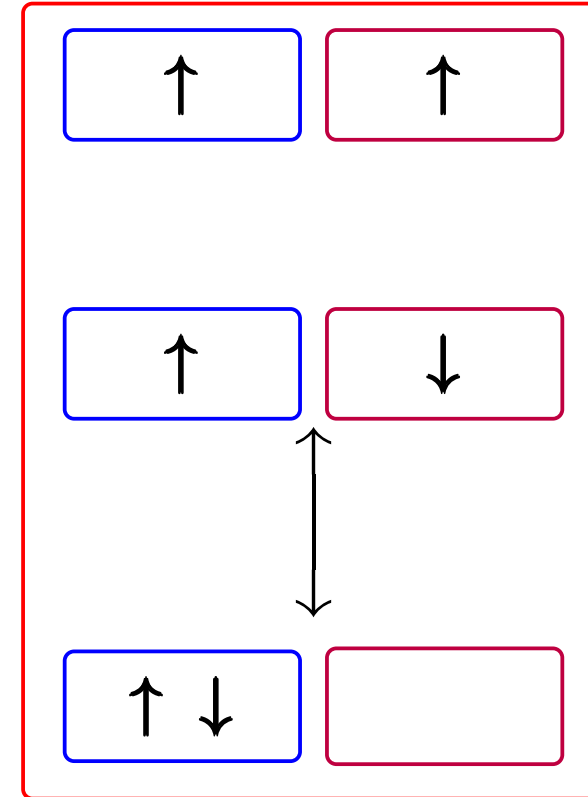
$$(E - H_e)^2 = t^2(1 - n_{2\uparrow})$$

Now apply this equation to various subspaces

Consider $N = 2, n_{1\uparrow} = 1$

Also,

$H_e = Un_{1\downarrow} - Un_{2\uparrow}n_{2\downarrow} + t(c_{2\downarrow}^\dagger c_{1\downarrow} + c_{1\downarrow}^\dagger c_{2\downarrow})$
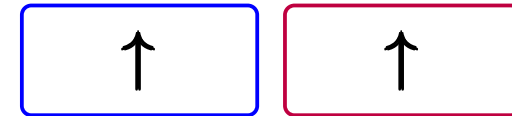
Notice the lonely subspace and the mixed subspace

Finding $\hat{E}$ in this subspace (up-up)

$$(E - H_e)^2 = t^2(1 - n_{2\uparrow})$$

$$n_{2\uparrow} = 1 \longrightarrow RHS = 0$$
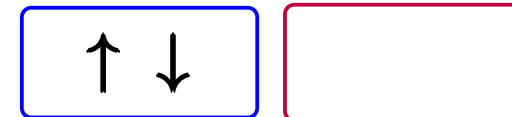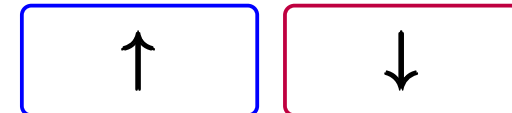
$$\downarrow$$

$$\hat{E} = H_e = 0$$

| ↑ | ↑ |

Finding $\hat{E}$ in this subspace (mixed)

$$(E - H_e)^2 = t^2(1 - n_{2\uparrow})$$

$$n_{2\uparrow} = 0 \longrightarrow RHS = \pm t\,\sigma_x$$

$$\downarrow$$

$$\hat{E} = H_e + t\,\sigma_x$$
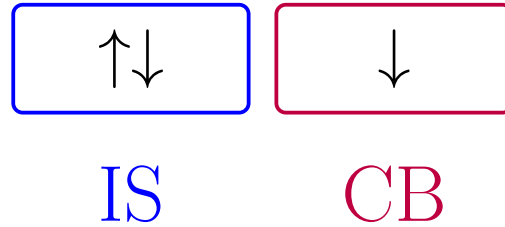
↑	↓
↑ ↓	

Transformation of Hamiltonian under URG (N=2)

$$\begin{pmatrix} 0 & & & & & \\ & 0 & & & & \\ & & 0 & & -t & t \\ & & & 0 & t & -t \\ & & -t & t & U & \\ & & t & -t & & U \end{pmatrix} \xrightarrow{\textbf{URG}} \begin{pmatrix} 0 & & & & & \\ & 0 & & & & \\ & & U & 2t & & \\ & & 2t & 0 & & \\ & & & & U & \\ & & & & & 0 \end{pmatrix}$$

Notice the *block-diagonalizing effect*

$$\mathcal{H} = \epsilon_s \hat{n}_2 + \epsilon_d \hat{n}_1 - t \sum_\sigma \left(c_{1\sigma}^\dagger c_{2\sigma} + c_{2\sigma}^\dagger c_{1\sigma} \right) + U \hat{n}_{1\uparrow} \hat{n}_{1\downarrow}$$

$\uparrow\downarrow$	$\downarrow$
IS	CB

Since this Hamiltonian is of the same form, the working equation again has the form

$$(E - H_e)^2 = t^2(1 - n_{2\uparrow})$$
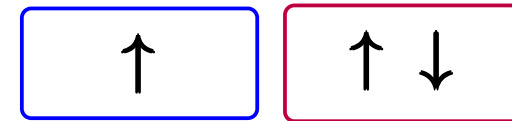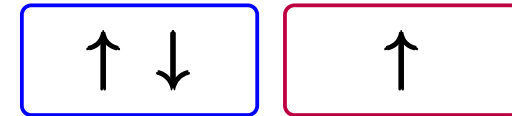
but the H_e is different.

Consider $N = 3$, with $n_{1\uparrow} = 1$

$n_{2\uparrow} = 1 \longrightarrow RHS = 0$

$\downarrow$

$\hat{E} = H_e$

$= \epsilon_s + \epsilon_d + \begin{pmatrix} \epsilon_d + U & -t \\ -t & \epsilon_s \end{pmatrix}$

| $\uparrow \downarrow$ | $\uparrow$ |

| $\uparrow$ | $\uparrow \downarrow$ |

$$H_e = \epsilon_d n_{1\downarrow} + \epsilon_s n_2 - t \left(c_{1\downarrow}^\dagger c_{2\downarrow} + c_{2\downarrow}^\dagger c_{1\downarrow} \right)$$

Transformation of the $N = 2$ subspace

$$
\begin{pmatrix}
-\frac{U}{2} & & & & & \\
& -\frac{U}{2} & & & & \\
& & -\frac{U}{2} & & t & -t \\
& & & -\frac{U}{2} & -t & t \\
& & t & -t & 0 & \\
& & -t & t & & 0
\end{pmatrix}
\xrightarrow{\textbf{URG}}
\begin{pmatrix}
-\frac{U}{2} & & & & & \\
& -\frac{U}{2} & & & & \\
& & -\frac{U}{2} & 2t & & \\
& & 2t & 0 & & \\
& & & & -\frac{U}{2} & \\
& & & & & 0
\end{pmatrix}
$$

Applying URG to Hubbard molecule (k-space)

$$\mathcal{H} = t\left(\hat{n}_\pi - \hat{n}_0\right) + \frac{U}{2}n_\uparrow n_\downarrow + \frac{U}{2}\prod_\sigma \left[c_{0,\sigma}^\dagger c_{\pi,\sigma} + c_{\pi,\sigma}^\dagger c_{0,\sigma}\right]$$

$$\left(E - H_h\right)^2 = \frac{U^2}{2}\hat{n}_{0\uparrow}\left(c_{0\downarrow}^\dagger c_{\pi\downarrow} + c_{\pi\downarrow}^\dagger c_{0\downarrow}\right)^2$$

$$\downarrow$$
$$\vec{k} = \pi$$

$$\uparrow\downarrow$$
$$\vec{k} = 0$$

The RHS now features U, instead of t

$\longrightarrow$ because in momentum space, the mixing of states is caused by the Hubbard term, not the kinetic term.
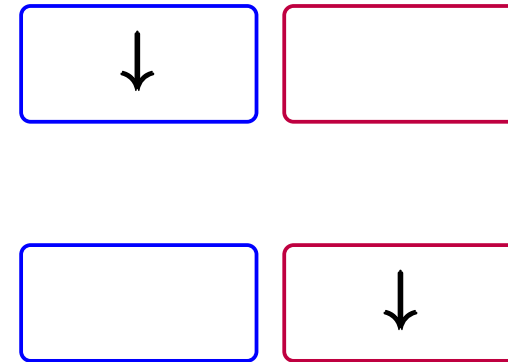
Consider $N = 1$, with $n_{1\uparrow} = 0$

$$n_{0\uparrow} = 0 \longrightarrow RHS = 0$$

$$\Downarrow$$

$$\hat{E} = H_h$$

$$= t \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

An issue I am unable to resolve...

$$N = 2$$
$$\left|\uparrow\downarrow, 0\right\rangle, \left|0, \uparrow\downarrow\right\rangle$$

Transformation of the $N = 2$ subspace

$$
\begin{pmatrix}
0 & & & & \\
& 0 & & & \\
& & \frac{U}{2} & -\frac{U}{2} & \\
& & -\frac{U}{2} & \frac{U}{2} & \\
& & & & \frac{U}{2} + 2t & -\frac{U}{2} \\
& & & & -\frac{U}{2} & \frac{U}{2} - 2t
\end{pmatrix}
\xrightarrow{\ \textbf{URG}\ }
\begin{pmatrix}
0 & & & & \\
& 0 & & & \\
& & 0 & & \\
& & & U & \\
& & & & \frac{U+\Delta}{2} & \\
& & & & & \frac{U-\Delta}{2}
\end{pmatrix}
$$

$$\mathcal{H} = \mathcal{H}_0 + V$$

$$\downarrow \quad e^{-S}\mathcal{H}e^{S}$$

$$\mathcal{H}_{\text{eff}} = \mathcal{H}_0 + \tfrac{1}{2}\left[V, \hat{S}\right]$$

Since $\hat{S}$ is of the order of V, there is no first order contribution

$$\left[\hat{S}, \mathcal{H}_0\right] = V$$

Schrieffer-Wolff Transf. (Anderson molecule)

$$
\begin{pmatrix}
-\frac{U}{2} & & t & -t \\
& -\frac{U}{2} & -t & t \\
t & -t & 0 & \\
-t & t & & 0
\end{pmatrix}
$$

$\xrightarrow{\text{swt}}$

$$
\begin{pmatrix}
-\frac{U}{2} - \frac{4t^2}{U} & \frac{4t^2}{U} & & \\
\frac{4t^2}{U} & -\frac{U}{2} - \frac{4t^2}{U} & & \\
& & \frac{4t^2}{U} & -\frac{4t^2}{U} \\
& & -\frac{4t^2}{U} & \frac{4t^2}{U}
\end{pmatrix}
$$

$\xrightarrow{\text{urg}}$

$$
\begin{pmatrix}
-\frac{U}{2} & 2t & & \\
2t & 0 & & \\
& & -\frac{U}{2} & \\
& & & 0
\end{pmatrix}
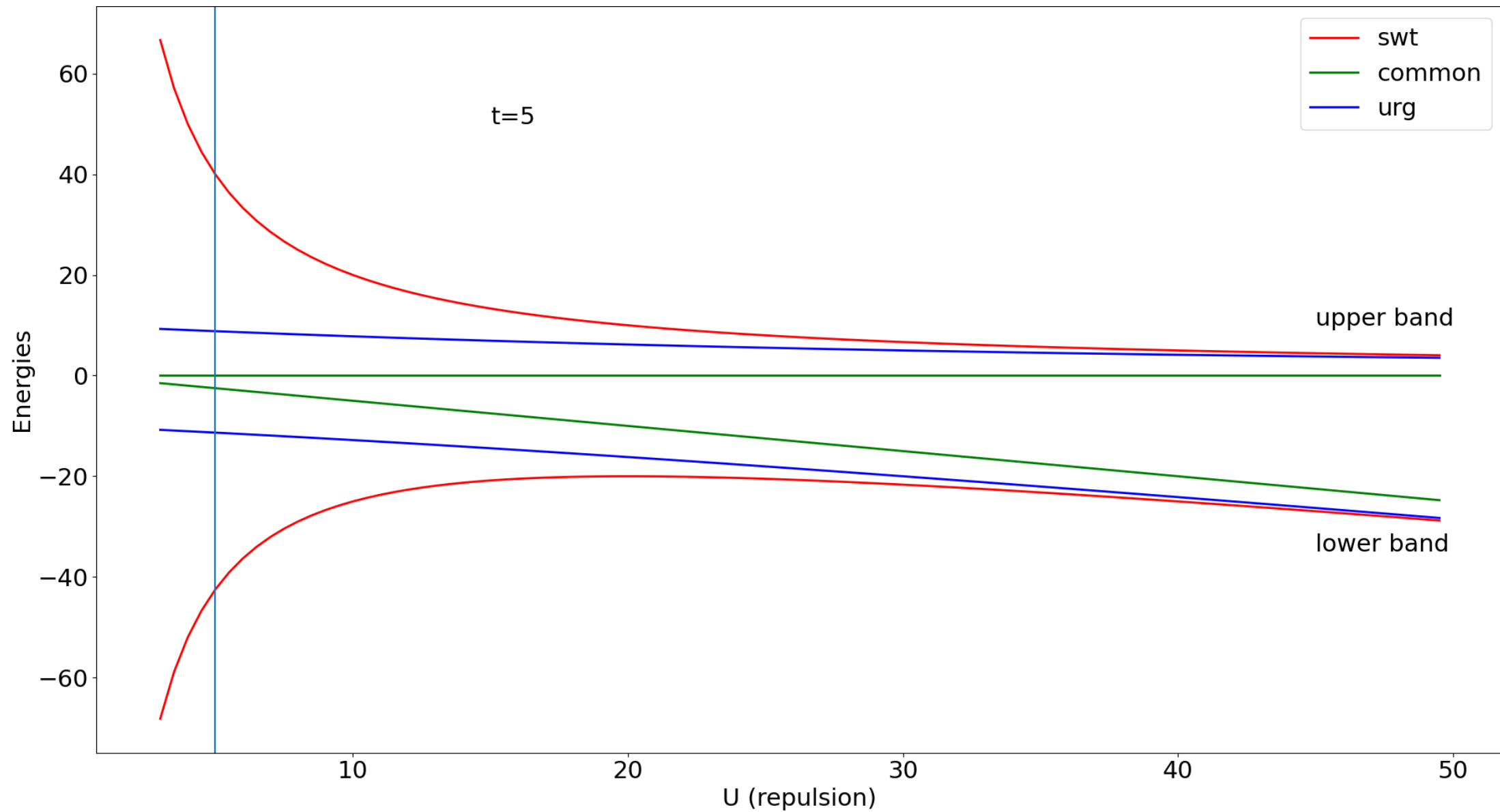$$

Schrieffer-Wolff Transf. (Anderson molecule)

About the SWT

- directly *drops terms* higher than t^2

- reduces to *antiferromagnetic Heisenberg model*

About the URG

- *All terms* are kept in the transformation

- reduces to antiferr. Heis. model *only at large U*

Schrieffer-Wolff Transf. (Anderson molecule)

Things I haven't understood(solved) yet

- Getting the effective Hamiltonian preserving the symmetries

- Solving the problem in one go (without needing to go into subspaces)

- Different choices lead to different effective Hamiltonians, although the final spectrum is the same