tDMRG   Schollwoeck

1

Zeitentwicklung eines Zustands in MPS-Form

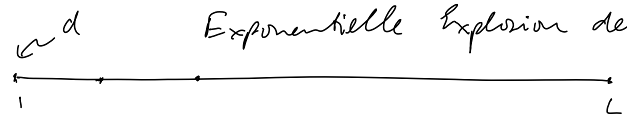
$\hat{H}$ $\quad |\psi(t)\rangle = e^{-i\hat{H}t}\,|\psi(0)\rangle \qquad \hbar = 1$

$$\hat{H}|n\rangle = E_n |n\rangle$$

$$|\psi(t)\rangle = \sum_n e^{-i\hat{H}t}\,|n\rangle\overbrace{\langle n|\psi(0)\rangle}^{c_n}$$

$$= \sum_n e^{-iE_nt}\,c_n|n\rangle$$

Exponentielle Explosion der Dimension: d^L



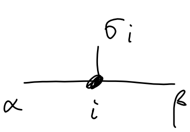
2

Zeitentwicklung eines MPS

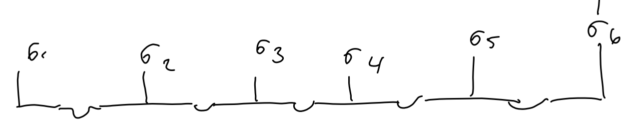
$$|\psi\rangle = \sum_{\underline{\sigma}} A^{\sigma_1}_{1\times D}\,A^{\sigma_2}_{D\times D}\,A^{\sigma_3}_{D\times D}\cdots A^{\sigma_L}_{D\times 1}\,|\underline{\sigma}\rangle$$

$\underline{\sigma} = \{\sigma_1 \ldots \sigma_L\}$

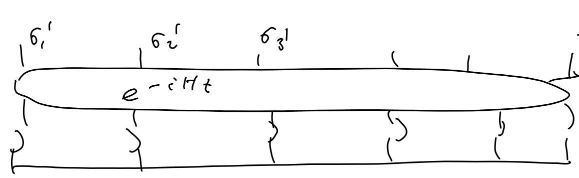
$A^{\sigma_i}_{\alpha\beta} =$



$|\psi\rangle =$



$e^{-iHt}|\psi\rangle$



$=$

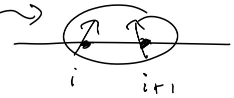
$=$

$$\langle\sigma'|\psi(t)\rangle = \sum_{\underline{\sigma}} \langle\underline{\sigma}'|e^{-iHt}|\underline{\sigma}\rangle\langle\underline{\sigma}|\psi(0)\rangle$$

Trick: meisten H's sind kurzreichweitig! ③

$$\hat{H} = \sum_{i=1}^{L-1} \underline{S}_i \cdot \underline{S}_{i+1} = \sum_i \frac{1}{2}\left(S_i^+ S_{i+1}^- + h.c. + S_i^z S_{i+1}^z \right)$$

$$= \sum_{i=1}^{L-1} \hat{h}_i$$



$$e^{-i\hat{H}t} = \prod_{j=1}^{N} e^{-i\hat{H}\Delta t} \qquad \Delta t = t/N$$

$$= \prod_{j=1}^{N} e^{-i\sum_i \hat{h}_i \Delta t} \overset{!}{=} \prod_{j=1}^{N} \prod_{i=1}^{L-1} e^{-i h_i \Delta t}$$

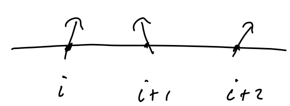
$e^{a+b} = e^a e^b$

$\hat{h}_{0.01}$

lokal

Aber: $e^{\hat{A}+\hat{B}} = e^{\hat{A}} e^{\hat{B}} e^{\frac{1}{2}[\hat{A},\hat{B}]}$ ④

und $\underbrace{[\hat{h}_i, \hat{h}_{i+1}]}_{\text{kommutieren nicht:}} \neq 0$



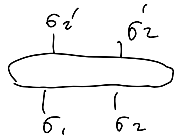
$$e^{i(h_1 \Delta t + h_2 \Delta t)} = e^{i h_1 \Delta t} e^{i h_2 \Delta t} \underbrace{e^{-\frac{1}{2}\underbrace{[h_1, h_2]}_{\text{const}}(\Delta t)^2}}_{\approx 1 - \frac{1}{2}\underbrace{[h_1,h_2](\Delta t)^2}_{\text{Fehler}}}$$

Wähle Δt klein $\Rightarrow$ Fehler klein!!

Nach $\frac{t}{\Delta t}$ Schritten: Fehler der Ordnung $\frac{t}{\Delta t}(\Delta t)^2 \sim \Delta t \to 0$

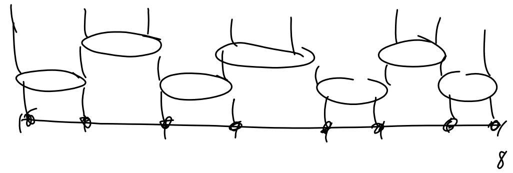
"Trotter-Zerlegung 1. Ordnung (in Δt)" Praxis: 4. Ordnung!

$e^{-i\hat{h}\Delta t}$:



, für $s = 1/2$, $|\uparrow\rangle$, $|\downarrow\rangle$ $d = 2$

$e^{-i\hat{h}t} = 4\times 4$ matrix, $\Rightarrow$ diagonalisierbar



} , infinitesimaler Zeitschritt Δt

$$A^{\sigma_1\sigma_1', \sigma_2\sigma_2'} \equiv U^{\sigma_1'\sigma_2', \sigma_1\sigma_2} \equiv \langle \sigma_1'\sigma_2' | e^{-ih\Delta t} | \sigma_1\sigma_2\rangle$$

Lineare Algebra : Singulärwertzerlegung:

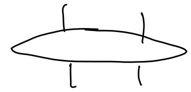
$$A = U\ D\ V$$

unitär → U ; D ← nicht-negativ ; V ← unitär

$$A^{\sigma_1\sigma_1', \sigma_2\sigma_2'} = \sum_{k=1}^{d^2} \underbrace{U^{\sigma_1\sigma_1', k}\sqrt{D^{k,k}}}\ \sqrt{D^{k,k}}\ V^{k, \sigma_2\sigma_2'}$$

$$\sum_{k=1}^{d^2} O_{1,k}^{\sigma_1'\sigma_1} \cdot O_{k,1}^{\sigma_2'\sigma_2}$$

$e^{-i\hat{h}\Delta t}$ =



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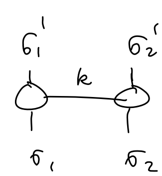
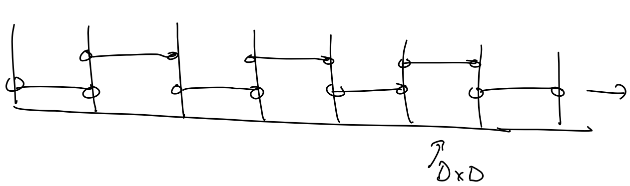
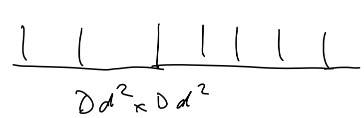
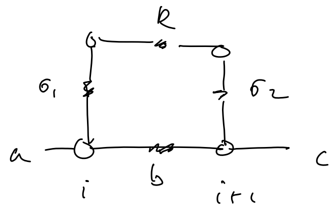


Zeitschritt:







$$= \sum_{\sigma_1\sigma_2} \sum_{b=1}^{D} \sum_{k=1}^{d^2} O^{\sigma_1'\sigma_1}_{1k} \, O^{\sigma_2\sigma_2'}_{k1} \, A^{\sigma_1}_{ab} \, A^{\sigma_2}_{bc}$$

$$= \sum_{b=1}^{D} \sum_{k=1}^{d^2} \left(\sum_{\sigma_1} O^{\sigma_1'\sigma_1}_{1k} A^{\sigma_1}_{ab} \right) \left(\sum_{\sigma_2} O^{\sigma_2\sigma_2'}_{k1} A^{\sigma_2}_{bc} \right)$$

$$\equiv B^{\sigma_1'}_{a(bk)} \qquad B^{\sigma_2'}_{(bk)c}$$

$$\uparrow\uparrow \; D \; d^2 \qquad \uparrow\uparrow \; D \; d^2$$

nach Zeitschritt Δt: $\quad |\psi(0)\rangle \longrightarrow |\psi(\Delta t)\rangle$

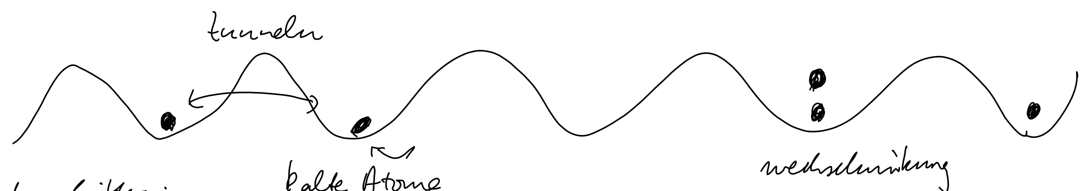
Dim D MPS $\qquad$ Dim Dd^2 MPS

Jeder Schritt lässt sich leicht programmieren!
Nach jedem Schritt, trunkieren:

$$\left\| \, |\psi_{Dd^2}(\Delta t)\rangle - |\psi_D(\Delta t)\rangle \, \right\|^2 \quad \text{minimal} \qquad \text{DMRG!}$$

Ausgangspunkt $\qquad$ gesuchter Endpunkt.

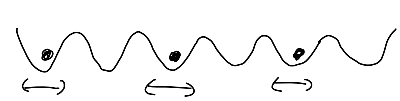
Anwendungen: ultrakalten Atomgase:



optisches Gitter:

$T \leq 100$ nK

- Quantenphasenübergänge
- Relaxation



- Quantenstatistik außerhalb des Gleichgewichts.