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:** $\hat{n} = \sum_{i,\sigma} \hat{n}_{i,\sigma}$
- **Total magnetization:** $\hat{S}_z = \sum_i (\hat{n}_{\uparrow} - n_{\downarrow})$
- **Site parity:** $\hat{P} : \Psi(i,j) \rightarrow \Psi(j,i)$

Exact diagonalization of Hubbard dimer

Some easy eigenstates using the commuting operators

- $\mathbf{N = 1} \implies |\uparrow, 0\rangle, |0, \uparrow\rangle, |\downarrow, 0\rangle, |0, \downarrow\rangle$

- $\mathbf{magnetization = up} \implies |\uparrow, 0\rangle, |0, \uparrow\rangle,$

  $\mathbf{magnetization = down} \implies |\downarrow, 0\rangle, |0, \downarrow\rangle$

- $\mathbf{parity = +ve} \implies |\uparrow, 0\rangle + |0, \uparrow\rangle, |\downarrow, 0\rangle + |0, \downarrow\rangle$

  $\mathbf{parity = -ve} \implies |\uparrow, 0\rangle - |0, \uparrow\rangle, |\downarrow, 0\rangle - |0, \downarrow\rangle$

Exact diagonalization of Hubbard dimer

Some easy eigenstates using the commuting operators

- $\mathbf{N = 3} \implies |\uparrow, \uparrow\downarrow\rangle, |\uparrow\downarrow, \uparrow\rangle, |\downarrow, \uparrow\downarrow\rangle, |\uparrow\downarrow, \downarrow\rangle$

- $\mathbf{magnetization = up} \implies |\uparrow, \uparrow\downarrow\rangle, |\uparrow\downarrow, \uparrow\rangle,$

  $\mathbf{magnetization = down} \implies |\downarrow, \uparrow\downarrow\rangle, |\uparrow\downarrow, \downarrow\rangle$

- $\mathbf{parity = +ve} \implies |\uparrow, \uparrow\downarrow\rangle + |\uparrow\downarrow, \uparrow\rangle, |\downarrow, \uparrow\downarrow\rangle + |\uparrow\downarrow, \downarrow\rangle$

  $\mathbf{parity = -ve} \implies |\uparrow, \uparrow\downarrow\rangle - |\uparrow\downarrow, \uparrow\rangle, |\downarrow, \uparrow\downarrow\rangle - |\uparrow\downarrow, \downarrow\rangle$

Exact diagonalization of Hubbard dimer

N = 2 requires a bit more work

- **magnetization** $= \pm 1$ is easy $\implies |\uparrow,\uparrow\rangle, |\downarrow,\downarrow\rangle$
- **magnetization = 0** $\implies |\uparrow,\downarrow\rangle, |\downarrow,\uparrow\rangle, |\uparrow\downarrow,0\rangle, |0,\uparrow\downarrow\rangle$

  parity = 1 $\implies |\uparrow,\downarrow\rangle + |\downarrow,\uparrow\rangle, \quad |\uparrow\downarrow,0\rangle + |0,\uparrow\downarrow\rangle \implies$ diagonal

  parity = -1 $\implies |\uparrow,\downarrow\rangle - |\downarrow,\uparrow\rangle, \quad |\uparrow\downarrow,0\rangle - |0,\uparrow\downarrow\rangle$

$$\begin{pmatrix} 0 & 2t \\ 2t & U \end{pmatrix} \implies \text{easily diagonalised}$$

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 of the Hamiltonian:

- **number of particles**
- **magnetization**
- **total spin angular momentum** $\hat{S}^2_{tot} = \sum_x \hat{S}^2_x$

(not showing the full thing here)

Formalism of unitary renormalization group

Given $\Longrightarrow$ some non-diagonal Hamiltonian $\rightarrow$ $\begin{pmatrix} \hat{A} & \hat{B} \\ \hat{C} & \hat{D} \end{pmatrix}$

Objective $\Longrightarrow$ a block-diagonal Hamiltonian $\rightarrow$ $\begin{pmatrix} \hat{E} & 0 \\ 0 & \hat{E}' \end{pmatrix}$

Equivalent Objective $\Longrightarrow$ find unitary U such that

$$\hat{U}^{\dagger} \begin{pmatrix} \hat{A} & \hat{B} \\ \hat{C} & \hat{D} \end{pmatrix} \hat{U} = \begin{pmatrix} \hat{E} & 0 \\ 0 & \hat{E}' \end{pmatrix}$$

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 $\hat{n}$.

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

$$\begin{aligned} \hat{H}_e &\Longrightarrow \textbf{occupied part of } \mathcal{H} \\ \hat{H}_h &\Longrightarrow \textbf{unoccupied part of } \mathcal{H} \\ \hat{T}, \hat{T}^\dagger &\Longrightarrow \textbf{transitions between } \hat{A} \ \& \ \hat{B} \end{aligned}$$

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

$$\eta : |1\rangle \otimes |\Psi_n\rangle \to |0\rangle \otimes |\Phi_n\rangle \qquad \begin{pmatrix} \Psi_n \\ 0 \end{pmatrix} \to \begin{pmatrix} 0 \\ \Phi_n \end{pmatrix}$$

Similarly, $\eta^\dagger$ takes an unoccupied state to an occupied state

$$\eta^\dagger : |0\rangle \otimes |\chi_n\rangle \to |1\rangle \otimes |\xi_n\rangle \qquad \begin{pmatrix} 0 \\ \chi_n \end{pmatrix} \to \begin{pmatrix} \xi_n \\ 0 \end{pmatrix}$$

Formalism of unitary renormalization group

Use the following

↓

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

Projection property of $\mathcal{P}$

Some linear algebra

↓ **to get** ↓

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