

ary Renormalization Group Approach to the Anderson m

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Overview

- The single-impurity Anderson model
- Motivation
- Formalism of the unitary renormalization group
- Results

Single-Impurity Anderson Model

$$\mathcal{H} = \underbrace{\sum_{k\sigma} \epsilon_k \hat{n}_{k\sigma}}_{\text{hopping term}} + \overbrace{U \sum_i \hat{n}_{i\uparrow} \hat{n}_{i\downarrow}}^{\text{Hubbard term}} \quad (1)$$

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 = \pm

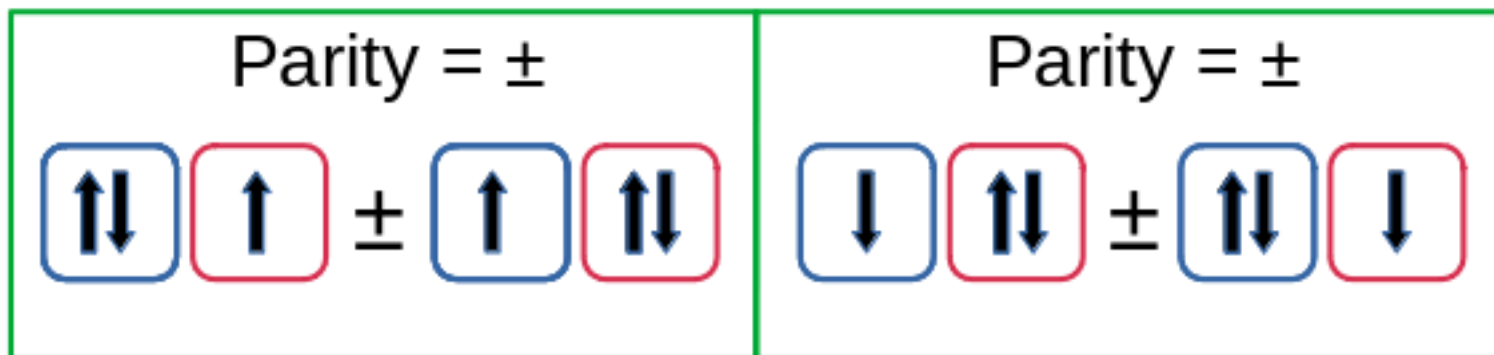


Parity = \pm



Exact diagonalization of Hubbard dimer

Similarly for $N = 3$



Exact diagonalization of Hubbard dimer

$N = 2$ requires a bit more work

$S_z = \pm 1$ magnetization is easy

$S_z = 0$



Magnetization = 0	
Parity = +	Parity = -
<p>↑↓ + empty + empty + ↑↓</p>	<p>↑↓ - empty - empty - ↑↓</p>
Already diagonal	Has to be diag.

Exact diagonalization of Anderson molecule

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

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

A

C

\bar{A}

Formalism of unitary renormalization group

Important: We are talking about *block*-diagonaliza

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

$$\mathcal{H}_{2N \times 2N} = \begin{pmatrix} |\hat{n} = 1\rangle & |\hat{n} = 0\rangle \\ (\hat{H}_e)_{N \times N} & (\hat{T})_{N \times N} \\ (\hat{T}^\dagger)_{N \times N} & (\hat{H}_h)_{N \times N} \end{pmatrix} \quad (3)$$

$\hat{H}_e \longrightarrow$ occupied
 $\hat{H}_h \longrightarrow$ unoccupied
 $\hat{T}, \hat{T}^\dagger \longrightarrow$ transition
 $\hat{A} \ \& \ \hat{B}$

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.

$$\mathcal{P} : \begin{pmatrix} H_e & T \\ T^\dagger & H_h \end{pmatrix} \xrightarrow{\text{rotation}} \begin{pmatrix} E & 0 \\ 0 & E' \end{pmatrix} \xrightarrow{\text{projection}} \begin{pmatrix} E & 0 \\ 0 & 0 \end{pmatrix} \quad (4)$$

Formalism of unitary renormalization group

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

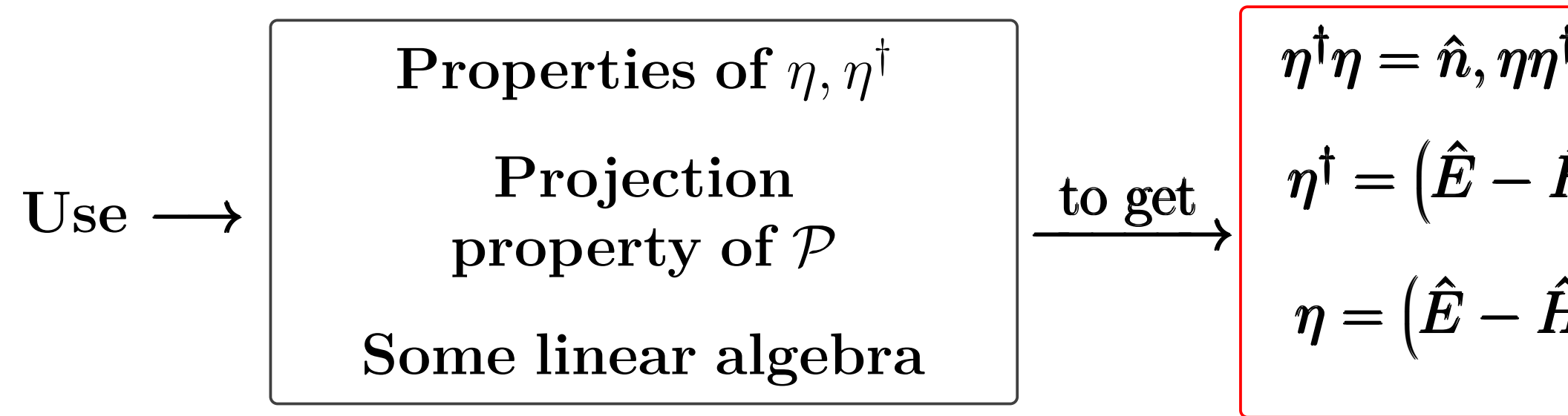
$$\mathcal{P} \sim 1 + \eta + \eta^\dagger$$

η takes an occupied state to an unoccupied state

$$/2/2\eta : |1\rangle \otimes |\Psi_n\rangle \rightarrow |0\rangle \otimes |\Phi_n\rangle$$

$$\begin{pmatrix} \Psi_n \\ 0 \end{pmatrix} \rightarrow \begin{pmatrix} 0 \\ \Phi_n \end{pmatrix} \quad (5)$$

Formalism of unitary renormalization group



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}

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

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

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

/2/2

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

Applying URG to Hubbard dimer

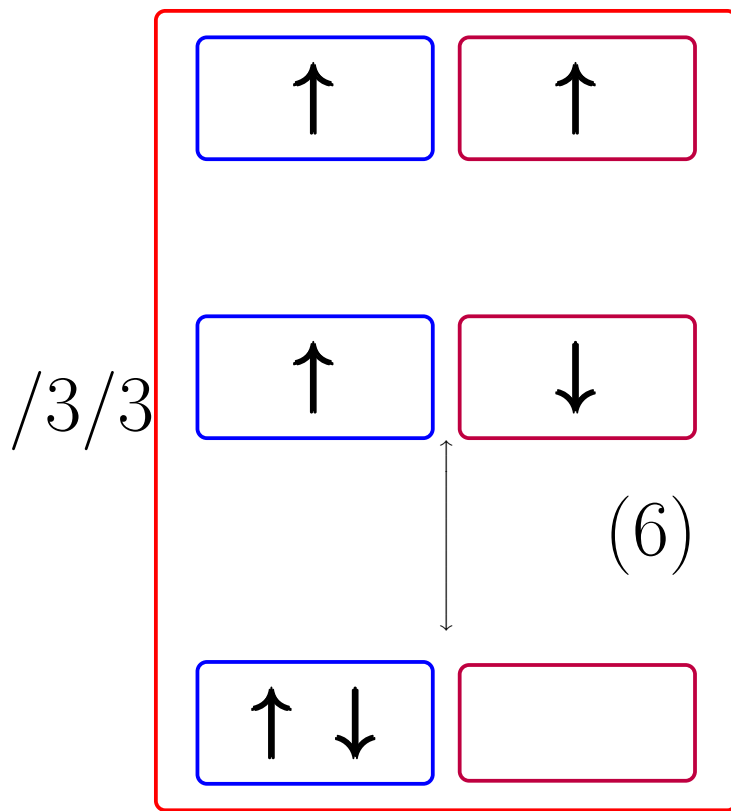
Now apply this equation to various subspaces

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)

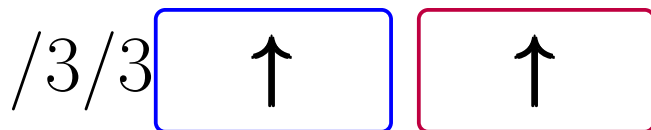
$$(E - H_e)^2 = t^2(1 - n_{2\uparrow})$$

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

/2/2



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



Applying URG to Hubbard dimer

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

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

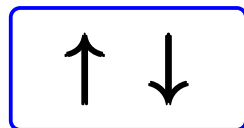
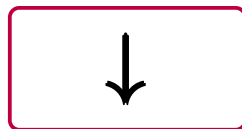
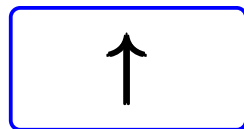
$$n_{2\uparrow} = 0 \longrightarrow RHS = \pm t \sigma_x$$

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

/3/3



Applying URG to Hubbard dimer

Transformation of Hamiltonian under URG (N=2)

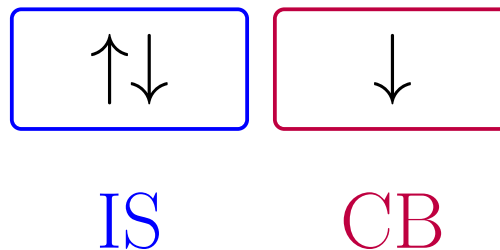
$$\begin{pmatrix} 0 & & & & \\ & 0 & & & \\ & & 0 & -t & t \\ & & & 0 & t \\ & & -t & t & U \\ & & t & -t & U \end{pmatrix} \xrightarrow{\text{URG}} \begin{pmatrix} 0 & & & & \\ & 0 & & & \\ & & U & 2t & \\ & & 2t & 0 & \\ & & & & U \\ & & & & & 0 \end{pmatrix}$$

(11)

Notice the *block-diagonalizing effect*

Applying URG to Anderson molecule

$$\mathcal{H} = \epsilon_s \hat{n}_2 + \epsilon_d \hat{n}_1 - t \sum_{\sigma} (c_{1\sigma}^{\dagger} c_{2\sigma} + c_{2\sigma}^{\dagger} c_{1\sigma}) + U \hat{n}_{1\uparrow} \hat{n}_{1\downarrow} \quad (12)$$



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 $n_{1\uparrow} = 1$

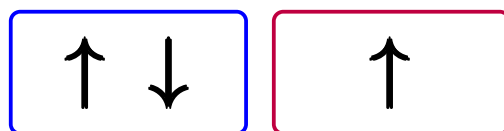
$$n_{2\uparrow} = 1 \longrightarrow RHS = 0$$



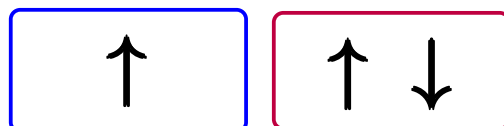
/2/2

$$\hat{E} = H_e$$

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



/3/3



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

Applying URG to Anderson molecule

Transformation of the $N = 2$ subspace

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

(16)

Applying URG to Hubbard molecule (k-space)

$$\mathcal{H} = t(\hat{n}_\pi - \hat{n}_0) + \frac{U}{2}n_\uparrow n_\downarrow + \frac{U}{2} \sum_{\sigma} [c_{0,\sigma}^\dagger c_{\pi,\sigma} + c_{\pi,\sigma}^\dagger c_{0,\sigma}] \quad (17)$$

/3/3

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

/3/3

↓

↑↓

$$\vec{k} = \pi \quad \vec{k} = 0$$

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 $n_{1\uparrow} = 0$

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

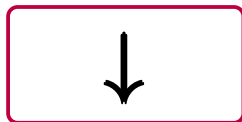
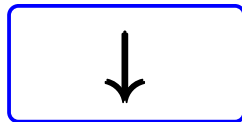
$$\Downarrow$$

$$\hat{E} = H_h$$

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

/2/2

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Schrieffer-Wolff Transformation

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

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

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

/2/2 Since \hat{S} is of the order of V , there is no first order contribution

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

Schrieffer-Wolff Transf. (Anderson molecule)

Schrieffer-Wolff Transf. (Anderson molecule)

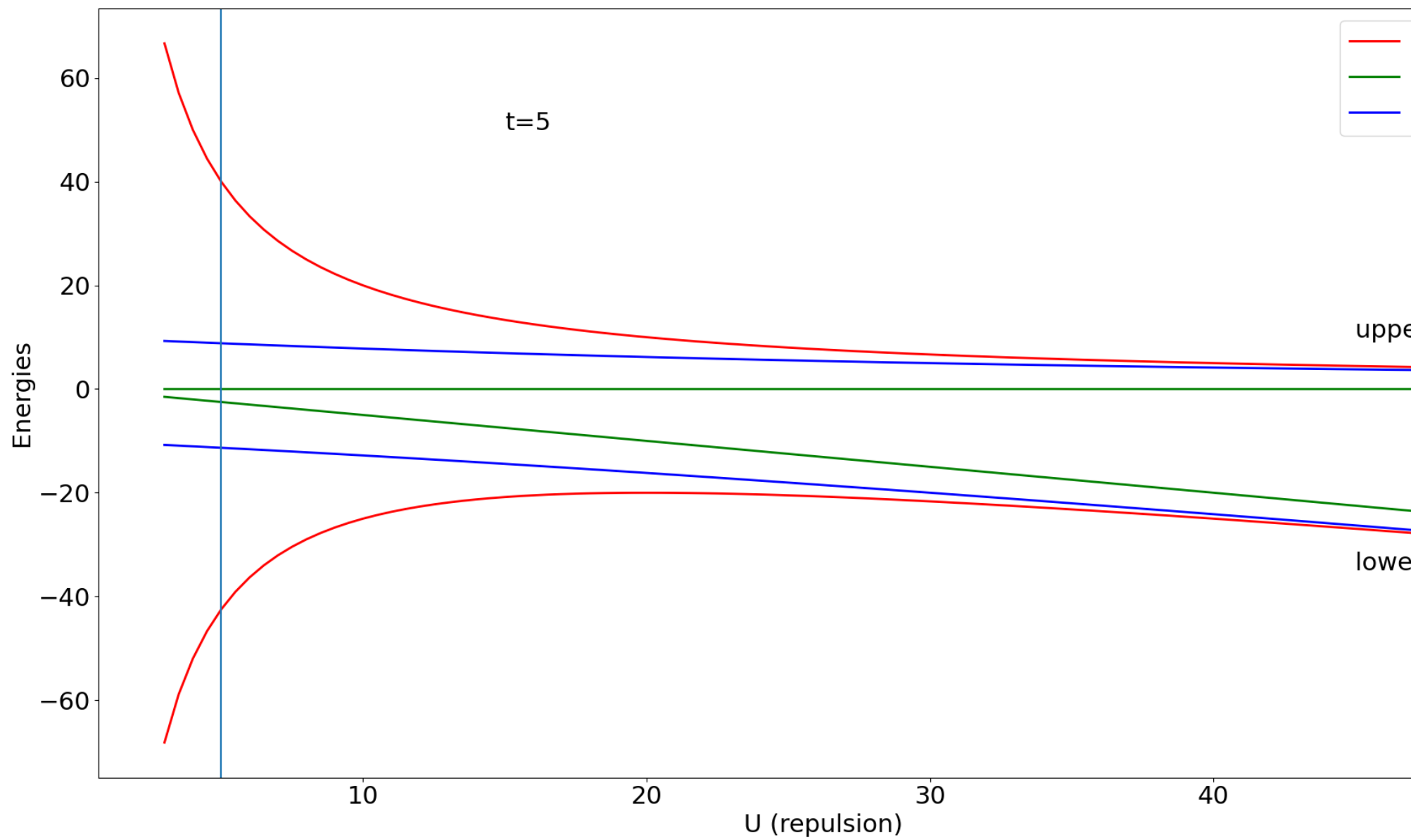
About the SWT

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

About the U

- *All terms* are transformation
- separates into bands
 $U \gg t$

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!