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**

Exact diagonalization of Hubbard dimer

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

Symmetries of the problem

- Total number of particles
- Total magnetization
- Site parity: $\hat{P} : \Psi(i,j) \rightarrow \Psi(j,i)$

Exact diagonalization of Hubbard dimer

Some easy eigenstates using the commuting operators

$N = 1$

Magnetization = **up**

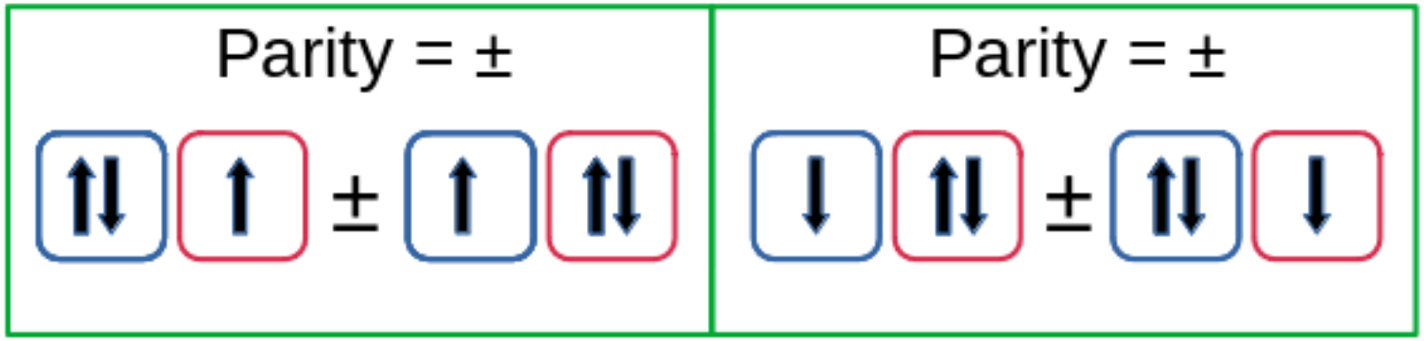
Magnetization = **down**

Parity = ±

Parity = ±

Exact diagonalization of Hubbard dimer

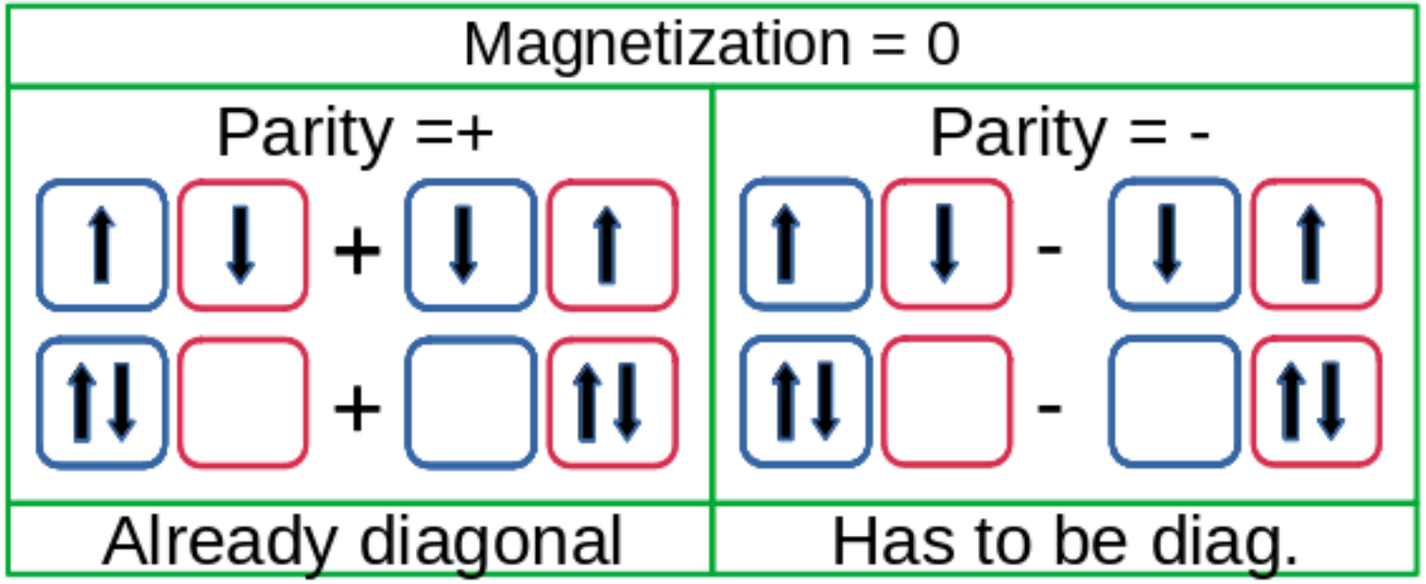
Similarly for $N = 3$



Exact diagonalization of Hubbard dimer

N = 2 requires a bit more work

magnetization = ±1 is easy



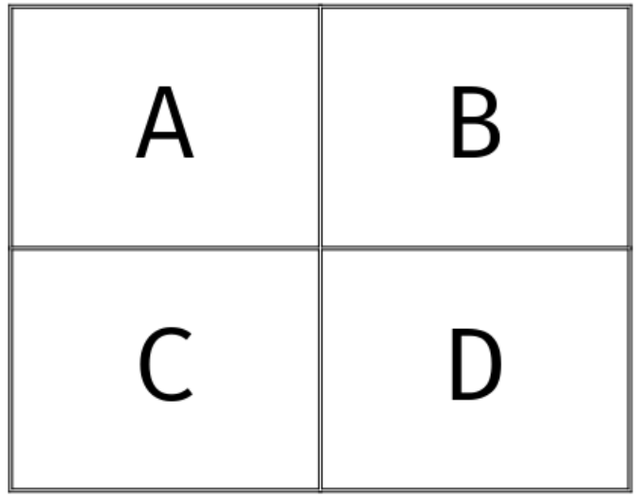
Exact diagonalization of Anderson molecule

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

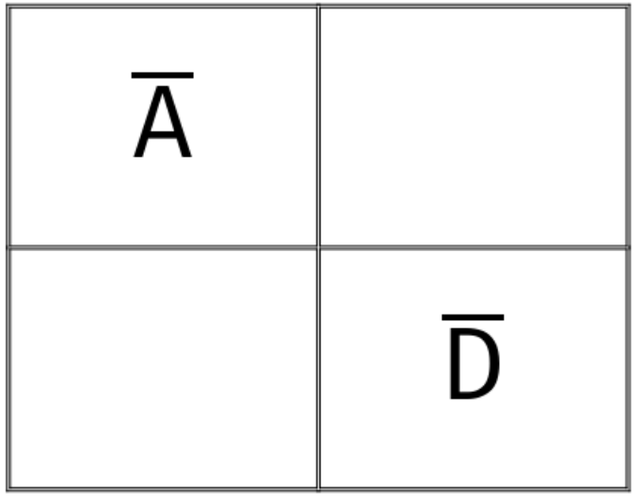
This also proceeds very similarly using the symmetries.

Formalism of unitary renormalization group

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



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



Formalism of unitary renormalization group

Important: We are talking about *block*-diagonalization

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

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

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

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

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

Formalism of unitary renormalization group

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.**

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

Formalism of unitary renormalization group

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

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

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

Formalism of unitary renormalization group

Use $\longrightarrow$

Properties of $\eta, \eta^\dagger$

Projection property of $\mathcal{P}$

Some linear algebra

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

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

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

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

Applying URG to Hubbard dimer

First determine the working equation

- **Choose $1\uparrow$ as the degree of freedom to disentangle.**
- **Calculate $\hat{H}_e, \hat{H}_h$ and $\hat{T}$**

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

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

$$T = Tr\left[\mathcal{H}\,c_{1\uparrow}\right]$$

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

Applying URG to Hubbard dimer

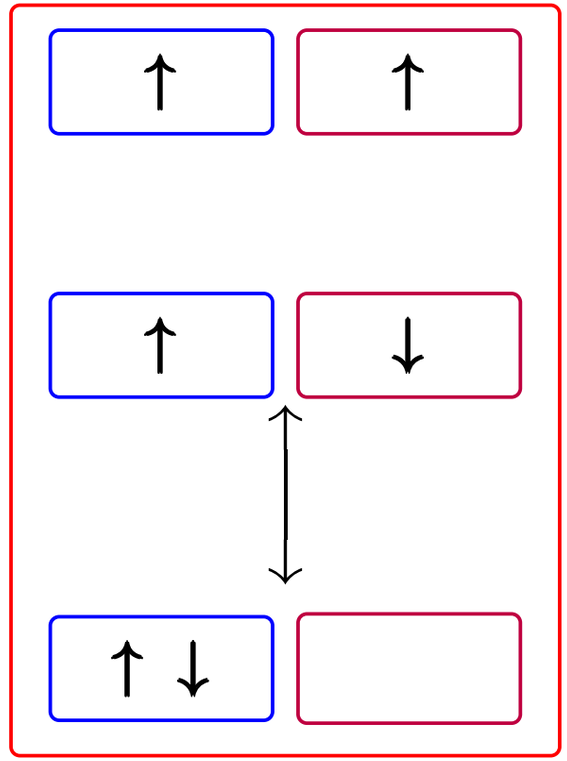
Now apply this equation to various subspaces

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

Also,

$$H_e = Un_{1\downarrow} - Un_{2\uparrow}n_{2\downarrow} + t(c^\dagger_{2\downarrow}c_{1\downarrow} + c^\dagger_{1\downarrow}c_{2\downarrow})$$

Notice the lonely subspace and the mixed subspace



Applying URG to Hubbard dimer

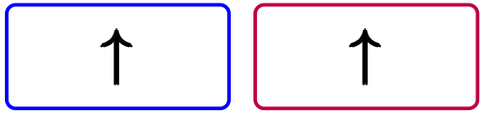
Finding $\hat{E}$ in this subspace (up-up)

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

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

$$\downarrow$$

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



Applying URG to Hubbard dimer

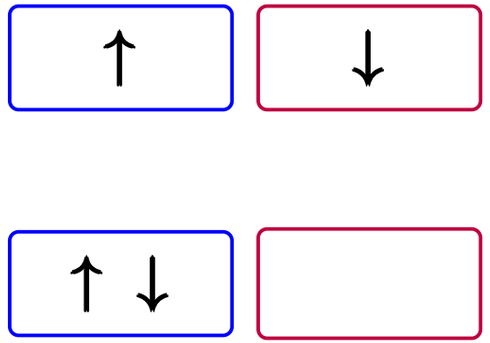
Finding $\hat{E}$ in this subspace (mixed)

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

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

$$\downarrow$$

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



Applying URG to Hubbard dimer

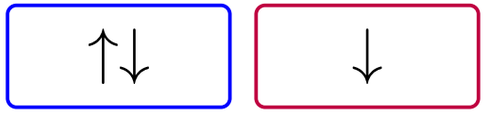
Transformation of Hamiltonian under URG (N=2)

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

Notice the *block-diagonalizing effect*

Applying URG to Anderson molecule

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



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.

Applying URG to Anderson molecule

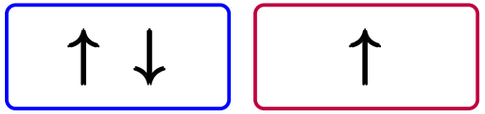
Consider $N = 3$, with $n_{1\uparrow} = 1$

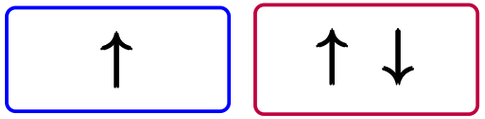
$$n_{2\uparrow} = 1 \longrightarrow RHS = 0$$

$$\downarrow$$

$$\hat{E} = H_e$$

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





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

Applying URG to Anderson molecule

Transformation of the $N = 2$ subspace

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

Applying URG to Hubbard molecule (k-space)

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

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

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

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.

Applying URG to Hubbard molecule (k-space)

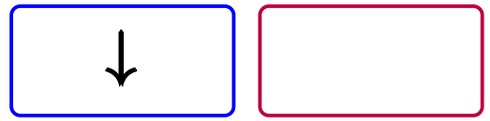
Consider $N = 1$, with $n_{1\uparrow} = 0$

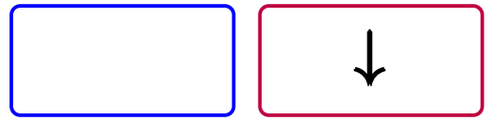
$$n_{0\uparrow} = 0 \longrightarrow RHS = 0$$

$$\Downarrow$$

$$\hat{E} = H_h$$

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





Schrieffer-Wolff Transformation

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

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

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

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)

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

swt

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

urg

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

Schrieffer-Wolff Transf. (Anderson molecule)

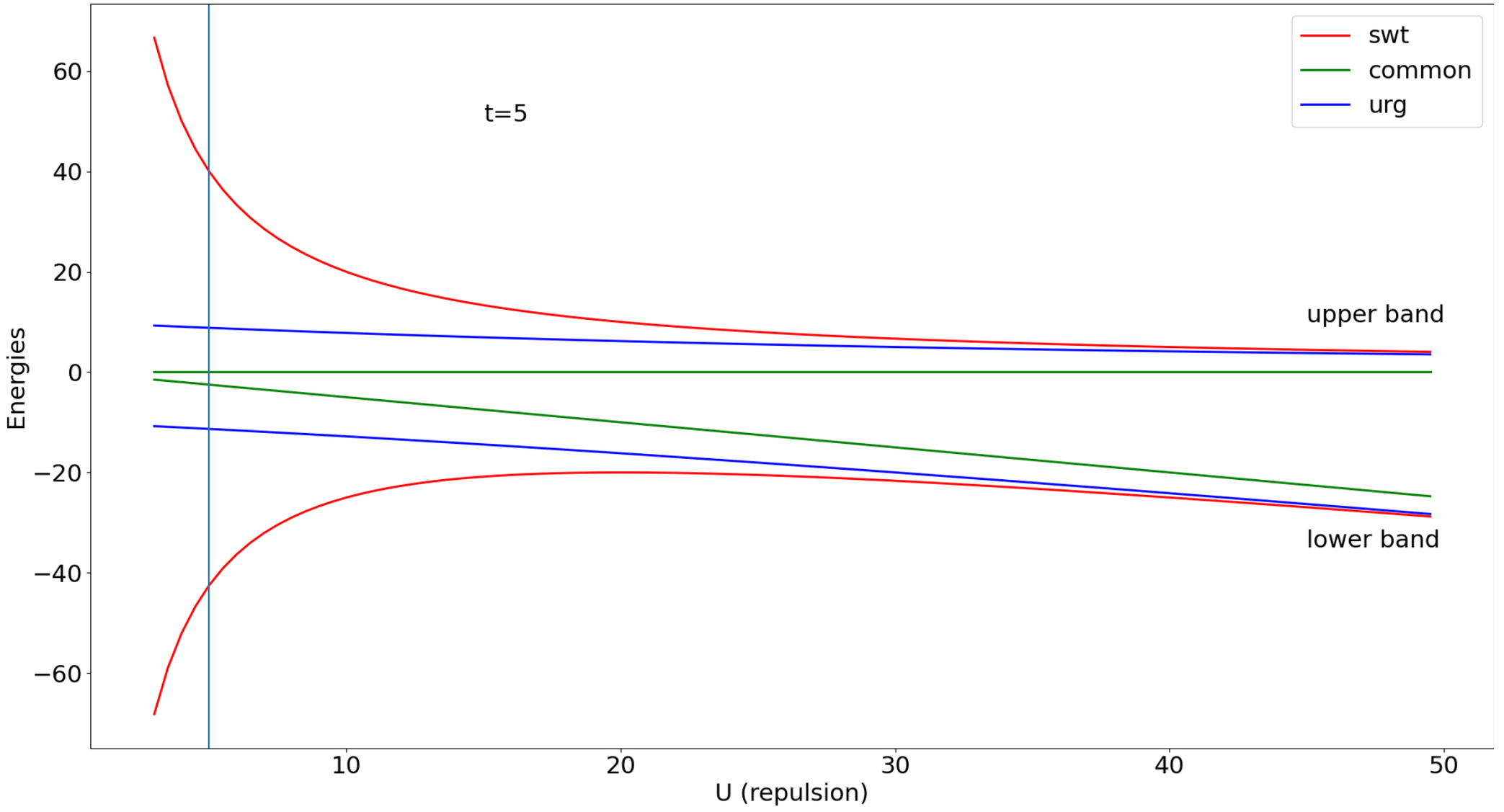
About the SWT

- directly ***drops terms*** higher than t^2
- separates into two bands, with a gap of $\frac{U}{2}$

About the URG

- ***All terms*** are kept in the transformation
- separates into bands only at $U \gg t$

Schrieffer-Wolff Transf. (Anderson molecule)



Things to do

- **Getting the effective Hamiltonian in operator form**
- **Writing the Hamiltonian in terms of the pseudo-spins and applying the URG in terms of them**

Thank you very much!