(Almost) 25 Years of DMRG - What Is It About?

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Concerning your talk (65min + 10 min for questions) we would prefer if you could provide a broad introduction into DMRG. This may include in particular:
1) Brief historic discussion
2) Why does one use DMRG?
3) Concept of entanglement and correlations and area laws
5) Details on how to implement DMRG/How does it work?
6) benchmark calculations and comparison to results obtained by resorting to different methods
7) comments on scaling behavior (w.r.t. number of electrons, dimension of truncated 1-particle Hilbert space and "bond length \( \chi \))
8) Open problems

While working out your presentation please be aware of related talks (for instance the one by Markus Reiher, "DMRG in Quantum Chemistry", building up on your presentation).
fundamental problem of solid state

- what do we need DMRG for? problem class:

**fundamental Hamiltonian** (without lattice vibrations...!):

\[
H = \sum_{j=1}^{e} \left( \frac{\mathbf{p}_j^2}{2m_e} + \frac{1}{2} \frac{1}{4\pi\varepsilon_0} \frac{q_e^2}{|\mathbf{r}_i - \mathbf{r}_j|} \right) + \sum_{j} V_{\text{eff}}(\mathbf{r}_j)
\]

kinetic energy  electron-electron interaction  lattice potential

- we don’t know how to solve the Schrödinger equation!

**problem**: electron-electron interactions
many-body problem of solid state I

- scenario I
  valence electrons well delocalized
  interactions well screened

  - electron cloud
  - lattice potential

  - energy
  - DOS
  - half-filled
  - conductor

- many metals, semiconductors: single-electron picture OK

  - density functional theory (DFT)
many-body problem of solid state II

- scenario II
  - valence electrons tightly bound
  - strong local interactions

- lattice potential

- many particle picture: strongly correlated materials

- model Hamiltonian methods - here DMRG comes in!

- insulator
  - eg. high-Tc parent compounds
why strong correlations?

0 dimensions
- magnetic impurity physics
- quantum dots

1 dimension
- spin chains & ladders
- Luttinger liquid

2 dimensions
- frustrated magnets
- high-$T_c$ superconductors

3 dimensions
- realistic modelling:
  - transition metal, rare earth compounds

realistic modelling:
- transition metal, rare earth compounds
transition metal oxides and rare earths

belated filling of the d- and f-shells
valence electrons quite tightly bound
cold atoms in optical lattices

- ultra-cold bosonic atoms form Bose-Einstein condensate

- standing laser waves: optical lattice
  - Greiner et al (Munich group), Nature ’02

- extension to fermions (spin = hyperfine levels)
  e.g. M. Köhl et al (Esslinger group), PRL ’05

interaction tunable via lattice depth

bosonic Hubbard model
tunability

- **controlled tuning** of interaction $U/t$ in time via lattice depth
- **adiabatic** change of $U/t$: quantum phase transition
  - momentum distribution function

\[ \begin{array}{cccccc}
\text{a} & \text{b} & \text{c} & \text{d} & \text{e} & \text{f} \\
\text{g} & \text{h} & \text{superfluid} & \text{adiabatic increase of interaction } U & \text{Mott insulator} \\
\end{array} \]

- **sudden** change of $U/t$ to Mott insulator: collapse and revival

\[ \begin{array}{cccccc}
\text{a} & \text{b} & \text{c} & \text{d} & \text{e} & \text{f} \\
\text{g} & \text{h} & \text{time} & \text{Mott insulator} \\
\end{array} \]

- „state engineering“ for generic quantum many-body systems
compression of information

- compression of information necessary and desirable
  - diverging number of degrees of freedom
  - emergent macroscopic quantities: temperature, pressure, ...

- classical spins
  - thermodynamic limit: $N \to \infty \quad 2N$ degrees of freedom (linear)

- quantum spins
  - superposition of states
  - thermodynamic limit: $N \to \infty \quad 2^N$ degrees of freedom (exponential)
classical simulation of quantum systems

- compression of exponentially diverging Hilbert spaces
- what can we do with classical computers?
  - exact diagonalizations
    - limited to small lattice sizes: 40 (spins), 20 (electrons)
  - stochastic sampling of state space
    - quantum Monte Carlo techniques
    - negative sign problem for fermionic systems
  - physically driven selection of subspace: decimation
    - variational methods
    - renormalization group methods
  - how do we find the good selection? DMRG!
DMRG: a young adult


> "This new formulation appears extremely powerful and versatile, and we believe it will become the leading numerical method for 1D systems; and eventually will become useful for higher dimensions as well."

~2004  old insight „DMRG is linked to MPS (Matrix Product States)“

goes viral


White, Feiguin, PRL 93, 076401 (2004), Verstraete, Porras, Cirac, PRL 93, 227205 (2004),

(some) reviews:

U. Schollwöck, Rev. Mod. Phys. 77, 259 (2005) - „old“ statistical physics perspective, applications
matrix product states: definitions

quantum system living on $L$ lattice sites

d local states per site $\{\sigma_i\}, \quad i \in \{1, 2, \ldots, L\}$

example: spin 1/2: $d=2 \quad |\uparrow\rangle, |\downarrow\rangle$

Hilbert space:

$$\mathcal{H} = \bigotimes_{i=1}^{L} \mathcal{H}_i \quad \mathcal{H}_i = \{|1_i\rangle, \ldots, |d_i\rangle\}$$

most general state (not necessarily 1D):

$$|\psi\rangle = \sum_{\sigma_1, \ldots, \sigma_L} c^{\sigma_1 \ldots \sigma_L} |\sigma_1 \ldots \sigma_L\rangle$$

abbreviations: $\{\sigma\} = \sigma_1 \ldots \sigma_L \quad c^{\{\sigma\}}$
(matrix) product states

exponentially many coefficients!
standard approximation: **mean-field approximation**

\[ c^{\sigma_1 \ldots \sigma_L} = c^{\sigma_1} \cdot c^{\sigma_2} \cdot \ldots \cdot c^{\sigma_L} \quad d^L \rightarrow dL \text{ coefficients} \]

often useful, but misses essential quantum feature: **entanglement**

consider 2 spin 1/2: \( \mathcal{H} = \mathcal{H}_1 \otimes \mathcal{H}_2 \quad \mathcal{H}_i = \{ | \uparrow_i \rangle, | \downarrow_i \rangle \} \)

\[ |\psi\rangle = c^{\uparrow\uparrow} | \uparrow\uparrow \rangle + c^{\uparrow\downarrow} | \uparrow\downarrow \rangle + c^{\downarrow\uparrow} | \downarrow\uparrow \rangle + c^{\downarrow\downarrow} | \downarrow\downarrow \rangle \]

**singlet state:** \[ |\psi\rangle = \frac{1}{\sqrt{2}} | \uparrow\downarrow \rangle - \frac{1}{\sqrt{2}} | \downarrow\uparrow \rangle \quad c^{\uparrow\downarrow} \neq c^{\uparrow} c^{\downarrow} \]

generalize product state to **matrix product state:**

\[ c^{\sigma_1} \cdot c^{\sigma_2} \cdot \ldots \cdot c^{\sigma_L} \rightarrow M^{\sigma_1} \cdot M^{\sigma_2} \cdot \ldots \cdot M^{\sigma_L} \]
matrix product states

useful generalization even for matrices of dimension 2: AKLT (Affleck-Kennedy-Lieb-Tasaki) model

general matrix product state (MPS):

$$|\psi\rangle = \sum_{\sigma_1, \ldots, \sigma_L} M^{\sigma_1} M^{\sigma_2} \ldots M^{\sigma_L} |\sigma_1 \sigma_2 \ldots \sigma_L\rangle$$

matrix dimensions:

$$(1 \times D_1), (D_1 \times D_2), \ldots, (D_{L-2} \times D_{L-1}), (D_{L-1} \times 1)$$

non-unique: gauge degree of freedom

$$XX^{-1} = 1 \quad M^{\sigma_i} \to M^{\sigma_i} X \quad M^{\sigma_{i+1}} \to X^{-1} M^{\sigma_{i+1}}$$
Why are matrix product states interesting?

- any state can be represented as an MPS (even if numerically inefficiently)
- MPS are hierarchical: matrix size related to degree of entanglement
- MPS emerge naturally in renormalization groups
- MPS can be manipulated easily and efficiently
- MPS can be searched efficiently: which MPS has lowest energy for a given Hamiltonian?
singular value decomposition (SVD)

key workhorse of MPS manipulation and generally very useful!

general matrix $A$ of dimension $(m \times n)$ \hspace{1cm} $k = \min(m, n)$

then \hspace{1cm} $A = USV^\dagger$

with $U$ \hspace{0.5cm} \dim. \hspace{0.5cm} (m \times k)$ \hspace{1cm} $U^\dagger U = I$ (ON col); if $m = k$: $UU^\dagger = I$

$S$ \hspace{0.5cm} \dim. \hspace{0.5cm} (k \times k)$ \hspace{0.5cm} diagonal: $s_1 \geq s_2 \geq s_3 \geq \ldots$ non-neg.: $s_i \geq 0$

\hspace{0.5cm} singular values, non-vanishing $= \text{rank } r \leq k$

$V^\dagger$ \hspace{0.5cm} \dim. \hspace{0.5cm} (k \times n) \hspace{1cm} $V^\dagger V = I$ (ON row); if $k = n$: $VV^\dagger = I$

popular notation: \text{(left) singular vectors} $|u_i\rangle$

$U = [|u_1\rangle |u_2\rangle \ldots]$
**SVD and EVD (eigenvalue decomp.)**

singular value decomposition (always possible):

\[ A = U S V^\dagger \quad s_1 \geq s_2 \geq s_3 \geq \ldots \quad s_i \geq 0 \]

eigenvalue decomposition (for special square matrices):

\[ A U = U \Lambda \quad \lambda_i \quad U = [|u_1\rangle|u_2\rangle \ldots] \quad \text{eigenvectors} \]

connection by „squaring“ \( A \): \( A^\dagger A \quad AA^\dagger \)

\[ AA^\dagger = U S V^\dagger V S U^\dagger = U S^2 U^\dagger \Rightarrow (AA^\dagger)U = U S^2 \]
\[ A^\dagger A = V S U^\dagger U S V^\dagger = V S^2 V^\dagger \Rightarrow (A^\dagger A)V = V S^2 \]

eigenvalues = singular values squared
eigenvectors = left, right singular vectors
any state can be decomposed as MPS

reshape coefficient vector into matrix of dimension \((d \times d^{L-1})\) and SVD:
\[ c^{\sigma_1 \sigma_2 \ldots \sigma_L} \rightarrow \Psi_{\sigma_1, \sigma_2 \ldots \sigma_L} = \sum_{a_1} U_{\sigma_1, a_1} S_{a_1, a_1} V_{a_1, \sigma_2 \ldots \sigma_L}^\dagger \]
slice \(U\) into \(d\) row vectors:
\[ U_{\sigma_1, a_1} \rightarrow \{ A_{\sigma_1}^1 \} \quad \text{with} \quad A_{1, a_1}^{\sigma_1} = U_{\sigma_1, a_1} \]
rearrange SVD result:
\[ c^{\sigma_1 \sigma_2 \ldots \sigma_L} = \sum_{a_1} A_{1, a_1}^{\sigma_1} c_{a_1 \sigma_2 \sigma_3 \ldots \sigma_L} \quad c_{a_1 \sigma_2 \sigma_3 \ldots \sigma_L} = S_{a_1, a_1} V_{a_1, \sigma_2 \ldots \sigma_L}^\dagger \]
reshape coefficient vector into matrix of dim. \((d^2 \times d^{L-2})\) and SVD:
\[ c_{a_1 \sigma_2 \sigma_3 \ldots \sigma_L} \rightarrow \Psi_{a_1 \sigma_2, \sigma_3 \ldots \sigma_L} = \sum_{a_2} U_{a_1 \sigma_2, a_2} S_{a_2, a_2} V_{a_2, \sigma_3 \ldots \sigma_L}^\dagger \]
slice \(U\) into \(d\) matrices:
\[ A_{a_1, a_2}^{\sigma_2} = U_{a_1 \sigma_2, a_2} \]
rearrange SVD result:
\[ c^{\sigma_1 \sigma_2 \ldots \sigma_L} = \sum_{a_1, a_2} A_{1, a_1}^{\sigma_1} A_{a_1, a_2}^{\sigma_2} c_{a_2 \sigma_3 \sigma_3 \ldots \sigma_L} \quad \text{and so on!} \]
bipartition of „universe“ AB into subsystems A and B:

\[ \{ |i\rangle_A \} \quad \{ |j\rangle_B \} \]

1 \quad \ell \quad \ell + 1 \quad L

\[ \dim \mathcal{H}_A \dim \mathcal{H}_B \]

\[ |\psi\rangle = \sum_{i=1}^{\dim \mathcal{H}_A} \sum_{j=1}^{\dim \mathcal{H}_B} \psi_{ij} |i\rangle_A |j\rangle_B \]

read coefficients as matrix entries, carry out SVD:

\[ |\psi\rangle = \sum_{\alpha=1}^{r} s_{\alpha} |\alpha\rangle_A |\alpha\rangle_B \]

Schmidt decomposition

\[ |\alpha\rangle_A = \sum_{i=1}^{\dim \mathcal{H}_A} U_{i\alpha} |i\rangle_A \]

\[ |\alpha\rangle_B = \sum_{j=1}^{\dim \mathcal{H}_B} V_{j\alpha}^* |j\rangle_B \]

orthonormal sets!
bipartite entanglement in MPS

measuring bipartite entanglement $S$: reduced density matrix

$$|\psi\rangle = \sum \psi_{ij} |i\rangle |j\rangle \quad \hat{\rho} = |\psi\rangle \langle \psi| \rightarrow \hat{\rho}_S = \text{Tr}_E \hat{\rho}$$

$$S = -\text{Tr}[\hat{\rho}_S \log_2 \hat{\rho}_S] = -\sum w_\alpha \log_2 w_\alpha$$

arbitrary bipartition

use Schmidt decomposition

reduced density matrix and bipartite entanglement

$$\hat{\rho}_S = \sum w_\alpha |\alpha_S\rangle \langle \alpha_S|$$

$$S = -\sum w_\alpha \log_2 w_\alpha \leq \log_2 M$$

codable maximum
entanglement scaling: gapped systems

- entanglement grows with system surface: area law
- for ground states! Eisert, Cramer, Plenio, RMP (10)

\[ S(L) \sim c \text{st.} \quad S(L) \sim L \quad S(L) \sim L^2 \]

\[ S \leq \log_2 M \Rightarrow M \geq 2^S \]

\[ M > 2^{c\text{st.}} \quad M > 2^L \quad M > 2^{L^2} \]
Hilbert space size: just an illusion?

- random state in Hilbert space: entanglement entropy extensive

- expectation value for entanglement entropy extensive and maximal

- states with non-extensive entanglement set of measure zero

- merit of MPS: parametrize this set efficiently!

ground states are here!
work with MPS: diagrammatics

matrix: vertical lines = physical states, horizontal lines = matrix indices

left edge               bulk                 right edge   complex conjug.

rule: connected lines are contracted (multiplied and summed)

matrix product state in graphical representation
block growth, decimation and MPS

RG schemes: grow blocks while decimating basis

\[ |a_\ell\rangle = \sum_{a_{\ell-1}, \sigma_\ell} \langle a_{\ell-1}, \sigma_\ell | a_\ell \rangle |a_{\ell-1}\rangle |\sigma_\ell\rangle \equiv \sum_{a_{\ell-1}, \sigma_\ell} M^\sigma_{a_{\ell-1}, a_\ell} |a_{\ell-1}\rangle |\sigma_\ell\rangle \]

simple rearrangement of expansion coefficients into matrices:

\[ M^\sigma_{a_{\ell-1}, a_\ell} = \langle a_{\ell-1}, \sigma_\ell | a_\ell \rangle \]

recursion easily expressed as matrix multiplication:

\[ |a_\ell\rangle = \sum_{\sigma_1, \ldots, \sigma_\ell} (M^{\sigma_1} M^{\sigma_2} \ldots M^{\sigma_\ell})_{1, a_\ell} |\sigma_1 \sigma_2 \ldots \sigma_\ell\rangle \]
(left and right) normalization

both state decomposition and block growth scheme give special gauge

\[ \delta_{a'_\ell, a_\ell} = \langle a'_\ell | a_\ell \rangle = \sum_{a'_{\ell-1}\sigma_{\ell}^* a_{\ell-1}\sigma_{\ell}} \langle a'_{\ell-1} \sigma_{\ell} | a_{\ell-1} \sigma_{\ell} \rangle \]

\[ = \sum_{a_{\ell-1}\sigma_{\ell}} M_{a_{\ell-1}, a'_{\ell}} \sigma_{\ell}^* M_{a_{\ell-1}, a'_{\ell}} \sigma_{\ell} \]

left normalization (called A); more compact representation:

\[ I = \sum_{\sigma_{\ell}} M_{\sigma_{\ell}}^\dagger M_{\sigma_{\ell}} \equiv \sum_{\sigma_{\ell}} A_{\sigma_{\ell}}^\dagger A_{\sigma_{\ell}} \]

right normalization (called B):

\[ I = \sum_{\sigma_{\ell}} B_{\sigma_{\ell}} B_{\sigma_{\ell}}^\dagger \]

mixed normalization:

AAAAAAMBBBBBBB
matrix product operators (MPO)

general operator:

\[ \hat{O} = \sum_{\{\sigma\}} \sum_{\{\sigma'\}} C^{\sigma_1 \ldots \sigma_L, \sigma'_1 \ldots \sigma'_L} |\sigma_1 \ldots \sigma_L\rangle \langle \sigma'_1 \ldots \sigma'_L| \]

rearrange indices:

\[ C^{\sigma_1 \ldots \sigma_L, \sigma'_1 \ldots \sigma'_L} \rightarrow C^{\sigma_1 \sigma'_1 \sigma_2 \sigma'_2 \ldots \sigma_L \sigma'_L} \]

„mean-field“ very useful: \[ C^{\sigma_1 \sigma'_1 \sigma_2 \sigma'_2 \ldots \sigma_L \sigma'_L} \rightarrow C^{\sigma_1 \sigma'_1} \cdot C^{\sigma_2 \sigma'_2} \cdot \ldots \cdot C^{\sigma_L \sigma'_L} \]

\[ \hat{S}^z_i \rightarrow \hat{I}_1 \otimes \hat{I}_2 \otimes \ldots \otimes \hat{S}^z_i \otimes \ldots \otimes \hat{I}_L \]

\[ C^{\sigma_1 \sigma'_1 \sigma_2 \sigma'_2 \ldots \sigma_L \sigma'_L} = \delta_{\sigma_1, \sigma'_1} \cdot \delta_{\sigma_2, \sigma'_2} \cdot \ldots \cdot (\hat{S}^z)_{\sigma_i, \sigma'_i} \cdot \ldots \cdot \delta_{\sigma_L, \sigma'_L} \]

matrix product operator:

\[ \hat{O} = \sum_{\{\sigma\}} \sum_{\{\sigma'\}} M^{\sigma_1 \sigma'_1} M^{\sigma_2 \sigma'_2} \ldots M^{\sigma_L \sigma'_L} |\sigma_1 \ldots \sigma_L\rangle \langle \sigma'_1 \ldots \sigma'_L| \]
applying an MPO to an MPS

graphical representation with ingoing and outgoing physical states:

\[ \tilde{M}_{(ab),(a'b')}^{\sigma_i} = \sum_{\sigma_i'} N_{aa'}^{\sigma_i \sigma_i'} M_{bb'}^{\sigma_i'} \]
problem: matrix dimensions of MPS grow under MPO application

solution: compression of matrices with minimal state distance

assume state is given in mixed normalized form:

$$|\psi\rangle = \sum_{\{\sigma\}} A^{\sigma_1} A^{\sigma_2} \ldots A^{\sigma_\ell} M^{\sigma_{\ell+1}} B^{\sigma_{\ell+2}} \ldots B^{\sigma_L} |\sigma_1 \ldots \sigma_L\rangle$$

stack $M$ matrices into one:

$$M_{a_\ell, \sigma_{\ell+1} a_{\ell+1}} = M^{\sigma_{\ell+1}}_{a_\ell, a_{\ell+1}}$$

carry out SVD, and use results: $M = USV^\dagger$

$$A^{\sigma_\ell} \leftarrow A^{\sigma_\ell} U$$

orthonormality of $U$!

$$B^{\sigma_{\ell+1}}_{a_\ell, a_{\ell+1}} = V^\dagger_{a_\ell, \sigma_{\ell+1} a_{\ell+1}}$$
normalization and compression II

now introduce orthonormal states:

\[ |a_\ell\rangle_A := \sum_{\sigma_1, \ldots, \sigma_\ell} (A^{\sigma_1} \ldots A^{\sigma_\ell})_{1,a_\ell} |\sigma_1 \ldots \sigma_\ell\rangle \]

\[ |a_\ell\rangle_B := \sum_{\sigma_{\ell+1}, \ldots, \sigma_L} (B^{\sigma_{\ell+1}} \ldots B^{\sigma_L})_{a_\ell,1} |\sigma_{\ell+1} \ldots \sigma_L\rangle \]

read off Schmidt decomposition:  

\[ |\psi\rangle = \sum_{a_\ell} s_{a_\ell} |a_\ell\rangle_A |a_\ell\rangle_B \]

compress matrices \( A^{\sigma_\ell}, B^{\sigma_{\ell+1}} \) by keeping \( D \) largest singular values

\[ A^{\sigma_\ell} S \rightarrow M^{\sigma_\ell} \]

\[ |\psi\rangle = \sum_{\{\sigma\}} A^{\sigma_1} A^{\sigma_2} \ldots A^{\sigma_{\ell-1}} [\boxed{M^{\sigma_\ell}} B^{\sigma_{\ell+1}} \ldots B^{\sigma_L}] |\sigma_1 \ldots \sigma_L\rangle \]

mixed rep shifted by 1 site: sweep through chain; also normalization
time-evolution

assume initial state in MPS representation; time evolution:

\[ |\psi(t)\rangle = e^{-i\hat{H}t} |\psi(0)\rangle \]

how to express the evolution operator as an MPO?

one solution: **Trotterization** of evolution operator into small time steps

\[ N \to \infty \quad \tau \to 0 \quad N\tau = T \quad \tau \sim 0.01 \]

Heisenberg model:

\[ \hat{H} = \sum_{i=1}^{L-1} \hat{h}_i \quad \hat{h}_i = \mathbf{S}_i \cdot \mathbf{S}_{i+1} \]

\[ e^{-i\hat{H}T} = \prod_{i=1}^{N} e^{-i\hat{H}_i \tau} = \prod_{k=1}^{N} e^{-i \sum_{i=1}^{L-1} \hat{h}_i \tau} \]

first-order Trotter decomposition
Trotter decomposition

calculation of $e^{-i\hat{h}_i\tau}$ as $(d^2 \times d^2)$ matrix:

$$H_i U = U \Lambda \quad H_i = U \Lambda U^\dagger \quad \Rightarrow \quad e^{-iH_i\tau} = U e^{-i\Lambda \tau} U^\dagger = U \cdot \text{diag}(e^{-i\lambda_1\tau}, e^{-i\lambda_2\tau}, \ldots) \cdot U^\dagger$$

problem: exponential does not factorize if operators do not commute

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

but error is negligible as $\tau \to 0$

$$[\hat{h}_i\tau, \hat{h}_{i+1}\tau] \propto \tau^2$$

convenient rearrangement:

$$\hat{H} = \hat{H}_{\text{odd}} + \hat{H}_{\text{even}}; \quad \hat{H}_{\text{odd}} = \sum_{i=1} \hat{h}_{2i-1}, \quad \hat{H}_{\text{even}} = \sum_{i} \hat{h}_{2i}$$

$$e^{-i\hat{H}T} = e^{-i\hat{H}_{\text{even}}\tau} e^{-i\hat{H}_{\text{odd}}\tau}; \quad e^{-i\hat{H}_{\text{even}}\tau} = \prod_{i} e^{-i\hat{h}_{2i}\tau}, \quad e^{-i\hat{H}_{\text{odd}}\tau} = \prod_{i} e^{-i\hat{h}_{2i-1}\tau}$$
bring local evolution operator into MPO form:

$$U^{\sigma_1\sigma_2,\sigma_1'\sigma_2'} = \langle \sigma_1\sigma_2|e^{-i\hat{H}_1\tau}|\sigma_1'\sigma_2'\rangle$$

$$U^{\sigma_1\sigma_2,\sigma_1'\sigma_2'} = \overline{U}_{\sigma_1\sigma_1',\sigma_2\sigma_2'} \overset{SVD}{=} \sum_b W_{\sigma_1\sigma_1',b}S_{b,b}W_{b,\sigma_2\sigma_2'}$$

$$= \sum_b M^{\sigma_1\sigma_1'}_{1,b} M^{\sigma_2\sigma_2'}_{b,1}$$

one time step: dimension grows as $d^2$

- apply one infinitesimal time step in MPO form
- compress resulting MPS
single-particle excitation

- quarter-filled Hubbard chain: $U/t=4$
- add spin-up electron at chain center at time=0
- measure charge and spin density

- separation of charge and spin

Kollath, US, Zwerger, PRL 95, 176401 (‘05)
real time evolution limited by entanglement growth:

\[ S(t) \leq S(0) + \nu t \quad \text{and} \quad S \sim \ln D \]

in the worst case, matrix dimensions grow exponentially!

**ground states** can be obtained by imaginary time evolution (SLOW!):

\[
|\psi\rangle = \sum_n c_n |n\rangle \quad \hat{H} |n\rangle = E_n |n\rangle \quad E_0 \leq E_1 \leq E_2 \leq \ldots
\]

\[
\lim_{\beta \to \infty} e^{-\beta \hat{H}} |\psi\rangle = \lim_{\beta \to \infty} \sum_n e^{-\beta E_n} c_n |n\rangle = \lim_{\beta \to \infty} e^{-\beta E_0} (c_0 |0\rangle + \sum_{n>0} e^{-\beta (E_n - E_0)} c_n |n\rangle)
\]

\[
= \lim_{\beta \to \infty} e^{-\beta E_0} c_0 |0\rangle
\]
overlaps

\[ \langle \psi(t) | \psi(0) \rangle \quad \langle S_i^z(t) \rangle = \langle \psi(t) | \hat{S}_i^z | \psi(t) \rangle \]

overlap contractions:

\[
\langle \phi | \psi \rangle = \sum_{\{\sigma\}} \sum_{\{\sigma'\}} \langle \{\sigma'\} | \tilde{M}^{\sigma_1'} \cdots \tilde{M}^{\sigma_L'} M^{\sigma_1} \cdots M^{\sigma_L} | \{\sigma\} \rangle = \sum_{\{\sigma\}} \tilde{M}^{\sigma_1} \cdots \tilde{M}^{\sigma_L} M^{\sigma_1} \cdots M^{\sigma_L}
\]

order of contractions: zip through the ladder; cost \( O(dL D^3) \)

two-point correlators: long-range or superposition of exponentials

\[
E^{(a_{\ell-1}a'_{\ell-1}), (a_{\ell},a'_{\ell})} := \sum_{\sigma_{\ell}} A^{\sigma_{\ell}*}_{a_{\ell-1},a_{\ell}} A^{\sigma_{\ell}}_{a'_{\ell-1},a'_{\ell}}
\]

hence: power laws only „by approximation“
dynamical quantum simulator

coherent dynamics! controlled preparation? local measurements?

first experiments:
period-2 superlattice
- double-well formation
- staggered potential bias

- pattern loading
- odd/even resolved measurement

(Fölling et al. (2007))

first theory proposals:
- prepare \( |\psi\rangle = |1, 0, 1, 0, 1, 0, \ldots\rangle \)
- switch off superlattice
- observe Bose-Hubbard dynamics

Cramer et al., PRL 101, 063001 (2008)
Flesch et al., PRA 78, 033608 (2008)
dynamical quantum simulator

Trotzky et al., Nat. Phys. 8, 325(2012)

45,000 atoms, $U=5.2$

momentum distribution
densities II

fully controlled relaxation in closed quantum system!

validation of dynamical quantum simulator

time range of experiment > 10 x time range of theory
real „analog computer“ that goes beyond theory

no free fit parameters!
nearest-neighbour correlators

\[ \langle \hat{b}^\dagger_n(t) \hat{b}_{n+1}(t) \rangle \]

- again three regimes
- \( U \approx 3 \): crossover regime
- at large \( U \), \( 1/U \) fit of relaxed correlator can be understood as perturbation to locally relaxed subsystems
currents

measurement: split in double wells, measure well oscillations

phase and amplitude

sloshing; no c.m. motion

current decay as power law?
nearest neighbour correlations

Visibility proportional to nearest neighbour correlations

Build-up of quantum coherence

General trend, I/U correct!

Momentum distribution
build-up of quantum coherence

long-time limit of nearest-neighbor correlations (here: visibility of momentum distribution)

discrepancy because original theory ignored trap:

\[ E_{\text{kin}} = -J \langle \hat{b}_i \hat{b}^\dagger_{i+1} + \hat{b}^\dagger_{i+1} \hat{b}_i \rangle \]
neutron scattering at $T>0$

structure function by neutron scattering (Broholm group)

high flux

precise lineshapes

- **problem:** experiment usually $T=4.2K$, energy scales at $J=O(10K)$
  definitely not at $T=0$!

- desired feature because of achievable field strengths:
  $H$ should be of order $J$ — rule of thumb $1K=1T$
finite-temperature dynamics

- purification

Density matrix of physical system:
Pure state of physical system plus auxiliary system

\[ \hat{\rho}_{phys} = \text{Tr}_{aux} |\psi\rangle \langle \psi| \]

- finite-temperature dynamics

Evolution of pure state in enlarged state space

Verstraete, Garcia-Ripoll, Cirac, PRL ‘04
purification and finite-T evolution

**purification:** any mixed state can be expressed by a pure state on a larger system (P: physical, Q: auxiliary state space)

\[
\hat{\rho}_P = \sum_n \rho_n |n\rangle_P \langle n| \quad |\psi\rangle_{PQ} = \sum_n \sqrt{\rho_n} |n\rangle_P |n\rangle_Q
\]

\[
\hat{\rho}_P = \text{tr}_Q |\psi\rangle_{PQ} P Q \langle \psi| \quad \text{simplest way: Q copy of P}
\]

**expectation values** as before:

\[
\langle \hat{O}_P \rangle_{\hat{\rho}_P} = \text{tr}_P \hat{O}_P \hat{\rho}_P = \text{tr}_P \hat{O}_P \text{tr}_Q |\psi\rangle_{PQ} P Q \langle \psi| = \text{tr}_P \hat{O}_P |\psi\rangle_{PQ} P Q \langle \psi| = P Q \langle \psi| \hat{O}_P |\psi\rangle_{PQ}
\]

**time evolution** as before:

\[
\hat{\rho}_P(t) = e^{-i\hat{H}t} \hat{\rho}_P e^{i\hat{H}t} = e^{-i\hat{H}t} \text{tr}_Q |\psi\rangle_{PQ} P Q \langle \psi| e^{+i\hat{H}t} = \text{tr}_Q |\psi(t)\rangle_{PQ} P Q \langle \psi(t)|
\]

\[
|\psi(t)\rangle_{PQ} = e^{-i\hat{H}t} |\psi\rangle_{PQ}
\]
time-evolution of thermal states

**Problem:** usually we do not have mixed state in eigenrepresentation

**Thermal states:** easy way out by imaginary t-evolution

\[
e^{-\beta \hat{H}} = e^{-\beta \hat{H}/2} \cdot \hat{I}_P \cdot e^{-\beta \hat{H}/2} = \text{tr}_Q e^{-\beta \hat{H}/2} |\rho_0\rangle_P Q \langle P Q | \rho_0 | e^{-\beta \hat{H}/2}
\]

**Purification of infinite-T state:** product of local totally mixed states

**Gauge degree of freedom:** arbitrary unitary evolution on Q

Lots of room for improvement:

Build MPOs and compress them:

\[
\langle \hat{B}(2t) \hat{A} \rangle_\beta = Z(\beta)^{-1} \text{tr} \left( e^{i \hat{H}t} e^{-\beta \hat{H}/2} \hat{B} e^{-i \hat{H}t} \right) \left( e^{-i \hat{H}t} \hat{A} e^{-\beta \hat{H}/2} e^{i \hat{H}t} \right)
\]
linear prediction

ansatz: data is linear combination of \( p \) previous data points

\[
\tilde{x}_n = - \sum_{i=1}^{p} a_i x_{n-i}
\]

find prediction coefficients by minimising error for available data

\[
E = \sum_{n} \frac{|\tilde{x}_n - x_n|^2}{w_n}
\]

iteratively continue time series from data using ansatz

(Barthel, Schollwöck, White, PRB 79, 245101 (2009))
some results of linear prediction

- transverse Ising model: prediction of $S(k,t)$

- spinons in spin-1/2 chain: experiment vs. numerics

extends time domain 10x
Barthel, US, White (2009)

perfect agreement with high-precision neutron scattering

Lake, ... Barthel, US, ... PRL 111, 137 (2013)
when does it work?

- why do we predict $S(k,t)$ in time and not e.g. $G(x,t)$ (and Fourier transform to momentum space later)?

  linear prediction works best for special time series

- superposition of exponential decays

  \[
  x_{n+m} = \sum_{\nu=1}^{p} c_\nu e^{i(\omega_\nu - \eta_\nu)m} x_n
  \]

- cf. pole structure of momentum-space of Green‘s functions

\[
G(k, \omega) = \frac{1}{\omega - \epsilon_k - \Sigma(k, \omega)} \quad G(k, t) = a_1 e^{-i\omega_1 t - \eta_1 t}
\]
variational ground state search: DMRG

problem: find MPS (of a given dimension) that minimizes energy

$$\min \frac{\langle \psi | \hat{H} | \psi \rangle}{\langle \psi | \psi \rangle} \iff \min \left( \langle \psi | \hat{H} | \psi \rangle - \lambda \langle \psi | \psi \rangle \right)$$

graphical representation of expression to be minimized:

variational minimization with respect to one matrix:

unnormalized MPS: generalized EV problem

mixed normalization MPS: eigenvalue problem
ground state DMRG

analytical representation of variational problem:

\[
\frac{\partial}{\partial M_{\sigma_i}} \left( \langle \psi | \hat{H} | \psi \rangle - \lambda \langle \psi | \psi \rangle \right) \mid_{\psi_0} = 0
\]

\[
\sum_{\sigma_i' a_{i-1}' a_i'} H_{\sigma_i a_{i-1} a_i, \sigma_i' a_{i-1}' a_i'} M_{\sigma_i' a_{i-1}' a_i'} \delta_{\sigma_i \sigma_i'} = \sum_{\sigma_i' a_{i-1}' a_i'} N_{a_{i-1} a_i, a_{i-1}' a_i'} \delta_{\sigma_i \sigma_i'} M_{\sigma_i a_{i-1} a_i'} \equiv \sum_{\sigma_i' a_{i-1}' a_i'} N_{\sigma_i a_{i-1} a_i, \sigma_i' a_{i-1}' a_i'} M_{\sigma_i' a_{i-1}' a_i'}
\]

\[
H m = \lambda N m
\]

DMRG algorithm:

- start with random or guess initial MPS
- maintaining mixed normalization, sweep "hot site" forth and back
- at each step, optimize local matrices by solving eigenvalue problem

convergence: monitor \( \langle \psi | \hat{H}^2 | \psi \rangle - (\langle \psi | \hat{H} | \psi \rangle)^2 \)
Hamiltonians in MPO form

construct Hamiltonian as automaton that moves through chain (e.g. from right to left) building Hamiltonian

\[ \hat{H} = \hat{M}^{[1]} \hat{M}^{[2]} \ldots \hat{M}^{[L]} \quad \hat{M}^{[i]} = \sum_{\sigma_i, \sigma'_i} M^{\sigma_i, \sigma'_i} |\sigma_i\rangle \langle \sigma'_i| \]

\[ \hat{H} = J \sum_{i=1}^{L-1} \frac{1}{2} (\hat{S}^{+}_i \hat{S}^{-}_{i+1} + \hat{S}^{-}_i \hat{S}^{+}_{i+1}) + \hat{S}^{z}_i \hat{S}^{z}_{i+1} + h \sum_{i=1}^{L} \hat{S}^{z}_i \]
Hamiltonians in MPO form II

short ranged Hamiltonians find very compact, exact representation!

\[
\hat{M}^{[i]} = \begin{bmatrix}
\hat{I} & 0 & 0 & 0 & 0 & 0 \\
\hat{S}^+ & 0 & 0 & 0 & 0 & 0 \\
\hat{S}^- & 0 & 0 & 0 & 0 & 0 \\
h\hat{S}^z & (J/2)\hat{S}^- & J^z\hat{S}^z & (J/2)\hat{S}^+ & \hat{I}
\end{bmatrix}
\]

\[
\hat{M}^{[1]} = \begin{bmatrix}
h\hat{S}^z & (J/2)\hat{S}^- & J^z\hat{S}^z & (J/2)\hat{S}^+ & \hat{I}
\end{bmatrix}
\]

\[
\hat{M}^{[L]} = \begin{bmatrix}
\hat{I} \\
\hat{S}^+ \\
\hat{S}^- \\
h\hat{S}^z
\end{bmatrix}
\]
frustrated magnetism in 2D

- „classic“ candidates (spin length $1/2$):

- $J_1$-$J_2$ model on a square lattice

- classical model
  - order only locally coplanar
  - extensive $T=0$ entropy

- agreement: no magnetic order for $S=1/2$

Yan et al, Science (2011)
Depenbrock et al, PRL (2012)

herbertsmithite $\text{ZnCu}_3(\text{OH})_6\text{Cl}_2$
DMRG in two dimensions

- map 2D lattice to 1D (vertical) "snake" with long-ranged interactions

- horizontally: ansatz obeys area law: easy axis, long at linear cost
- vertically: ansatz violates area law: hard axis, long at exponential cost
- consider long cylinders of small circumference $c$: mixed BC

\[
S \sim \log_2 M^L = L \log_2 M
\]

\[
S \sim \log_2 (M^2)^L = 2L \log_2 M
\]

\[
S \sim \log_2 M \quad \rightarrow \quad M \sim 2^L
\]
ground state energies

- fully $SU(2)$ invariant DMRG code
- up to 3,800 representatives ($16,000 U(1)$ DMRG states) 100% increase
- cylinders up to circumference $c=17.3, N=726$ 50% increase
- tori up to $N=(6\times6)\times3=108$ sites ED: 48 sites

TD limit energy estimate: $-0.4386(5)$

iDMRG (infinite cylinder) upper bounds below HVBC; YC8: $-0.4379$

fully $SU(2)$ invariant DMRG code

eliminates need for special edge manipulations of $U(1)$ DMRG: ground state of $S=1$ sector

bond energy deviations from mean

bulk excitation

much smoother gap curve

triplet gap estimate: $0.13(1)$

triplet gap for infinitely long cylinders

singlet gap estimate: approx $0.05$ (Yan et al. (2011))
topological entanglement entropy (TEE)

- Ground state in 2D obeying area law
- For smooth (circular) surface of bipartition
  \[ S(L) = aL - \gamma \]
- Topological entanglement entropy (TEE) \( \gamma \)
  \[ \gamma = \log_2 D \]
  Quantum dimension
  Torus degeneracy: \( D^2 \)
  \[ D = \sqrt{2} \quad \text{chiral QSL} \quad D = \sqrt{3} \]
- Reduces conventional entanglement entropy
- Global property
- Can be used to detect topological phases (complete classification)

Preskill, Kitaev, PRL 2006
Levin, Wen, PRL 2006

\( D = 2 \) \( Z_2 \) QSL
Double semion phase
topological entanglement and DMRG

- MPS structure of DMRG gives direct access to reduced density operator
- entanglement entropy for free
- in 1D mapping: cut of arbitrary link of path

- smooth surface minimizes subleading corrections
- one optimal cut for XC,YC cylinders each

![Diagrams](X)n (Y)n

2D view: 2 cylinders A, B
TEE with DMRG: Renyi entropies

- MPS: $M$ non-zero eigenvalues of $\rho_A$ only
- tail of spectrum not captured well?
- von Neumann entropy correct?

- Renyi entropy $S_\alpha(\rho) = \frac{1}{1 - \alpha} \log_2 \text{tr} \rho^\alpha \quad (0 \leq \alpha < \infty)$
  
  $S_0(\rho) = \text{rank } \rho \quad S_1(\rho) = -\text{tr } \rho \log_2 \rho \quad S_\infty(\rho) = -\log_2 w_1$

- low-$\alpha$ Renyi: focus on tail
- high-$\alpha$ Renyi: focus on head of spectrum - measured accurately!

- theorems:

  topological entanglement entropy independent of alpha
TEE in the kagome lattice

- Extrapolate Renyi entropies to circumference $c=0$
- Negative intercept is TEE
- Find topological order!

$$\gamma \approx 0.94 \quad D \approx 2$$

- TEE extracted from random state in GS manifold lower bound
- True value for so-called minimum entropy state
- DMRG seems to systematically pick those

conclusions

- **1D: DMRG/MPS currently most powerful method**
  - ground states
  - time-evolution, also at non-zero temperature
  - limitation: exponential growth of resources; entanglement growth

- **2D: DMRG/MPS starts making very interesting forays**
  - long cylinders
  - suboptimal ansatz, but numerically extremely stable

- Barring new ideas, key challenges for powerful codes:
  - parallelization
  - (non-)Abelian quantum numbers
  - non-trivial geometries (impurity solvers, quantum chemistry)
  - convergence of ground states