

# 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

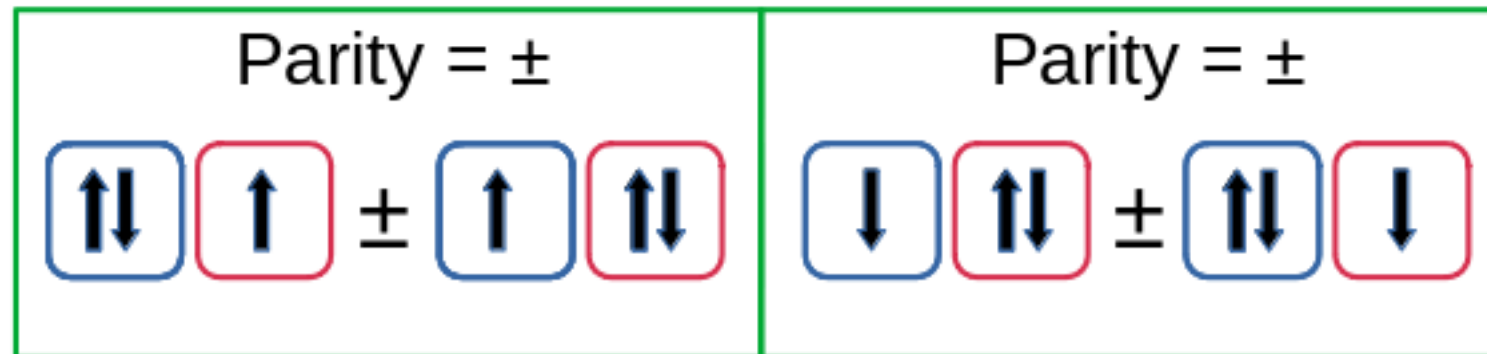
$N = 1$     

Magnetization = <b>up</b>	Magnetization = <b>down</b>
	

Parity = $\pm$	Parity = $\pm$
	

# Exact diagonalization of Hubbard dimer

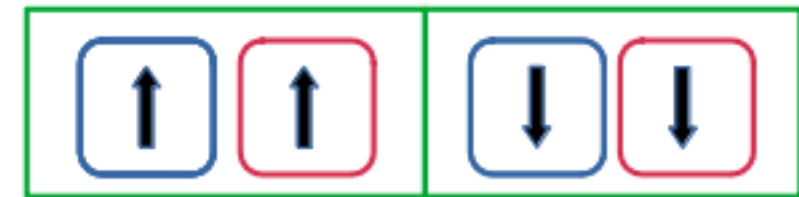
Similarly for  $N = 3$



# Exact diagonalization of Hubbard dimer

$N = 2$  requires a bit more work

magnetization =  $\pm 1$  is easy



Magnetization = 0	
Parity = +	Parity = -
$\begin{array}{cc} \uparrow & \downarrow \\ \uparrow\downarrow & \end{array} + \begin{array}{cc} \downarrow & \uparrow \\ & \uparrow\downarrow \end{array}$	$\begin{array}{cc} \uparrow & \downarrow \\ \uparrow\downarrow & \end{array} - \begin{array}{cc} \downarrow & \uparrow \\ & \uparrow\downarrow \end{array}$
Already diagonal	Has to be diag.

# Exact diagonalization of Anderson molecule

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

This also proceeds very similarly using the symmetries.

# Formalism of unitary renormalization group

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

A	B
C	D

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

$\bar{A}$	
	$\bar{D}$



# 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  $\hat{n}$ .

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

$\hat{H}_e \longrightarrow$  **occupied part**  
 $\hat{H}_h \longrightarrow$  **unoccupied part**  
 $\hat{T}, \hat{T}^\dagger \longrightarrow$  **transitions between**  
 $\hat{A} \ \& \ \hat{B}$

# 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.

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

# Formalism of unitary renormalization group

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

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

$\eta$  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

to get  $\longrightarrow$

$$\begin{aligned}\eta^\dagger \eta &= \hat{n}, \eta \eta^\dagger = 1 - \hat{n} \\ \eta^\dagger &= (\hat{E} - \hat{H}_e)^{-1} c^\dagger T \\ \eta &= (\hat{E} - \hat{H}_h)^{-1} T^\dagger c\end{aligned}$$

# 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  $\hat{T}$

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

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

$$T = \text{Tr} [\mathcal{H} c_{1\uparrow}]$$

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

# Applying URG to Hubbard dimer

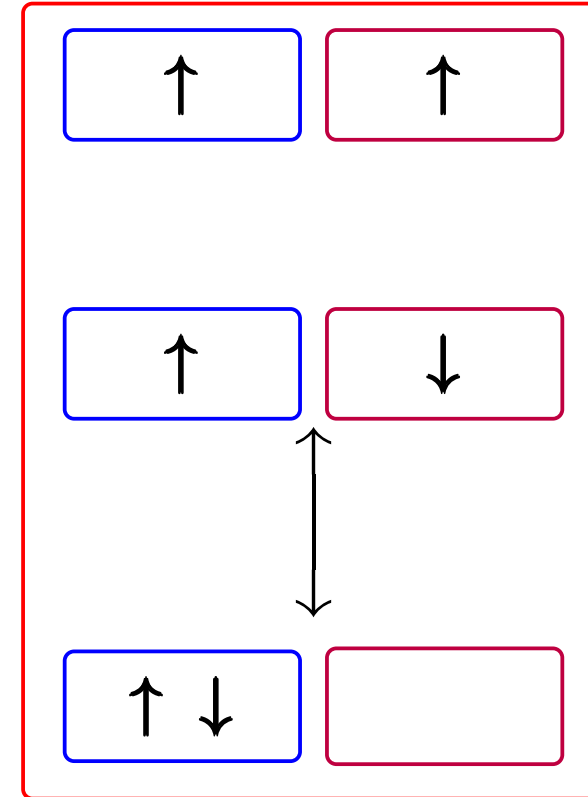
Now apply this equation to various subspaces

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

Also,

$$H_e = U n_{1\downarrow} - U n_{2\uparrow} n_{2\downarrow} + t(c_{2\downarrow}^\dagger c_{1\downarrow} + c_{1\downarrow}^\dagger c_{2\downarrow})$$

Notice the lonely subspace  
and the mixed subspace



# Applying URG to Hubbard dimer

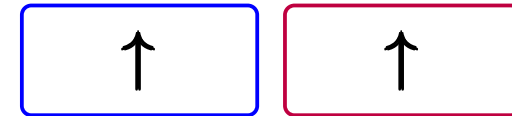
Finding  $\hat{E}$  in this subspace (up-up)

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

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



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



# Applying URG to Hubbard dimer

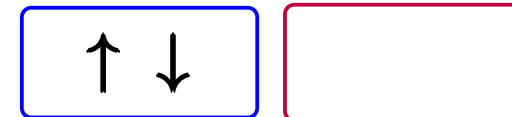
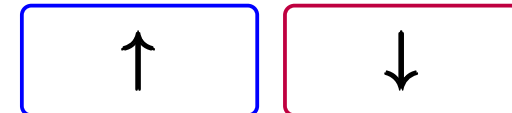
Finding  $\hat{E}$  in this subspace (mixed)

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

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



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





# Applying URG to Hubbard dimer

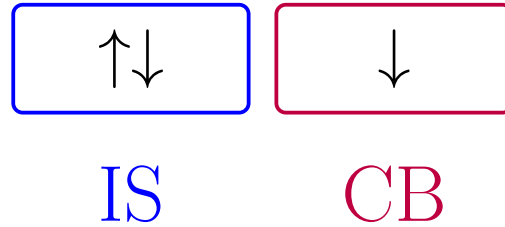
Transformation of Hamiltonian under URG (N=2)

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

Notice the *block-diagonalizing effect*

# Applying URG to Anderson molecule

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



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

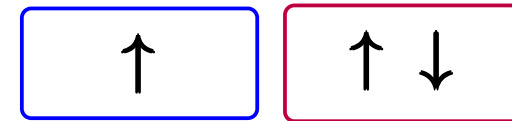
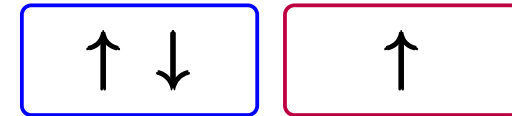
Consider  $N = 3$ , with  $n_{1\uparrow} = 1$

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



$$\hat{E} = H_e$$

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



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

# Applying URG to Anderson molecule

Transformation of the  $N = 2$  subspace

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

# Applying URG to Hubbard molecule (k-space)

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

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

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

The RHS now features  $U$ , instead of  $t$   
→ 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)

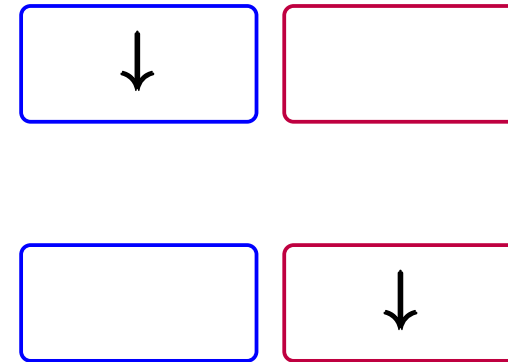
Consider  $N = 1$ , with  $n_{1\uparrow} = 0$

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

$\Downarrow$

$$\hat{E} = H_h$$

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



# Schrieffer-Wolff Transformation

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

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

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

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

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

# Schrieffer-Wolff Transf. (Anderson molecule)

$$\begin{pmatrix} -\frac{U}{2} & t & -t \\ -\frac{U}{2} & -t & t \\ t & -t & 0 \\ -t & t & 0 \end{pmatrix} \begin{matrix} \xrightarrow{\text{swt}} \\ \xrightarrow{\text{urg}} \end{matrix} \begin{pmatrix} -\frac{U}{2} - \frac{4t^2}{U} & \frac{4t^2}{U} & & \\ \frac{4t^2}{U} & -\frac{U}{2} - \frac{4t^2}{U} & & \\ & & \frac{4t^2}{U} & -\frac{4t^2}{U} \\ & & -\frac{4t^2}{U} & \frac{4t^2}{U} \end{pmatrix}$$
$$\begin{pmatrix} -\frac{U}{2} & 2t \\ 2t & 0 \\ & -\frac{U}{2} \\ & & 0 \end{pmatrix}$$



# Schrieffer-Wolff Transf. (Anderson molecule)

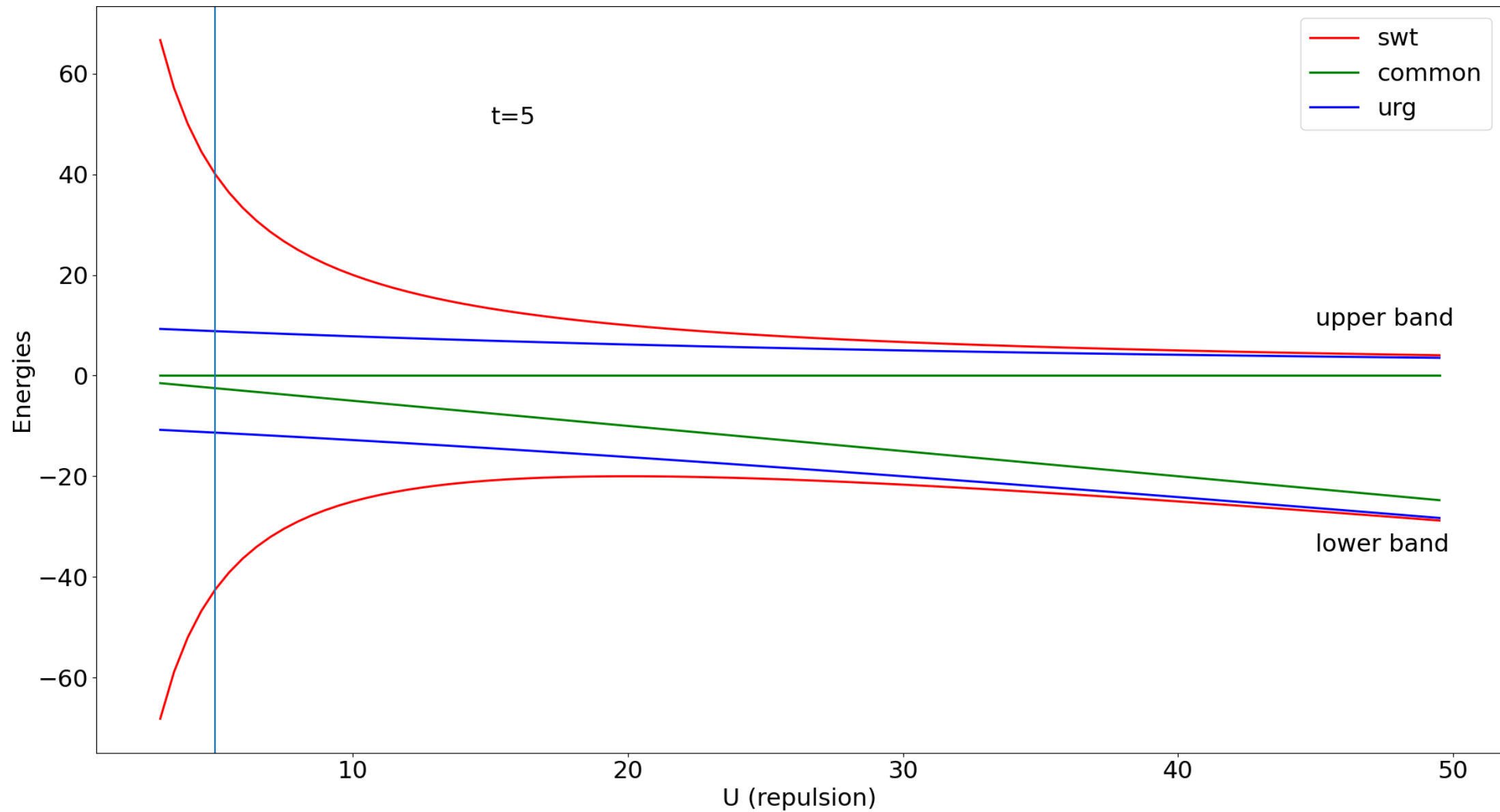
## About the SWT

- 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