**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


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 $\psi$ 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

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

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

$$A = \sum_{ii'j} A_{ii'} |\varphi_i\rangle |j\rangle \langle \varphi_i| \langle j| = \sum_{ii'} A_{ii'} |\varphi_i\rangle \langle \varphi_i| \otimes 1_j$$

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

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

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

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

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

Thus projection with density matrix $\rho$, i.e., $\text{Tr} \rho$, keep in most probable eigenvalue $w_\alpha$. 

\[\sum_{ij} \psi_{ij}^* \psi_{ij'} = 1\]
Key DMRG Idea

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 $H_{\text{system}}$ to get ground state $\psi$ (Lanczos or Davidson).

2. Calculate density matrix

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

3. Diagonalize $\rho_{ii'}$ to get eigenstates $v^{\alpha}$.

4. New basis is most probable $m$ $v^{\alpha}$'s. Change basis with $\tilde{H} = \tilde{A} H \tilde{A}^T$, etc.
DMRG Algorithm

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. Which state is more entangled?

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

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

**Answer:** (b) is perfectly entangled,
(a) is unentangled

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

$n |x\rangle \otimes |x\rangle$

In general, how do you tell?

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

$2 |i\rangle |j\rangle \text{ like a matrix}$

**Singular Value Decomposition — Matrix Factorization**

- works for any matrix

$Y = UDV$

$m \times n \text{ } m \times m \text{ } m \times n \text{ } m \times m \text{ }$ rows are orthogonal
0 has diagonal, $\geq 0$ - singular value

QI: Schmidt decomposition

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

Normalisation: $\sum_{\alpha} \lambda_{\alpha} = 1$  $\lambda_{\alpha} = \text{prob. of state}

\rho = \psi \psi^T = U \rho_U (U^T \rho^T U') 

= U \rho U^T \text{ diag. form}

So $\omega_{\alpha} = \lambda_{\alpha}$ density matrix $\text{idea same as Schmidt - decorr.}$

DMRG is very natural from QI point of view -

DMRG = Low entanglement approximate algorithm
Matrix Product State

First transform

\[ |\alpha_2\rangle = \sum_{\alpha_1} O_2[\epsilon_{\alpha_2}] |\alpha_1\rangle \quad |\alpha_1\rangle = |5,\rangle \]

Second

\[ |\alpha_3\rangle = \sum_{\alpha_2} O_3[\epsilon_{\alpha_3}] |\alpha_2\rangle \quad |\alpha_2\rangle = |5,\rangle \]

\[ = \sum_{\alpha_2} O_3[\epsilon_{\alpha_3}] O_2[\epsilon_{\alpha_2}] |\alpha_3\rangle \quad |\alpha_3\rangle = |5,\rangle \]

All the way across (at step ...)

\[ |\psi\rangle = \sum_{\alpha_2} O_4[\epsilon_{\alpha_4}] \cdots O_2[\epsilon_{\alpha_2}] |\alpha_4\rangle \cdots |\alpha_3\rangle \]

This is a matrix product state:

\[ Y(\epsilon_{s_2}, -\epsilon_{s_2}) = A_1[\epsilon_{\alpha_4}] \cdots A_5[\epsilon_{\alpha_3}] \]

1st + last A's = Vectors

Rest = Matrices

Specify \( s_2, -s_2 \), multiply matrices, get number that is \( Y(s_2, -s_2) \)

Another form

\[ Y(s_2, -s_2) = Tr \sum A_1[\epsilon_{s_1}] \cdots A_5[\epsilon_{s_3}] \cdots \]
Diagrams

Let $A[A_1 \cdots A_{d-1}] \leftrightarrow A[\sum_{s_1} \cdots \sum_{s_d}]$

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

Then $|14\rangle \leftrightarrow \sum_{s_1, s_2} A_1 A_2 |s_1, s_2\rangle$

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

Contracts $\langle \phi | 14 \rangle$ Both MPS's

But algebraically, this is a mess:

$$\sum_{s_1, \ldots, s_L} \phi(s_1, \ldots, s_L) = \sum_{s_1, s_2} (A_1 \cdots A_{d-1})(B_1 \cdots B_{d-1})$$

$$= \sum_{s_1, s_2} A_{11} A_{21} \cdots B_{11} B_{21} \cdots$$
Operators

Single Site e.g. \[ S_{\uparrow}^z \sim S_{\uparrow}^z \{ S_{\uparrow}, S'_{\uparrow} \} \]

\[ \langle \uparrow | S_{\uparrow}^z | \uparrow \rangle \rightarrow \]

\[ \begin{array}{c}
\begin{array}{c}
\vdots
\end{array}
\end{array} \]

Two Site

\[ \begin{array}{c}
\begin{array}{c}
\vdots
\end{array}
\end{array} \]

Matrix Product Basis: (New term)

\[ \begin{array}{c}
\begin{array}{cccc}
S_{1} & S_{2} & S_{3} & S_{4}
\end{array}
\end{array} \]

\[ |15,7\rangle \]

\[ \{ |x\rangle \} = \text{set of states, regard as basis} \]

\[ \text{We'd like them to be orthonormal:} \]

\[ \Omega = \begin{array}{c}
\begin{array}{c}
\vdots
\end{array}
\end{array} \]

\[ \text{Want } \Omega |x\rangle = |x\rangle \]

The DMRG algorithm produces orthonormal bases

\[ \begin{array}{c}
\begin{array}{c}
\vdots
\end{array}
\end{array} \]

\[ L \quad \text{DMRG with } R \]

\[ 1 = \begin{array}{c}
\begin{array}{c}
\vdots
\end{array}
\end{array} \]
DMRG steps with diagrams

More general form allowed during Davidson/Lanczos

New m

New $A_l[s]$

New $A_{l+1}[s]$

Not orthogonal