

LECTURE

TIME-DEPENDENT DMRG

Literature:

- 1) DMRG - U. Schollwöck, Rev. Mod. Phys. 77, 259 (2005)
 - 2) time-dependent DMRG - Trotter-based, $T=0, T>0$
 - G. Vidal, PRL 93 ~~040502~~, 040502 (2004)
 - A.J. Daley, C. Kollath, U. Schollwöck, G. Vidal, J. Stat. Mech.: Theor. Exp. P04005 (2004)
 - A. Feiguin, S.R. White, PRL 93, 076401 (2004)
 - F. Verstraete, D. Porras, J.I. Cirac, PRL 93, 227204 (2004) ($T>0$)
 - 3) time-dependent DMRG - Krylov-based
 - S.R. White, talk 2004, <http://komet337.physik.uni-mainz.de/Teichmann/DMRG/workshop/proceedings/white.pdf>
- (Krylov: S. Manmana et. al.)

calculate

- $|\psi(t)\rangle = e^{-i\hat{H}t} |\psi(0)\rangle$
- $\langle \hat{O}_1(t) \hat{O}_2(0) \rangle = \langle \psi | e^{+i\hat{H}t} \hat{O}_1 e^{-i\hat{H}t} \hat{O}_2 | \psi \rangle$
 $= \langle \psi(t) | \hat{O}_1 | \psi(t) \rangle$ where $|\psi(t)\rangle = e^{-i\hat{H}t} |\psi(0)\rangle$
 $|\psi(0)\rangle = \hat{O}_2 | \psi \rangle \Rightarrow$ FT to structure function and other frequency-dependent quantities!

TIME-DEPENDENT DMRG

Problem: given $|\psi(t=0)\rangle$, $\hat{H}(t)$, what is $|\psi(t)\rangle$?

assume \hat{H} for simplicity

$$|\psi(t)\rangle = e^{-i\hat{H}t} |\psi(0)\rangle \qquad \hat{H}|n\rangle = E_n|n\rangle$$

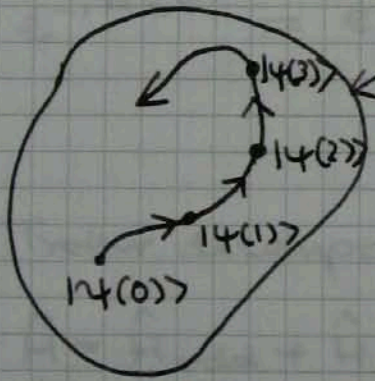
$$= \sum_n e^{-iE_n t} c_n |n\rangle \qquad c_n = \langle n | \psi(0) \rangle$$

eigenbasis unknown

$$= \sum_{n\tilde{m}} e^{-iE_n t} c_n a_{n\tilde{m}} |\tilde{m}\rangle \qquad a_{n\tilde{m}} = \langle \tilde{m} | n \rangle$$

$$= \sum_{\tilde{m}} \left(\sum_n e^{-iE_n t} c_n a_{n\tilde{m}} \right) |\tilde{m}\rangle$$

↑ some other basis
↑ unknown
changes in value



Hilbert space

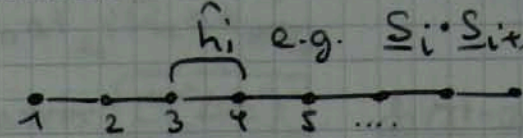
time-evolving quantum state 'explores' Hilbert space

$$|\psi(t)\rangle \longleftrightarrow \sum_{\{\sigma_i\}} A_1^{\sigma_1}(t) A_2^{\sigma_2}(t) \dots A_L^{\sigma_L}(t) |\sigma_1 \dots \sigma_L\rangle$$

time-dependent matrix product state that - for given dimension D - has minimal distance

$$\| |\psi(t)\rangle - |\psi_{MPS}^D(t)\rangle \|_2$$

Strongly correlated quantum problems often have short-ranged Hamiltonians

$$\hat{H} = \sum_i \hat{h}_i$$


- ① global finite-t evolution → global infinitesimal-t evolution

$$e^{-i\hat{H}t} = \underbrace{e^{-i\hat{H}\Delta t} e^{-i\hat{H}\Delta t} \dots e^{-i\hat{H}\Delta t}}_{N = t/\Delta t}$$

- ② global infinitesimal-t evolution → local infinitesimal-t evolution

$$e^{-i\hat{H}\Delta t} = e^{-i\sum \hat{h}_i \Delta t} \neq \prod e^{-i\hat{h}_i \Delta t}$$

\uparrow
 $[\hat{h}_i, \hat{h}_{i+1}] \neq 0$

Trotter decomposition:

$$\hat{H} = \hat{H}_{\text{odd}} + \hat{H}_{\text{even}}$$

$$\hat{H}_{\text{odd}} = \sum_{j=0} \hat{h}_{2j+1} \quad \hat{H}_{\text{even}} = \sum_{j=1} \hat{h}_{2j}$$

these all commute, so the problem is separating odd from even in factorizing

Baker-Campbell-Hausdorff:

$$e^{\hat{X}} e^{\hat{Y}} = e^{\hat{Z}} \quad \hat{Z} = \hat{X} + \hat{Y} + \frac{1}{2} [\hat{X}, \hat{Y}] + \frac{1}{12} ([\hat{X}, [\hat{X}, \hat{Y}]] + [\hat{Y}, [\hat{Y}, \hat{X}]]) + \dots$$

assume $[\hat{X}, \hat{Y}]$ comm. with \hat{X}, \hat{Y} :

$$\text{Glauber formula } e^{\hat{X} + \hat{Y}} = e^{\hat{X}} e^{\hat{Y}} e^{-\frac{t}{2} [\hat{X}, \hat{Y}]}$$

reflected in naive factorization

$$e^{-\frac{1}{2}[\hat{X}, \hat{P}]} = 1 - \frac{1}{2} \boxed{O(\Delta t)^2}$$

(4)

error of first order - Trotter decomp.: $O(\Delta t)^2$
 $e^{i\hat{H}\Delta t} = e^{i\hat{H}_0\Delta t} e^{i\hat{H}_1\Delta t}$

over $\frac{T}{\Delta t}$ time steps: error $\boxed{O(\Delta t)}$ first-order in Δt .

generalizes to

$$e^{i\hat{H}\Delta t} = e^{a_{m+1}\hat{H}_0\Delta t} \underbrace{\left(\prod_{n=1}^m e^{b_n\hat{H}_e\Delta t} e^{a_n\hat{H}_0\Delta t} \right)}_{\text{approximate, decomposed time evol.}} + O(\Delta t^{p+1})$$

$$\sum a_n = \sum b_n = 1$$

huge variety, characterized by order of error Δt^p

Trotter second order: $e^{-i\hat{H}_0\Delta t/2} e^{-i\hat{H}_e\Delta t} e^{-i\hat{H}_0\Delta t/2}$

Trotter fourth order: $\hat{S}(w_1) \hat{S}(w_2) \hat{S}(w_3)$ ~~with~~ with

$$\hat{S}(w_i) = e^{-i\hat{H}_0 w_i \Delta t/2} e^{-i\hat{H}_e w_i \Delta t} e^{-i\hat{H}_0 w_i \Delta t/2}$$

and $w_1 = w_2 = \frac{1}{4-4^{1/3}}$, $w_3 = 1 - 2w_1 - 2w_2$. (Suzuki)

in any case, how do we implement

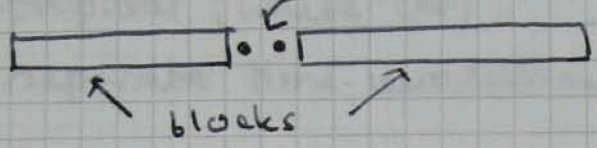
$$|\varphi\rangle = e^{-i\hat{h}_i\Delta t} |\psi\rangle,$$

i.e. find an optimal representation of $|\varphi\rangle$ given $|\psi\rangle$?

1)

answer (in "DMRG"-language):

- consider finite-system DMRG with sweeping (at position of bond)



- carry out infinitesimal local time evolution exactly:

$$|\psi\rangle = \sum_{m_L m_R} \sum_{\sigma_L \sigma_R} \Psi_{m_L m_R \sigma_L \sigma_R} |m_L\rangle |\sigma_L \sigma_R\rangle |m_R\rangle$$

$$e^{-i\hat{H}\Delta t} = \sum_{\sigma_L \sigma_R \sigma'_L \sigma'_R} |\sigma_L \sigma_R \sigma'_L \sigma'_R| U_{\sigma_L \sigma_R \sigma'_L \sigma'_R}$$

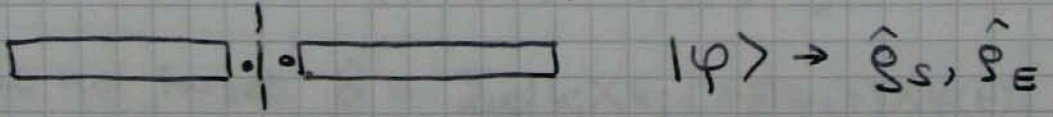
(diagonalize \hat{h} , exponentiate, transform back - 2 site problem...)

$$|\psi\rangle = \sum_{m_L m_R} \sum_{\sigma_L \sigma_R} \Psi_{m_L m_R \sigma_L \sigma_R} |m_L\rangle |\sigma_L \sigma_R\rangle |m_R\rangle$$

where

$$\Psi_{m_L m_R \sigma_L \sigma_R} = \sum_{\sigma'_L \sigma'_R} U_{\sigma_L \sigma_R \sigma'_L \sigma'_R} \Psi_{m_L m_R \sigma'_L \sigma'_R}$$

- continue sweeping to next bond in usual DMRG procedure: calculate new blocks by reduced density operator analysis:



keep M highest-weight eigenstates!

- carry out Trotter steps while sweeping forth/back

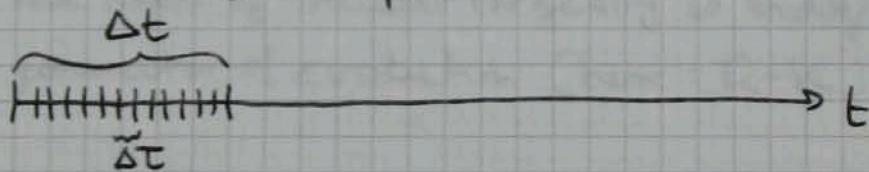
Krylov-time evolution

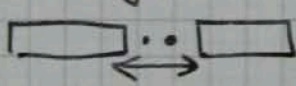
what can we do if \hat{H} is not short-ranged?

proposal (White '04):

separate time-evolution and state selection

- from $|\psi(t)\rangle$, calculate approximately $|\psi(t+\Delta t)\rangle$ (and other states in near future) to obtain suitable ^{approximate state} ~~state~~ space (multiple targeting)
- carry out high-precision time evolution in this state space.



at time t , carry out standard finite-system sweeps (), generating and targeting at each step:

$$\begin{aligned} |k_1\rangle &= -i\Delta t \hat{H} |\psi(t)\rangle \\ |k_2\rangle &= -i\Delta t \hat{H} (|\psi(t)\rangle + \frac{1}{2}|k_1\rangle) \\ |k_3\rangle &= -i\Delta t \hat{H} (|\psi(t)\rangle + \frac{1}{2}|k_2\rangle) \\ |k_4\rangle &= -i\Delta t \hat{H} (|\psi(t)\rangle + |k_3\rangle) \end{aligned} \quad \left. \begin{array}{l} \text{approx:} \\ \text{Runge-Kutta} \\ \text{vectors} \end{array} \right\}$$

do not target $\hat{\rho} = \sum_i \alpha_i |k_i\rangle\langle k_i| + \beta |\psi(t)\rangle\langle\psi(t)|$ ($\sum \alpha_i + \beta = 1$)
but better

$$|\psi(t + \frac{1}{3} \Delta t)\rangle = |\psi(t)\rangle + \frac{1}{162} (31|k_1\rangle + 14(|k_2\rangle + |k_3\rangle) - 5|k_4\rangle)$$

$$|\psi(t + \frac{2}{3} \Delta t)\rangle = |\psi(t)\rangle + \frac{1}{81} (16|k_1\rangle + 20(|k_2\rangle + |k_3\rangle) - 2|k_4\rangle)$$

$$|\psi(t + \Delta t)\rangle = |\psi(t)\rangle + \frac{1}{6}|k_1\rangle + \frac{1}{3}|k_2\rangle + \frac{1}{3}|k_3\rangle + \frac{1}{6}|k_4\rangle$$

and target $\hat{g} = \sum_{i=1}^4 |\psi(t_i)\rangle \langle \psi(t_i)|$

$(t_1 = t, t_2 = t + \frac{1}{3} \Delta t, t_3 = t + \frac{2}{3} \Delta t, t_4 = t + \Delta t)$

after some sweeps, basis adapted to these states.

Now high precision time-evolution e.g. Runge-Kutta
 $\Delta \tau = \frac{\Delta t}{10}$ (R-K error $O(\Delta \tau^5)$)

The idea of multi-targeting is independent of generator of evolution (here: R-K).

Best: Krylov time-evolution

$$e^{-i\hat{H}\Delta t}$$

huge exponential can't be calculated!

but $e^{-i\hat{H}\Delta t} |v\rangle$ is quite easy: Lanczos...

~~Useful idea~~

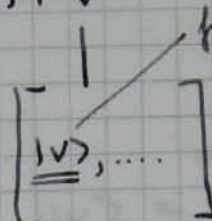
idea: Taylor expansion gives error $O(\Delta t^{n+1})$ if we calculate orders up to $\hat{H}^n |v\rangle$ - but does it give the best prefactor for the computational cost?

No, one can show that the answer is a Krylov sequence.

just consider \hat{H} for simplicity.

tridiagonalization: $T = V^\dagger H V$

unitary $V^{-1} = V^\dagger$



free, we take $|v\rangle$

Krylov = Lanczos vectors formed iteratively

approximately: $T_{n \times n} = V_n^\dagger H V_n$

the first n Lanczos vectors, starting from $|v\rangle$

$$e^{i\hat{H}} |v\rangle = e^{iVTV^\dagger} |v\rangle = V e^{iTV} V^\dagger |v\rangle = V e^{iTV} \begin{bmatrix} 1 \\ 0 \\ \vdots \end{bmatrix}$$

first column of e^{iTV}

no proof: \approx optimal $\approx V_n e^{iT_{n \times n}} \begin{bmatrix} 1 \\ 0 \\ \vdots \end{bmatrix}$

n small, ... early diagonalized and exponentiated.

result: first n Krylov vectors, weighted by first column entries of e^{iTV} .

construction of density operator:

How can we represent density operators as pure states? — finite-T DMRG.

bipartite system AB

$$|\psi\rangle_{AB} = \sum_{ij} \psi_{ij} |i\rangle_A |j\rangle_B$$

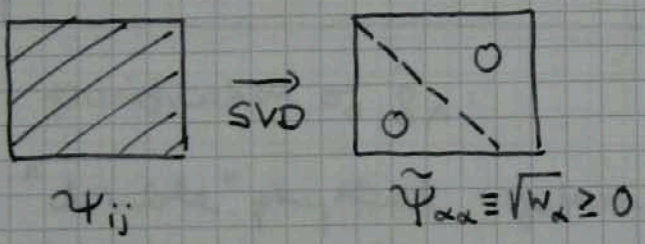
(Schmidt decomposition)

dimension state space A, B

$$|\psi\rangle_{AB} = \sum_{\alpha} \sqrt{w_{\alpha}} |\alpha\rangle_A |\alpha\rangle_B$$

$\min(D_A, D_B)$
 ≥ 0

IF normalized: $1 = \sum_{\alpha} (\sqrt{w_{\alpha}})^2 = \sum w_{\alpha}$



$$\hat{S}_{AB} = |\psi\rangle_{AB} \langle\psi|_{AB} = \sum_{\alpha} w_{\alpha} |\alpha\rangle_A |\alpha\rangle_B \langle\alpha|_A \langle\alpha|_B \quad (\text{tr } \hat{S}_{AB} = 1)$$

$$\begin{aligned} \hat{S}_A &= \text{tr}_B \hat{S}_{AB} = \sum_{\beta} \langle\beta|_B \left(\sum_{\alpha} w_{\alpha} |\alpha\rangle_A |\alpha\rangle_B \langle\alpha|_A \langle\alpha|_B \right) |\beta\rangle_B \\ &= \sum_{\alpha} w_{\alpha} |\alpha\rangle_A \langle\alpha|_A \quad w_{\alpha} \geq 0 \end{aligned}$$

pure state on AB \rightarrow mixed state on A

purification: invert this procedure!

A \equiv physical system (dimension D_A)

$$\hat{S} = \hat{S}_A = \sum_{\alpha} w_{\alpha} |\alpha\rangle_{(A)} \langle\alpha|_{(A)} \quad (\text{density op. in eigenbasis})$$

introduce fictitious

B \equiv auxiliary system (dimension $D_B \geq D_A$)

\swarrow loc on $D_B = D_A$

(arbitrary) basis $\{|\alpha\rangle_B\}$

Then

$$\hat{S}_A = \text{tr}_B \hat{S}_{AB} \text{ with}$$

$$\hat{S}_{AB} = \sum_{\alpha} w_{\alpha} |\alpha\rangle_A \langle\alpha|_B \langle\alpha|_A |\alpha\rangle_B = |\psi\rangle_{AB} \langle\psi|$$

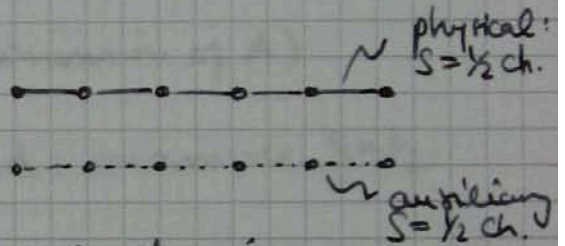
and

$$|\psi\rangle_{AB} = \sum_{\alpha} \sqrt{w_{\alpha}} |\alpha\rangle_A |\alpha\rangle_B$$

$$\hat{S}_A = \sum_{\alpha} w_{\alpha} |\alpha\rangle_A \langle\alpha|_A \Rightarrow |\psi\rangle_{AB} = \sum_{\alpha} \sqrt{w_{\alpha}} |\alpha\rangle_A |\alpha\rangle_B$$

purification of \hat{S}_A :

"double" physical system:



so, e.g., a density operator on a spin chain can be mapped to a pure state on a spin ladder.

calculation of observables connects seamlessly to pure state case:

$$\begin{aligned} \langle \hat{O} \rangle_{\hat{S}_A} &= \text{tr}_A (\hat{O}_A \hat{S}_A) \\ &= \text{tr}_A \hat{O}_A \text{tr}_B \hat{S}_{AB} \\ &= \text{tr}_A \text{tr}_B \hat{O}_A |\psi\rangle_{AB} \langle\psi| \\ &= \langle \psi | \hat{O}_A | \psi \rangle_{AB} \end{aligned}$$

- no new routine needed!

problem: $\hat{\rho}_A = \sum w_\alpha |\alpha\rangle_A \langle\alpha|$

unknown for general complex many-body problem \Rightarrow naive purification fails

solution for thermal density operators:

① infinite-temperature ($\beta=0$) density operator

$$\hat{\rho}_A(0) = \frac{1}{Z(0)} e^{-0 \cdot \hat{H}_A} = \frac{1}{Z(0)} \cdot \hat{\mathbb{1}}$$

$$Z(0) = \text{tr}_A \hat{\mathbb{1}} = \text{dim } D_A \quad (\text{dimension of } A)$$

but $\hat{\rho}_A(0)$ is easily constructed: example $S=1/2$



$$\hat{\rho}_A(0) = \bigotimes_i \hat{\rho}_i(0) \quad (\text{for } \beta=0 \text{ only})$$

$$\hat{\rho}_i(0) = \frac{1}{\sqrt{2}} \frac{1}{2} (|\uparrow\rangle_i \langle\uparrow| + |\downarrow\rangle_i \langle\downarrow|)$$

D_i : local dimension properly normalized!

purification:

$$|\psi\rangle_{AB}(0) = \bigotimes_i |\psi\rangle_{AB,i}(0) \quad (\text{for } \beta=0 \text{ only})$$

$$|\psi\rangle_{AB,i}(0) = \frac{1}{\sqrt{2}} (|\uparrow\uparrow\rangle_{A_i B_i} + |\downarrow\downarrow\rangle_{A_i B_i})$$

● A \rightarrow ● A physical
 ● B auxiliary

not unique: also $\frac{1}{\sqrt{2}} (|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle), \dots$

feasible - advantageous if good quantum numbers used

② imaginary time-evolution

up to normalization:

$$\hat{S}_A(\beta) \propto e^{-\beta \hat{H}} = e^{-\beta \hat{H}/2} \hat{\mathbb{1}} e^{-\beta \hat{H}/2}$$

$$\propto e^{-\beta \hat{H}/2} \hat{\rho}_A(0) e^{-\beta \hat{H}/2}$$

$$= e^{-\beta \hat{H}/2} \text{tr}_B(|\psi\rangle_{AB}(0) \langle \psi|_{AB}(0)) e^{-\beta \hat{H}/2}$$

Tracts only on A = $\text{tr}_B (e^{-\beta \hat{H}/2} |\psi\rangle_{AB}(0) \langle \psi|_{AB}(0) e^{-\beta \hat{H}/2})$

$$= \text{tr}_B (|\psi\rangle_{AB}(\beta) \langle \psi|_{AB}(\beta))$$

So, up to normalization, the purification of $\hat{S}_A(\beta)$ is given by

$$|\psi\rangle_{AB}(\beta) = \underbrace{e^{-\beta \hat{H}/2}}_{\text{by time-evolution}} \underbrace{|\psi\rangle_{AB}(0)}_{\text{by hand}}$$

actually numerically stable: errors are damped out exponentially!

normalization:

$$1 \stackrel{!}{=} \text{tr}_A \hat{S}_A(\beta) = \text{tr}_A \text{tr}_B |\psi\rangle_{AB}(\beta) \langle \psi|_{AB}(\beta)$$

$$= \langle \psi(\beta) | \psi(\beta) \rangle_{AB}$$

simply by normalizing $|\psi(\beta)\rangle_{AB}$

monitoring normalization factors gives $\frac{Z(\beta)}{Z(0)}$.

③ dynamical quantities by real-time evolution:

$$\begin{aligned}
 & \langle \hat{O}_1(t) \hat{O}_2(0) \rangle_{\hat{\rho}_A(\beta)} \\
 &= \text{tr}_A \hat{O}_1(t) \hat{O}_2(0) \hat{\rho}_A(\beta) \\
 &= \text{tr}_A \text{tr}_B \hat{O}_1(t) \hat{O}_2(0) |\Psi_{AB}^{(\beta)}\rangle \langle \Psi_{AB}^{(\beta)}| \\
 &= \langle \Psi_{AB}^{(\beta)} | \hat{O}_1(t) \hat{O}_2(0) | \Psi_{AB}^{(\beta)} \rangle_{AB} \\
 &= \langle \Psi(\beta) | \underbrace{e^{+i\hat{H}_A t} \hat{O}_1 e^{-i\hat{H}_A t}}_{\hat{O}_1(t)} \underbrace{\hat{O}_2}_{\hat{O}_2(0)} | \Psi(\beta) \rangle_{AB} \\
 &= \langle \Psi(\beta; t) | \hat{O}_1 | \Psi(\beta; t) \rangle_{AB} \quad | \Psi(\beta; 0) \rangle_{AB}
 \end{aligned}$$

again, no change with respect to old algorithm!

All so far holds independent of state representation (i.e. use of matrix product states)!

Last step: represent $|\Psi\rangle_{AB}(0)$ as MPS.

$|\Psi\rangle_{AB}(0) = \bigotimes_i |\Psi\rangle_{AB;i}(0) \Rightarrow$ "mean field" or "product state"

\Rightarrow matrix dimension ①

$|\Psi\rangle_{AB;i}(0) = \frac{1}{\sqrt{d}} \sum_{\sigma_i, \tau_i} |\sigma_i, \tau_i\rangle \equiv \sum_{\sigma_i, \tau_i} A_i^{\sigma_i, \tau_i} |\sigma_i, \tau_i\rangle \Rightarrow$

phys. auxiliary

$A_i^{\sigma_i, \tau_i} = \frac{1}{\sqrt{d}} \delta_{\sigma_i, \tau_i}$

\uparrow
d² matrices

-that's it! we can construct state by hand and start!