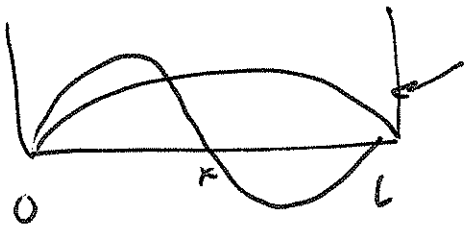
Density-Matrix Renormalization Group Algorithm

Sources: Master Thesis of Ahmet Keleş (Bilkent U.)
A.L. Malvezzi: "An Introduction to Numerical Methods in Low-Dimensional Quantum Systems" (Brazilian Journal of Physics, 33 55 (2003))

- standard renormalization group methods are not applicable to quantum systems
  - as discussed by White and Noack: the boundary conditions in quantum systems prevent a straightforward application of real-space renormalization techniques such as decimation, etc.

example: particle in a box



wavefunctions are zero at $x=0$ and $x=L$

if we try to build the ground state of the 2L-box system we fail, since the ground state of the 2L system is a function which is periodic in 2L but not periodic in L

- density-matrix renormalization group gets around this problem at least in one-dimension
- first: define reduced density matrix
  - given a wavefunction $|\psi\rangle$, the density matrix is

$$\rho_{ij} = \langle i|\psi\rangle\langle\psi|j\rangle$$

$$|\psi\rangle = \sum_i |i\rangle\langle i|\psi\rangle = \sum_i a_i |i\rangle$$

$$\rho_{ij} = a_i a_j^* \qquad \mathrm{Tr}\,\rho = \sum_i |a_i|^2 = 1$$

  - given a subsystem which can be in two states

$$p_1|\psi_1\rangle\langle\psi_1| + p_2|\psi_2\rangle\langle\psi_2|$$

such that $p_1 + p_2 = 1 \qquad p_1, p_2 \geq 0$

$$\rho_{ij} = p_1\langle i|\psi_1\rangle\langle\psi_1|j\rangle + p_2\langle i|\psi_2\rangle\langle\psi_2|j\rangle$$

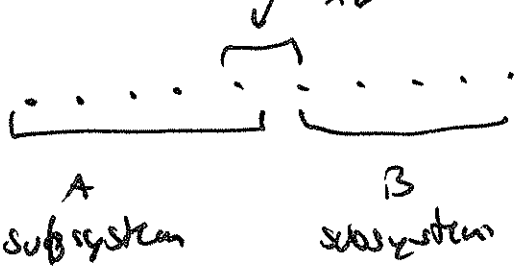
$$= p_1 a_i^{(1)} a_j^{(1)*} + p_2 a_i^{(2)} a_j^{(2)*}$$

$$\mathrm{Tr}\,\rho = p_1 \sum_i |a_i^{(1)}|^2 + p_2 \sum_i |a_i^{(2)}|^2 = p_1 + p_2 = 1$$

- $\langle\hat{O}\rangle = p_1\langle\psi_1|\hat{O}|\psi_1\rangle + p_2\langle\psi_2|\hat{O}|\psi_2\rangle = \mathrm{Tr}(\hat{\rho}\hat{O})$
- reduced density matrix
  - suppose that the Hamiltonian of a system is given by $H = H_A + H_B + C_{AB}$

$A, B \rightarrow$ refer to two subsystems of the total system

for example: spin-model



Suppose that the model under scrutiny is the Heisenberg model

$$H = \sum_i \vec{S}_i \cdot \vec{S}_{i+1}$$

$$\vec{S}_i \cdot \vec{S}_{i+1} = S_x^i S_x^{i+1} + S_y^i S_y^{i+1} + S_z^i S_z^{i+1}$$

$$= \frac{1}{2}\left(S_i^+ S_{i+1}^- + S_i^- S_{i+1}^+\right) + S_z^i S_z^{i+1}$$

$$S_x^i = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad S_y = \begin{pmatrix} 0 & i \\ -i & 0 \end{pmatrix} \quad S_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

using tensors we can construct $S_y^i S_x^{i+1}$ and the other components as

$$S_x^i S_x^{i+1} = \underset{1}{\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}} \otimes \underset{2}{\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}} \cdots \otimes \underset{i}{\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}} \otimes \underset{i+1}{\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}} \otimes \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \cdots \underset{L}{\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}}$$

identities everywhere but "i" and "i+1"; S_x at "i" th position; S_x at "i+1"-th position; L sites

- we can also write Hamiltonian $H = H_A + H_B + C_{AB}$ for this case in terms of sub-Hamiltonians H_A, H_B and coupling C_{AB} represented by tensor products

$$H = H_A \otimes I_B + I \otimes H_B + C_{AB}$$

$$C_{AB} = \underset{1}{\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}} \otimes \cdots \otimes \underset{N_A-1}{\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}} \otimes \underset{S_x}{\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}} \otimes \underset{S_x}{\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}} \otimes \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \cdots \otimes \underset{L}{\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}}$$

$$+ \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \cdots \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \otimes \begin{pmatrix} 0 & i \\ -i & 0 \end{pmatrix} \otimes \begin{pmatrix} 0 & i \\ -i & 0 \end{pmatrix} \otimes \cdots \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

$$+ \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \cdots \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \otimes \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \otimes \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \cdots \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

the ground state of H H(Ψ) can be represented as a linear combination of ~~states~~ product states, where the product is of one state from subsystem A one from subsystem B

$$\Rightarrow \quad |\Psi\rangle = \sum_{i,j} \Psi_{ij} \, |i\rangle_A \, |j\rangle_B$$

in this case we can define a reduced density matrix which allows expressing operators which act in one of the subsystems $\Rightarrow$

$$\hat{O}_A = \underbrace{(\ )\otimes(\ )\otimes \dots \otimes(\ )}_{\text{A subsystem}} \otimes \underbrace{\begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix} \dots \otimes \begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix}}_{\text{B subsystem (identities)}}$$

$$= O_A \otimes I_B \Rightarrow O_A \ 2^{N_A}\times 2^{N_A}, \quad I \ 2^{N_B}\times 2^{N_B}$$

$$\text{Tr}\ \langle O_A\rangle = \text{Tr}(\hat{\rho}\, \hat{O}_A \otimes I_B)$$

$$= \sum_{i,j} |\Psi_{ij}|^2 \, {}_A\langle i| \, {}_B\langle j| \, \hat{O}_A \, |j\rangle_B \, |i\rangle_A$$

$$= \sum_{i,j} |\Psi_{ij}|^2 \, \langle i|\hat{O}_A|i\rangle \, {}_B\langle j| \, \hat{I} \, |j\rangle_B$$

$$= \sum_{i,j} |\Psi_{ij}|^2 \langle i|\hat{O}_A|i\rangle$$

reduced density matrix $\quad \rho^{(A)}_{ij} = \sum_k \Psi^*_{ik} \Psi^*_{jk}$

$$= \text{Tr}_B\ \hat{\rho}$$

- the reduced density matrix plays a very important role in the density matrix renormalization group algorithm

  → it determines how to truncate and reduce the number of states used to calculate the properties of the system under study

- consider the exact ground state of a system

$$|\psi\rangle = \sum_{i,j} \psi_{ij}^{\dagger} |i\rangle_A |j\rangle_B$$

if the dimension of the A subsystem is M_A and that of the B subsystem is M_B

$$\Rightarrow |\psi\rangle = \sum_{i=1}^{M_A} \sum_{j=1}^{M_B} \psi_{ij} |i\rangle_A |j\rangle_B$$

suppose I want to represent the ground state, but reduce the number of states which represent the A subsystem

$$|\psi'\rangle = \sum_{\alpha=1}^{M_A'} \sum_{j=1}^{M_B} \psi'_{\alpha j} |\alpha_i\rangle_A |j\rangle_B$$

$M_A' < M_A$

$$|\alpha_i\rangle_A = \sum_i |i'\rangle_A \underbrace{{}_A\langle i'|\alpha_i\rangle_A}_{u_{\alpha i'}} = \sum_{i'} |i'\rangle_A u_{\alpha i'}$$

- the question is how do I decide which states should be thrown away?

to answer this question, minimize

$$(\langle\Psi| - \langle\Psi'|)(|\Psi\rangle - |\Psi'\rangle)$$
$$= \langle\Psi|\Psi\rangle - \langle\Psi'|\Psi\rangle - \langle\Psi|\Psi'\rangle + \langle\Psi'|\Psi'\rangle$$

$\langle\Psi|\Psi\rangle = 1$

$$\langle\Psi|\Psi'\rangle = \sum_{ij\alpha k} \Psi_{ij}\, \Psi'_{\alpha k}\, \underbrace{\langle i|\alpha\rangle}_{A}\, \underbrace{\langle j|k\rangle}_{B}$$

$$= \sum_{ij\alpha} \Psi_{ij}\, \Psi'_{\alpha j}\, u_{\alpha i}$$

$$\langle\Psi'|\Psi'\rangle = \sum_{ij} \Psi'^{2}_{ij}$$

- here it was assumed that Ψ'_{ij} are real, for simplicity

$$\Rightarrow (\langle\Psi| - \langle\Psi'|)(|\Psi\rangle - |\Psi'\rangle) = 1 - 2\sum_{ij\alpha} \Psi_{ij}\, \Psi'_{\alpha j}\, u_{\alpha i} + \sum_{ij} \Psi'^{2}_{ij}$$

minimize with respect to Ψ'_{ij}

$$\Rightarrow \Psi'_{ij} = \sum_{n} \Psi_{nj}\, u_{in}$$

- substituting back we obtain

$$(\langle\Psi| - \langle\Psi'|)(|\Psi\rangle - |\Psi'\rangle) = 1 - 2\sum_{ij\alpha k} \underbrace{\Psi_{ij}\, \Psi_{kj}}_{\text{reduced density matrix}}\, u_{\alpha k}\, u_{\alpha i} + \sum_{ijkl} \Psi_{kj}\, u_{ik}\, \Psi_{lj}\, u_{il}$$

$$= 1 - \sum_{\alpha ik} u_{\alpha i} \Big[\sum_{j} \Psi_{ij}\, \Psi_{kj}\Big] u_{\alpha k} = 1 - \sum_{\alpha ik} u_{\alpha i}\, \delta^{(4)}_{in}\, u_{\alpha k}$$

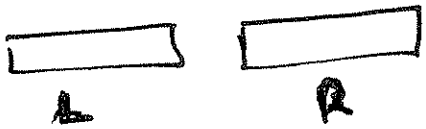
$$= 1 - \sum_{\alpha} \langle\alpha|\delta_4|\alpha\rangle \Rightarrow$$

$(\langle\psi| - \langle\tilde{\psi}|)(|\psi\rangle - |\tilde{\psi}\rangle)$ is minimized if the basis used corresponds to the eigenvectors of the reduced density matrix $\Rightarrow$ truncation: keep states with largest eigenvalues

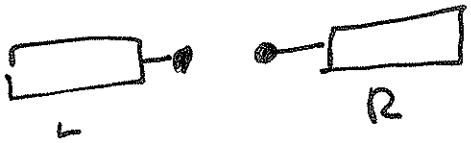
DMRG algorithm

- here the infinite system size algorithm is described, first, the finite system size is outlined afterwards

- outline of infinite system size algorithm
  - start with two blocks (left and right)

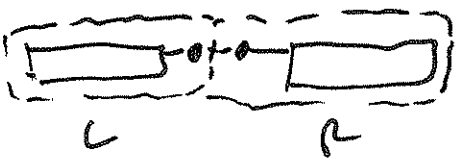


  - add one site to each block as



  - form a superblock

  - by keeping a desired number of eigenstates (largest eigenvalues of the reduced density matrix) form matrix of new left block and new right block



in more detail, use Heisenberg model as an example

- suppose left-block / right-block at the start have N_L and N_R sites

  ⇓ ⇓

  this means that the Hamiltonians which represent each are of dimension $2^{N_L} \times 2^{N_L}$ and $2^{N_R} \times 2^{N_R}$

  let's choose $N_L = N_R = N$:

- adding a site to the right of the left block and to the left of the right block

$$H_L^{N+1} = H_L^N \otimes \text{new site}$$

$$H_L^{N+1} = H_L^N \otimes I + \underbrace{I \otimes \cdots \otimes I}_{N-1} \otimes S_z \otimes S_z + \underbrace{I \otimes \cdots \otimes I}_{N-1} \otimes S_x \otimes S_x + \underbrace{I \otimes \cdots \otimes I}_{N-1} \otimes S_z \otimes S_z \Rightarrow \text{dimension } 2^{N+1} \times 2^{N+1}$$

$$H_R^{N+1} = I \otimes H_R^N + S_z \otimes S_z \otimes I \otimes \cdots \otimes I + S_x \otimes S_x \otimes I \otimes \cdots \otimes I + S_z \otimes S_z \otimes I \otimes \cdots \otimes I \quad \text{dimension } 2^{N+1} \times 2^{N+1}$$

- forming superblock Hamiltonian

$$H_L^{2N+2} = H_L^{N+1} \otimes I^{N+1} + I^{N+1} \otimes H_R^{N+1} + I \otimes \cdots \otimes I \otimes S_z \otimes S_z \otimes I \cdots \otimes I \quad \text{dimension } 2^{2N+2} \times 2^{2N+2}$$

- diagonalize superblock Hamiltonian

- calculate reduced density matrix of the new left-block $\Rightarrow N+1$ left sites and that of the new right block $\Rightarrow N+1$ right sites

- using the states corresponding to the largest eigenvalues of the reduced density matrix on each side, truncate the Hamiltonians H_L^{N+1} and H_R^{N+1}

  - in other words: H_L^{N+1} has dimensions $2^{N+1} \times 2^{N+1}$

  - after diagonalizing the reduced density matrix on the left side, keep the largest 2^N eigenvalues and their eigenvectors

$$\Rightarrow \left(H_L^{N+1}\right)_{\text{truncated}} = \left(\equiv\right)\left(H_L^{N+1}\right)\left(||||\right)$$

2^N by 2^{N+1} matrix; 2^{N+1} by 2^N matrix

as a result $\left(H_L^{N+1}\right)_{\text{truncated}}$ is

$$2^N \times 2^N$$

- do the same for H_R^{N+1}

using the truncated $(H_L)_{tr}$ and $(H_R)_{tr}$ one can start the procedure all over, and increase the size of the blocks, BUT one needs not only $(H_L)_{tr}$ at each step, but also the spin on the right most edge of the left block, and the leftmost edge of the right block

$$\Rightarrow \quad (H_L^{N+1})_{tr} \xrightarrow{\text{enlarge}} H_L^{N+2} = (H_L^{N+1})_{tr} \otimes I$$

$$+ \; (S_x)_{tr}^{N+1} \otimes S_x$$

$$+ \; (S_y)_{tr}^{N+1} \otimes S_y$$

$$+ \; (S_z)_{tr}^{N+1} \otimes S_z$$

$$(S_x)_{tr}^{N+1} = (\underbrace{I \otimes \ldots \otimes I}_{N} \otimes S_x)_{tr}$$ in the ~~truncated~~ truncated basis

- formed by $(\Xi)(I \otimes \ldots \otimes \underset{N}{I} \otimes \underset{N+1}{S})((\Xi)^{\dagger})$

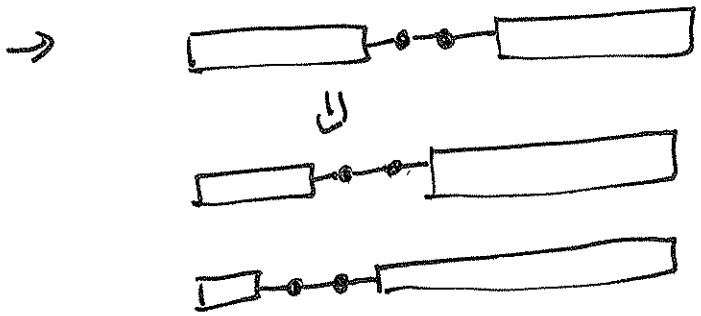
↑ matrix of eigenvectors of reduced density matrix

- similarly on the right side

using this algorithm one keeps increasing
U until averages converge → we take that
to mean the thermodynamic limit

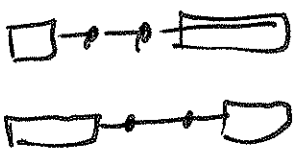
- finite system algorithm

starts with some size for superblock $2N+2$
increase using the same procedure as the
infinite system size algorithm, but once
~~that size~~ desired size is reached, "sweep"
to the left



in other words: enlarge right block, but for
left block use a smaller H_L (stored from
the earlier part of the calculation, in
which the blocks were grown to the desired
size)

after one should also sweep to the right



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and back to center

the key advantage for both infinite and finite system algorithm is provided by truncation

- consider the step of enlarging both blocks

$\Rightarrow$ superblock Hamiltonian has dimensions 2^{2N+2}

~~next~~ H_L^{N+1}, H_R^{N+1} have dimensions $2^{N+1} \times 2^{N+1}$

but after truncation $(H_L^{N+1})_{tr}$ has dimensions $2^N \times 2^N$

in the next step we will use the truncated left block Hamiltonian ($2^N \times 2^N$ matrix) to represent $N+1$ sites (also true for the right side)

enlarge 

$\Rightarrow$ new superblock will still be $2^{N+2} \times 2^{2N+2}$ even though the number of sites in the system are $2N+4$

- largest matrix to diagonalize is always $2^{2N+2} \times 2^{2N+2}$