

Interacting Systems

Now we want to generalize to interacting systems. This primarily consists of adding sites with an \otimes , not an \oplus .

Most of the DMRG procedure outlined before needs little change. The main question:

How do we project out a state for a block from a state of the entire lattice? Problem: the projection is many-valued.

Let $|i\rangle$ be the states of the block, and $|j\rangle$ be the states of the rest of the lattice. A state of the entire lattice can be written as

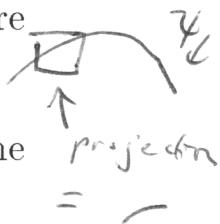
$$|\psi\rangle = \sum_{ij} \psi_{ij} |i\rangle |j\rangle$$

In general, there is no way to pick states $|\tilde{i}\rangle$ and $|\tilde{j}\rangle$ so that

$$|\psi\rangle = |\tilde{i}\rangle |\tilde{j}\rangle$$

Example: if the block has an average of N particles, it can still fluctuate into states with $N \pm 1, N \pm 2$, particles. Need at least one state for each number of particles. (A state without a definite N , such as the BCS wavefunction, doesn't help, either.)

We will need an *approximate* projection. What is the best projection? It comes from the density matrix.



Density Matrices

Reference: R.P. Feynman, *Statistical Mechanics: A Set of Lectures*

Let $|i\rangle$ be the states of the block (the *system*), and $|j\rangle$ be the states of the rest of the lattice (the rest of the *universe*). If ψ is a state of the entire lattice,

$$|\psi\rangle = \sum_{ij} \psi_{ij} |i\rangle |j\rangle$$

The reduced density matrix for the system is

$$\rho_{ii'} = \sum_j \psi_{ij}^* \psi_{i'j}$$

An operator A which acts only on the system can be written as

$$A = \sum_{ii'j} A_{ii'} |\cancel{\psi}_i\rangle \langle \cancel{\psi}_j| \langle \cancel{\psi}_{i'}| = \sum_{ii'} A_{ii'} |\cancel{\psi}_i\rangle \langle \cancel{\psi}_{i'}| \otimes \mathbf{1}_j$$

The expectation value of A can be written in terms of the density matrix

$$\langle A \rangle = \sum_{ii'j} A_{ii'} \psi_{ij}^* \psi_{i'j} = \sum_{ii'} A_{ii'} \rho_{ii'} = \text{Tr} \rho A$$

A nice way of representing ρ is through its eigenstates $|v_\alpha\rangle$ and eigenvalues $w_\alpha \geq 0$ ($\sum_\alpha w_\alpha = 1$)

$$\begin{aligned} \sum_\alpha w_\alpha &= \text{Tr } \rho = \text{Tr} \left[\sum_{ij} \rho_{ij} \right] \\ &= \sum_{ij} |\rho_{ij}|^2 \\ &= 1 \text{ by normalization} \end{aligned}$$

$\rho = \sum_\alpha w_\alpha |v_\alpha\rangle \langle v_\alpha|$

$v_\alpha^\dagger v_\alpha = 1$

$w_\alpha = \text{prob of system being in state } V_\alpha$

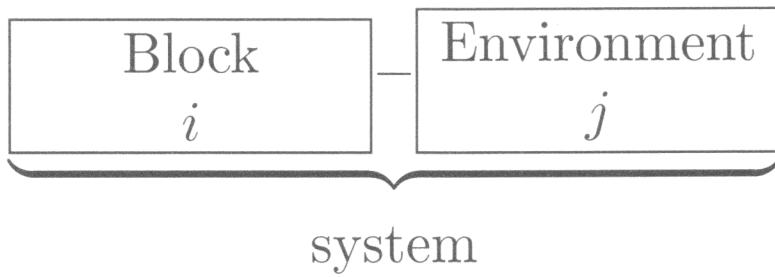
$= \sum_{ij} V_i^* \rho_{ij} V_j$

The $|v_\alpha\rangle$ provide the best way to project out important states of the block. We can argue several ways. Notice that

$$\langle A \rangle = \sum_\alpha w_\alpha \langle v_\alpha | A | v_\alpha \rangle$$

If for a particular α , $w_\alpha \approx 0$, we make no error in $\langle A \rangle$ if we discard $|v_\alpha\rangle$.

Thus projection with density matrix: diag ρ , keep
in most probable eigenvalues w_α



Both the Block and the Environment are represented by a reduced basis. We will find a new reduced basis for the Block.

Procedure

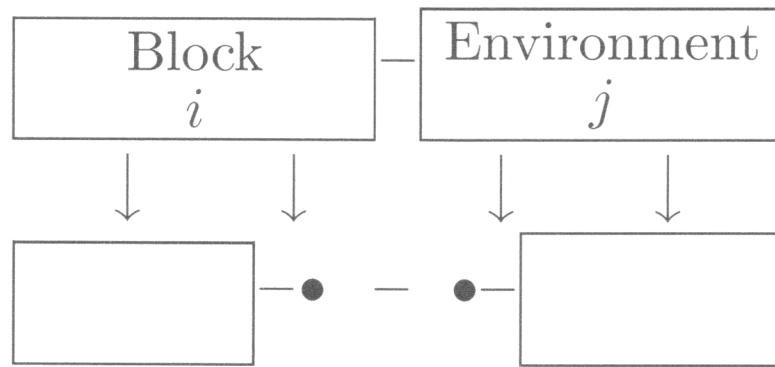
1. Diagonalize H_{system} to get ground state ψ (Lanczos or Davidson).
2. Calculate density matrix

$$\rho_{ii'} = \sum_j \psi_{ij} \psi_{i'j}$$

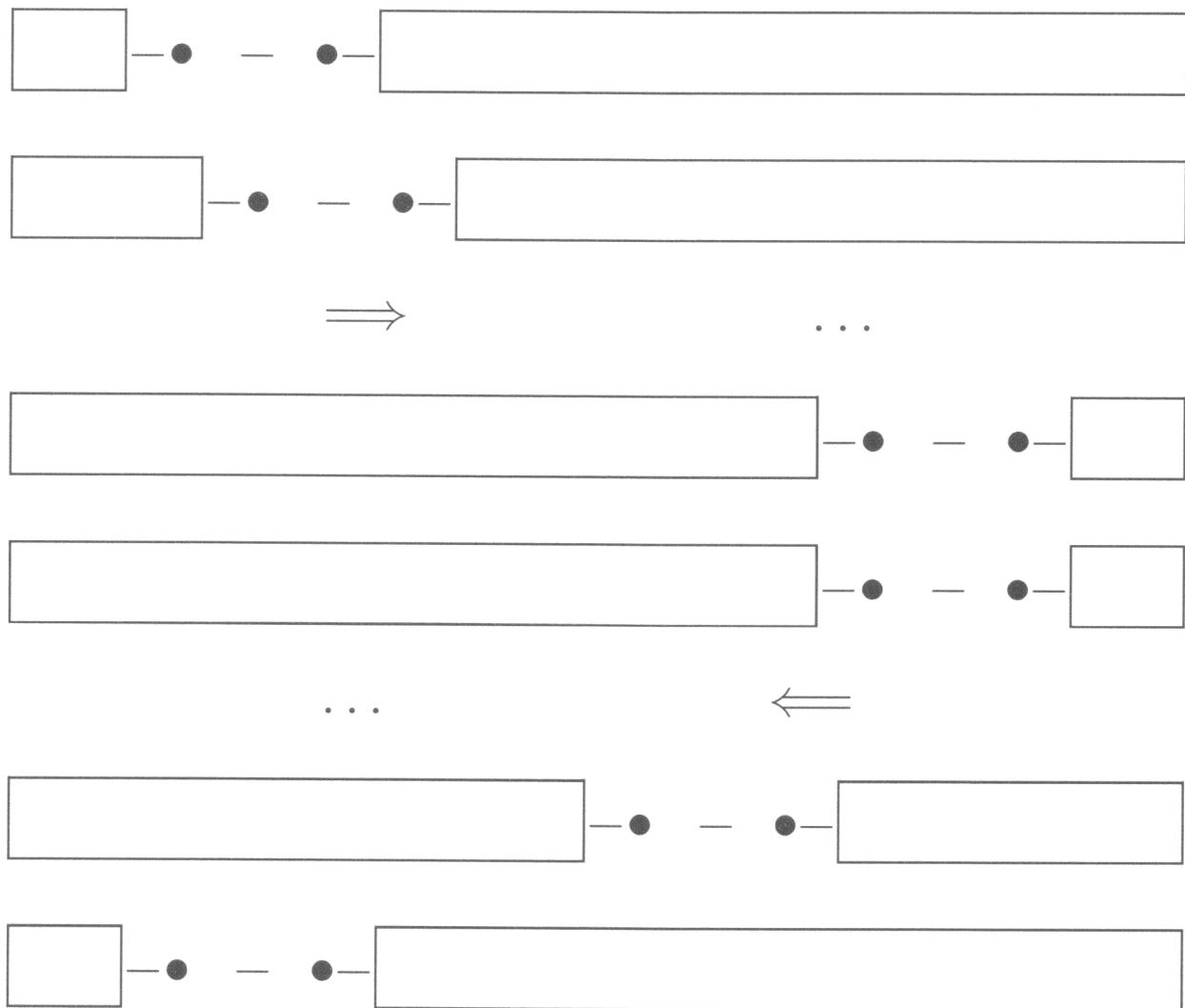
3. Diagonalize $\rho_{ii'}$ to get eigenstates v^α .
4. New basis is most probable m v^α 's. Change basis with $\bar{H} = \bar{A} H \bar{A}^T$, etc.

DMRG Algorithm

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The basic DMRG step generates a new reduced basis for a block that is one site larger than the previous block.



Entanglement

Entanglement is a property of a state divided into 2 parts — how quantum-correlated are the two parts?

Example: Two $S=\frac{1}{2}$'s. Q. Which state is more ~~more~~ entangled?

$$(a) | \uparrow \downarrow \rangle + | \uparrow \uparrow \rangle + | \downarrow \downarrow \rangle + | \downarrow \uparrow \rangle$$

$$(b) | \uparrow \uparrow \rangle + | \downarrow \downarrow \rangle$$

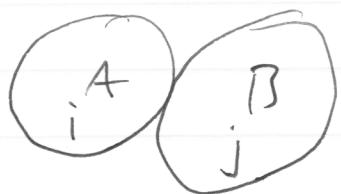
Answer: (b) is perfectly entangled.

(a) is unentangled

$$(| \uparrow \rangle + | \downarrow \rangle) \otimes (| \uparrow \rangle + | \downarrow \rangle) \quad \text{product state}$$

$$\cong | X-\uparrow \rangle \otimes | X-\uparrow \rangle$$

In general, how do you tell?



$$|\Psi\rangle = \sum_{ij} F_{ij} |i\rangle |j\rangle$$

F_{ij} like a matrix

Singular Value Decomposition — Matrix Factorization
— works for any matrix

$$A = U D V^T$$

$m \times n \quad m \times m \quad m \times n \quad - \text{rows are}$
 $\text{ortho diag} \quad \text{ortho}$

Numerical
Recipes

~~16~~ 16

\mathbf{D} has diag. elts, ≥ 0 - singular values

QI: ~~Schmidt~~ Schmidt-decomposition Schmidt
numbers,
vectors

Untangled: only one sig. value $\neq 0$

Normalization: $\sum_{\alpha} \lambda_{\alpha}^2 = 1$ $\lambda_{\alpha}^2 = \text{prob of state}$

$$|\alpha\rangle \langle \beta|_R$$

Density matrices:

$$\rho = \Psi \Psi^T = U D V (V^T D^T U^T) \\ = U D^2 U^T \text{ diag. form}$$

So $W_{\alpha} = \lambda_{\alpha}^2$ Density matrix idea same as Schmidt-decomp.

- DMRG is very natural from QI point of view -

DMRG = Low entanglement approximation algorithm

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Matrix Product States

1st transform



$$|\alpha_2\rangle = \sum_{\alpha_1} O_2[s_2]_{\alpha_2 \alpha_1} |s_2\rangle |\alpha_1\rangle$$

$$|\alpha_1\rangle = |s_1\rangle$$

2nd

$$|\alpha_3\rangle = \sum_{\alpha_2} O_3[s_3]_{\alpha_3 \alpha_2} |s_3\rangle |\alpha_2\rangle$$

$$= \sum_{\alpha_2 \alpha_1} O_3[s_3]_{\alpha_3 \alpha_2} O_2[s_2]_{\alpha_2 \alpha_1} |s_3\rangle |s_2\rangle |s_1\rangle$$

All the w's across (at step $\square \dots$)

$$|Y\rangle = \sum_{\alpha_2 \dots \alpha_L} O_{L-1}[s_L]_{\alpha_L \alpha_{L-1}} \dots O[|s_2\rangle]_{\alpha_2 \alpha_1} |s_L \dots s_1\rangle$$

This is a matrix product state:

$$Y(s_1 \dots s_L) = A_1(s_1) \dots A_L(s_L) \quad \begin{matrix} \leftarrow \text{Set of 2} \\ \text{matrices} \end{matrix}$$

1st + last A's = vectors

rest = matrices

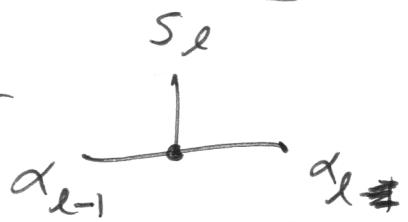
Ostlund &
Rommer
1995

Specify $s_1 \dots s_L$, Multiply m'tr's, get numer -
that is $Y(s_1 \dots s_L)$

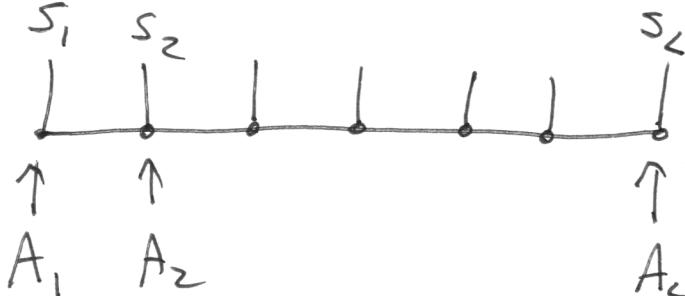
Another form

$$Y(s_1 \dots s_L) = \text{Tr} \{ A_1(s_1) \dots A_L(s_L) \}$$

Diagrams

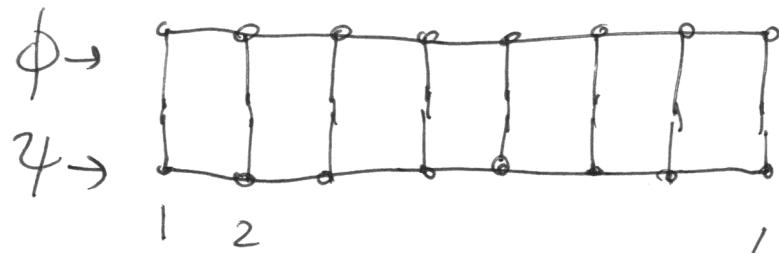
Let  $\longleftrightarrow A[s_l]_{d_l \times d_{l-1}}$

This is a very general notation for tensor networks. We contract over internal lines, and intersections/vertices represent the matrices/tensors.

Then $| \Psi \rangle \longleftrightarrow$ 

The diagrams are much easier to work with than the algebraic notation!

Contract $\langle \phi | \Psi \rangle$ Both MPS's



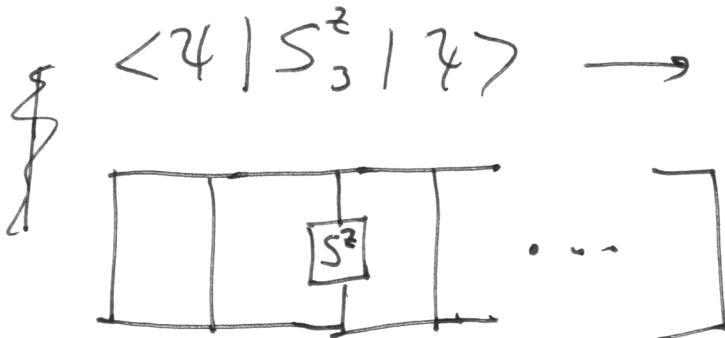
But algebraically, this is a mess:

$$\sum_{s_1, s_L} \Psi(s_1 \dots s_L) \phi(s_1 \dots s_L) = \sum_{\{s\}} (\hat{A}_1[s_1] \dots \hat{A}_L[s_L]) (\hat{B}_1[s_1] \dots \hat{B}_L[s_L])$$

$$= \sum_{\{s\}} \sum_{\{i\}} \sum_{\{j\}} A_{1i_1}^{s_1} A_{2i_1 i_2}^{s_2} \dots B_{1j_1}^{s_1} B_{2j_1 j_2}^{s_2} \dots$$

Operators

Single Site e.g. $S_3^z \sim S_3^z [S_3, S_3']$



Two-Site



Matrix Product Basis: (New term)



$\{| \alpha \rangle\}$ = set of states, we'd like them to be regarded as basis orthonormal:

$$\text{Or } \begin{array}{c} \text{---} \\ | & | & | & | \\ \alpha' & & & & \end{array} \quad \text{Want } O_{\alpha \alpha'} = \delta_{\alpha \alpha'}$$

The DMRG algorithm produces orthonormal bases

$$\begin{array}{ccc} | & | & | \\ L & & & \end{array} \quad \begin{array}{c} | & | \\ \text{DMRG wth} & \end{array} \quad \begin{array}{c} | & | \\ R & \end{array}$$

$$\begin{array}{c} | \\ L \end{array} \cdot \begin{array}{c} | & | \\ R & \end{array} = 1 \quad 1 = \begin{array}{c} | & | \\ R & \end{array}$$

DMRG steps with diagrams

