

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

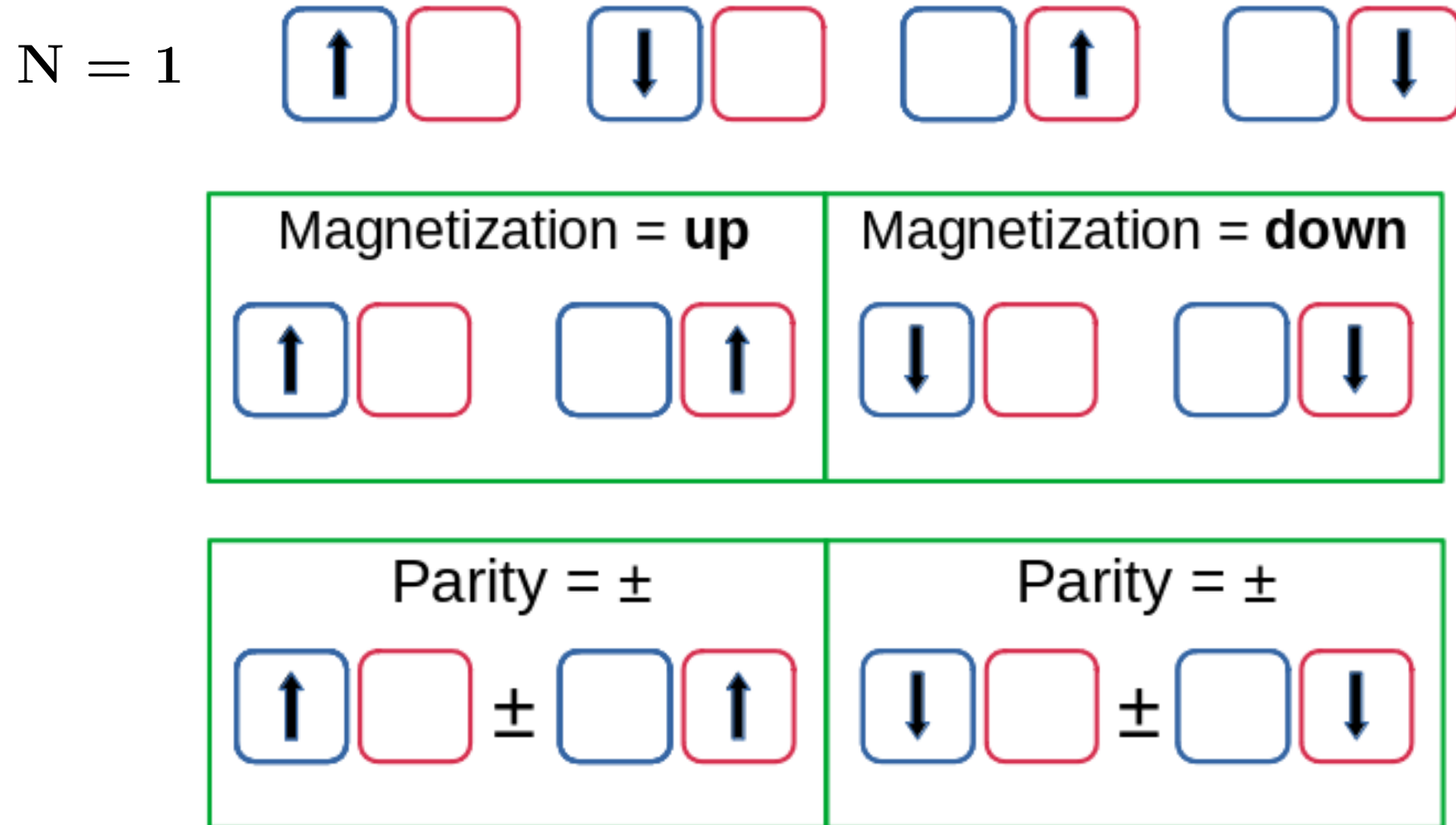
$$\mathcal{H} = \underbrace{-t \sum_{\sigma} \left(c_{1\sigma}^{\dagger} c_{2\sigma} + c_{2\sigma}^{\dagger} c_{1\sigma} \right)}_{\text{hopping term}} + \overbrace{U \sum_i \hat{n}_{i\uparrow} \hat{n}_{i\downarrow}}^{\text{Hubbard term}}$$

Symmetries of the problem

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

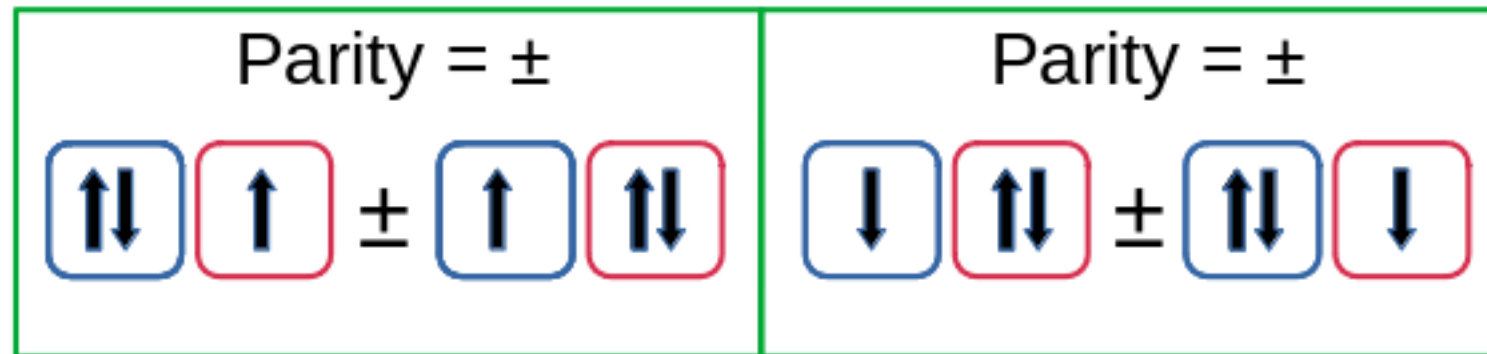
Exact diagonalization of Hubbard dimer

Some easy eigenstates using the commuting operators



Exact diagonalization of Hubbard dimer

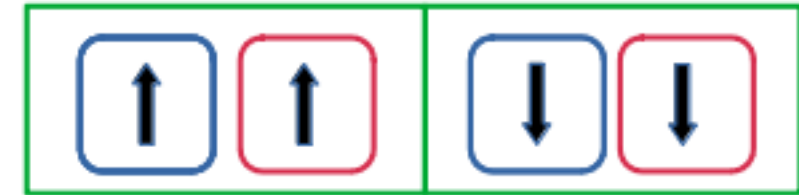
Similarly for $N = 3$



Exact diagonalization of Hubbard dimer

$N = 2$ requires a bit more work

magnetization = ± 1 is easy



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

E	
	<u>\tilde{E}</u>

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:

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

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 η, η^\dagger
Projection
property of \mathcal{P}
Some linear algebra

to get \longrightarrow

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

Applying URG to Hubbard dimer

First step: Determine the working equation

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

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

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

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

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

Applying URG to Hubbard dimer

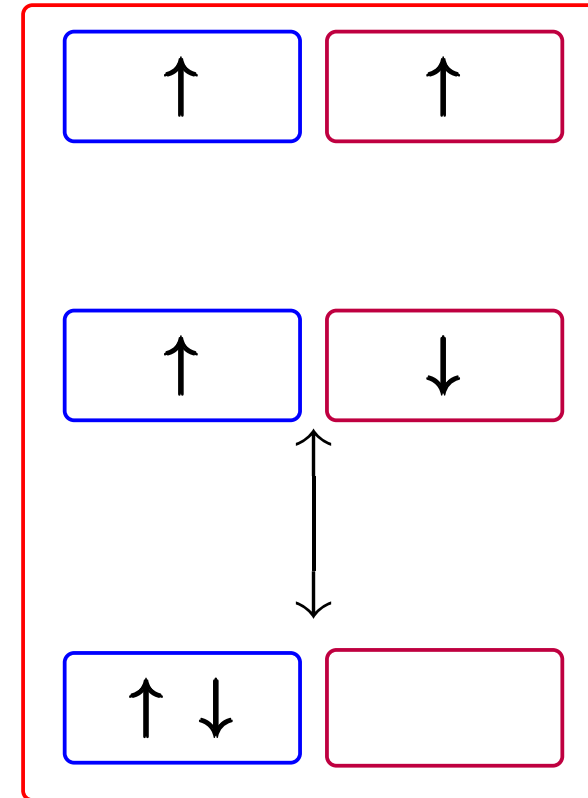
Now apply this equation to various subspaces

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

Also, $H_e =$

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

Notice the lonely subspace
and the mixed subspace



Applying URG to Hubbard dimer

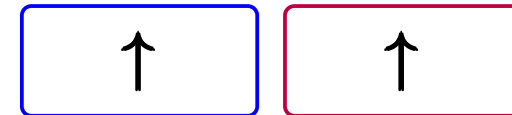
Finding \hat{E} in this subspace (up-up)

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

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



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



Applying URG to Hubbard dimer

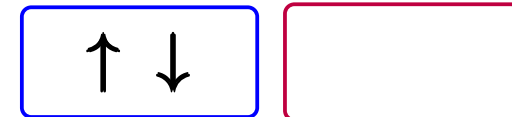
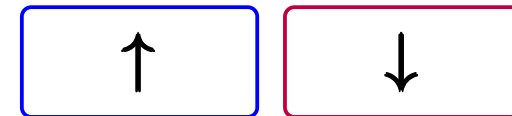
Finding \hat{E} in this subspace (mixed)

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

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



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



Applying URG to Hubbard dimer

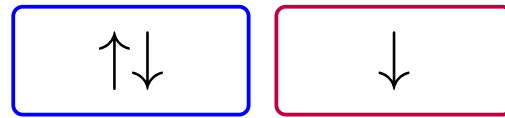
Transformation of Hamiltonian under URG (N=2)

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

Notice the *block-diagonalizing effect*

Applying URG to Anderson molecule

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



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

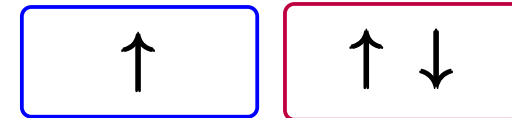
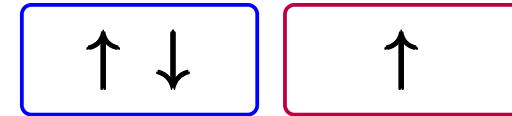
Consider $N = 3$, with $n_{1\uparrow} = 1$

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



$$\hat{E} = H_e$$

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



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

Applying URG to Anderson molecule

Transformation of the $N = 2$ subspace

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

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)

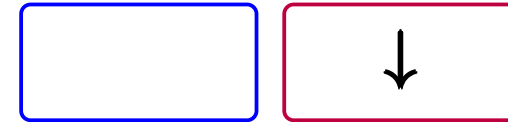
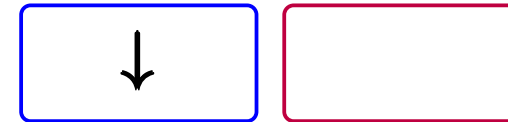
Consider $N = 1$, with $n_{1\uparrow} = 0$

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

\Downarrow

$$\hat{E} = H_h$$

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



Schrieffer-Wolff Transformation

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



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

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
- 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)

