Classical simulation of open quantum systems

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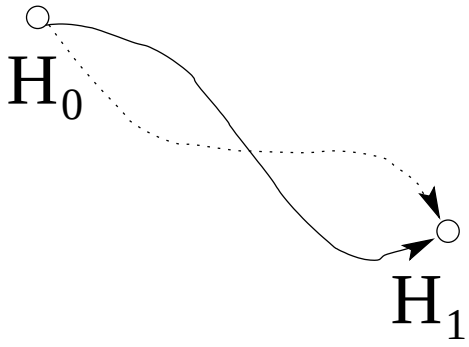
Outline

One wants to solve hardest problems with best algorithms!

- **Quantum adiabatic algorithm** (hard instances):
  - Computational complexity: worst vs. average performance.
  - 3-SAT: hardest instances at small m/n.
  - Exponentially small gap: many almost-solutions.
- **Classical simulation of quantum many-body systems** (good algo.):
  - MPS/MPO algorithms for local 1D: entanglement!
  - Evolution of pure states (“always” bad).
  - Evolution of operators (“mostly” bad).
  - Equilibrium ρ (good).
  - Nonequilibrium steady states (“often” good).

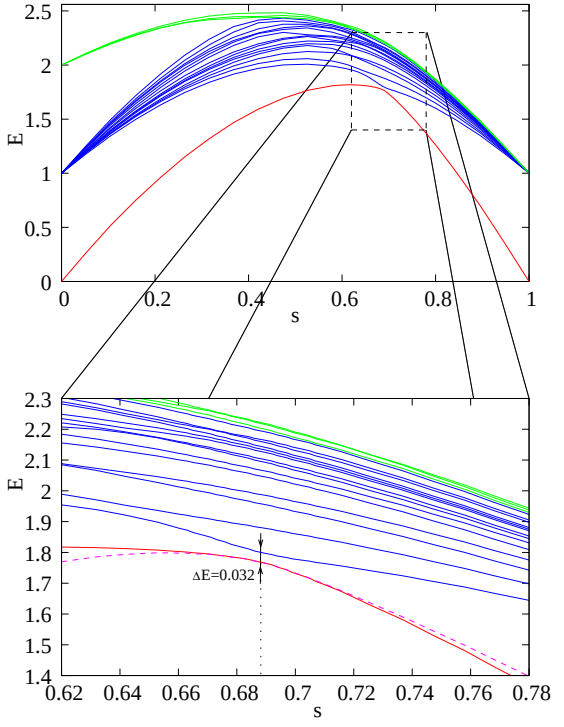
Quantum adiabatic algorithm



- H_0 is the initial Hamiltonian. Independent of the problem and with known ground state.
- H_1 is the final Hamiltonian. Depends on the problem - ground state gives the solution.

Procedure:

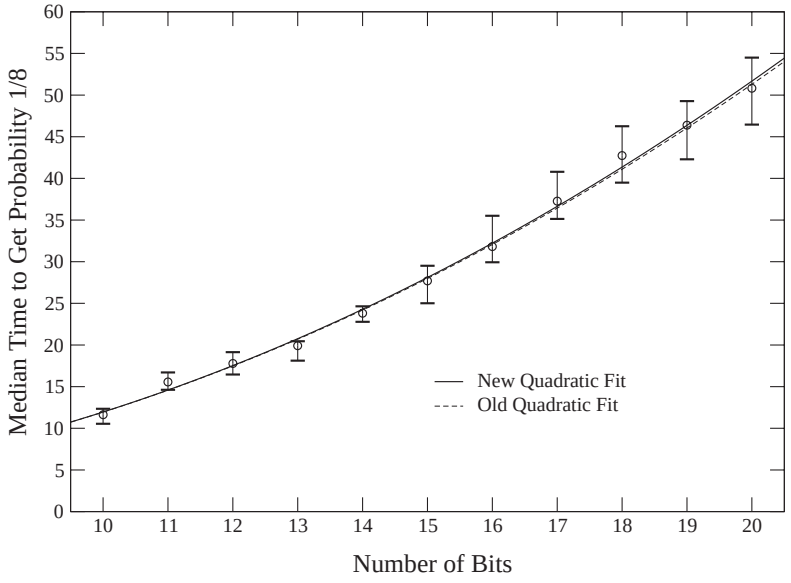
- set the system into ground state of H_0
- adiabatically change the Hamiltonian, $H_0 \to H(t) = (1 - \frac{t}{T})H_0 + \frac{t}{T}H_1 \to H_1$
- the final state encodes the solution



3-SAT: $n = 14$, $m = 42$ $(m/n = 3)$

MIT result for NP-complete problem

Numerical study of adiabatic algorithm for NPC problem.



Farhi *et. al.*, Science **292** (2001)

- random instances of exact cover
- quadratic time dependence for small sizes

Is quantum adiabatic algorithm for NPC problems polynomial?

of an NP-complete problem. For the small examples that we could simulate, the quantum adiabatic algorithm worked well, providing evidence that quantum computers (if large ones can be built) may be able to outperform ordinary computers on hard sets of instances of NP-complete problems.

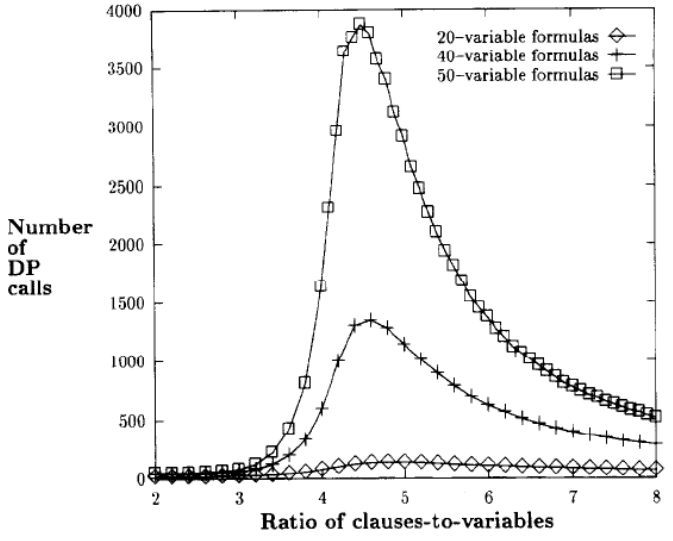
algorithms. Most of the instances we have generated lie near the "phase transition" for Exact Cover. The phase transition region

Random 3-SAT

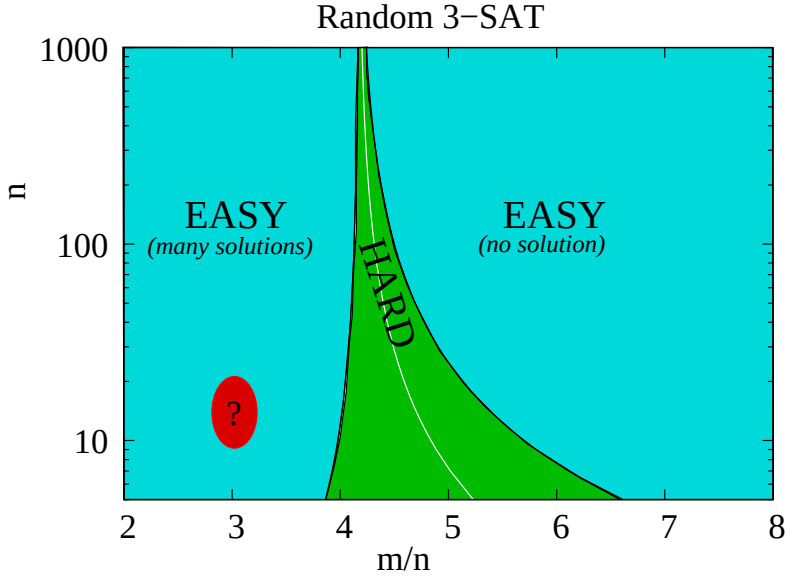
How to generate “hard” 3-SAT instances?

(Complexity is defined with respect to the *hardest* cases.)

- well known classical problem, e.g. artificial intelligence.
- “common wisdom/approach”: **random 3-SAT ensemble**, hard instances near phase transition (random 3-SAT for m/n)



B. Selman *et. al.*, Artificial Intelligence **81**, 17 (1996)

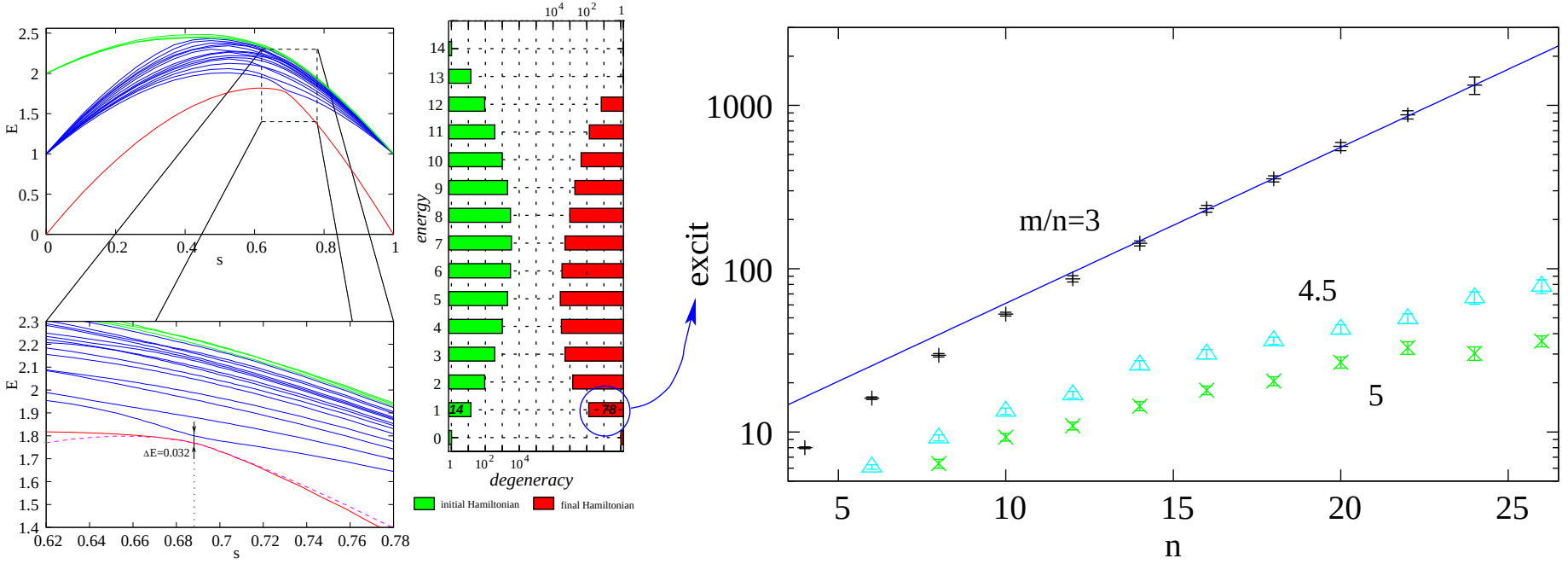


scheme after: S. Kirkpatrick, B. Selman, Science **264**, 1297 (1994)

For 3-SAT there is no “natural” measure!

3-SAT with exactly one solution

It seems that the degeneracy of the first excited state matters.

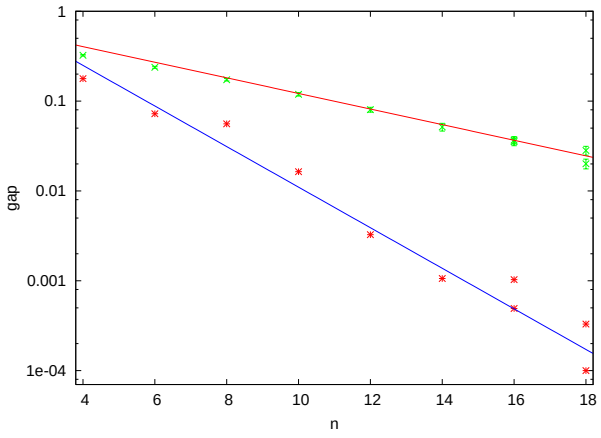


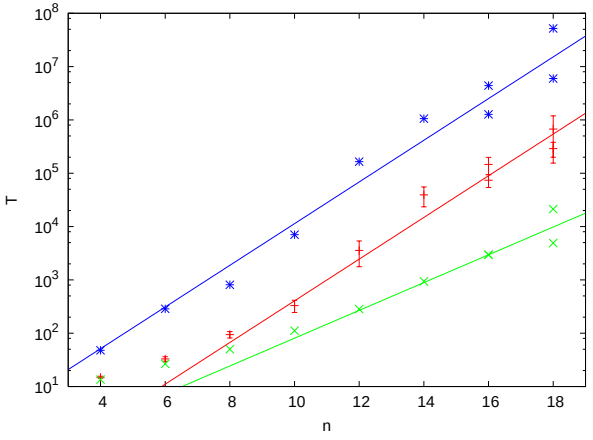
- For $m/n = 3$ the degeneracy grows exponentially with n!
- For larger m/n (at the phase transition!) the growth is slower.

  (asymptotics might not have been reached yet)

Energy gap for single-solution 3-SAT

[M. Žnidarič PRA **71**, 062305 (2005)]

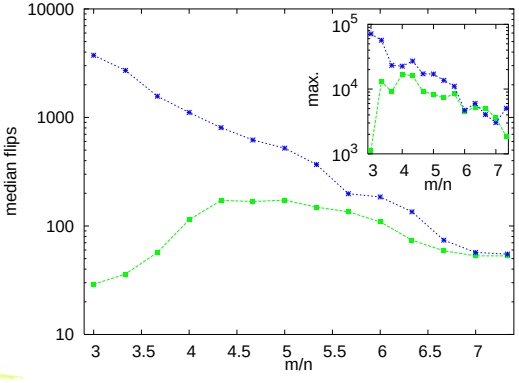


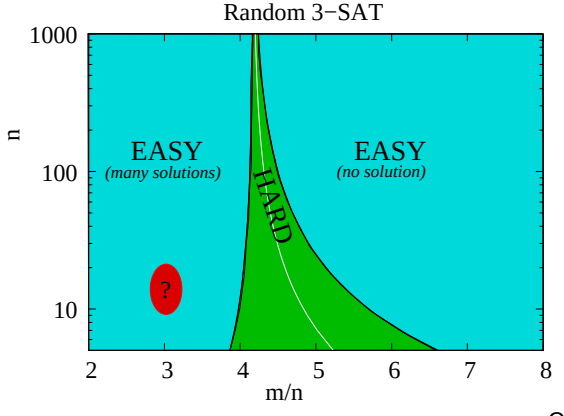


- Left : average and minimal gap for $m/n = 3$ (100 instances).
- Right : AQC running time (from Landau-Zener).

[See also R. Schützhold & G. Schaller, PRA **74**, 060304 (2006)]

time grows exponentially with n





Exact exponentially small gap

Can we analytically calculate Δ? YES [M. Žnidarič and M. Horvat, PRA **73**, 022329 (2006)]

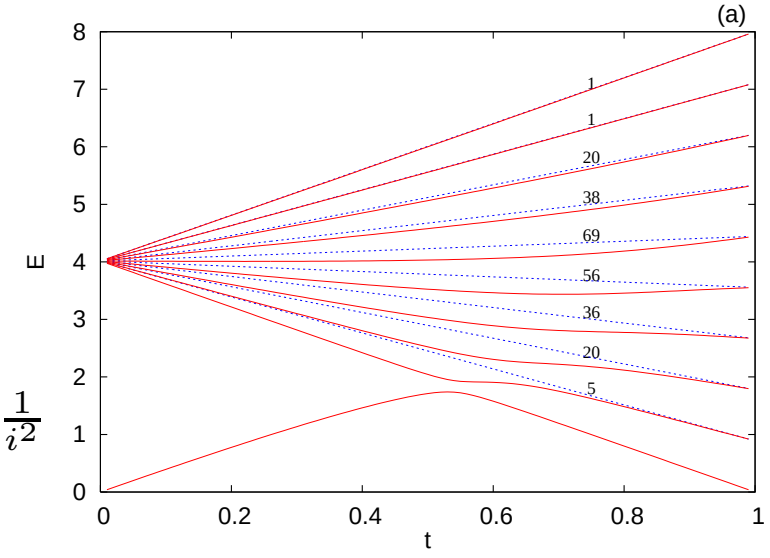
- Projector to the ground state:

$$H_0 = b(\mathbb{1} - |\psi\rangle\langle\psi|)$$

$$|\psi\rangle = \frac{1}{\sqrt{N}} \sum_{i=0}^{N-1} |i\rangle, \qquad b = \frac{n}{2} \frac{N}{N-1}$$

$$\Delta \approx \frac{n\sqrt{d_0}}{2\sqrt{N}} f(n), \qquad f(n) = \frac{2}{1+\gamma\gamma_{-1}} \sqrt{\frac{\gamma_{-1}^2}{\gamma_{-2}}}$$

$$\gamma = \sum_{i=0}^{D} \frac{d_i}{N} i \approx \frac{n\alpha}{8}, \quad \gamma_{-1} := \sum_{i=1}^{D} \frac{d_i}{N} \frac{1}{i}, \quad \gamma_{-2} := \sum_{i=1}^{D} \frac{d_i}{N} \frac{1}{i^2}$$



- B. Altshuler, H. Krovi & J. Roland, PNAS **107**, 12446 (2010).
- M. H. S. Amin, PRL **100**, 130503 (2008).

Worst vs. average performace

1. For computational complexity the worst-case performance matters (the hardest instance of a given size n).
   - the measure does not matter.

2. For average performance (median,...) the choice of the measure is absolutely crucial!
   - with a “biased” measure one can easily “demonstrate” efficiency.

Efficient classical simulation

Part II.

Representing states

MPS (matrix product state, Fannes, Nachtergaele, Werner ('92))

$$|\psi\rangle = \sum c_{s_1 \ldots s_n} |s_1 \ldots s_n\rangle$$

$$c_{s_1 \ldots s_n} = \mathrm{tr}[A^{s_1} A^{s_2} \cdots A^{s_n}],$$

where A^{s_i} are matrices of dimension $D \times D$.

- For each qubit we have two matrices, $A^{s_i=0}$ in $A^{s_i=1}$, all-together $2 \times D^2 \times n$ parameters!
- What is the necessary dimension D?
  - D for A on $i-$th site equals to the number of nonzero Schmidt coefficients (for bipartition $[s_1 \ldots s_i][s_{i+1} \ldots s_n]$)!

Schmidt decomposition

$$|\psi\rangle = \sum_{i=0}^{N_{\mathrm{A}}-1} \sqrt{\lambda_i} |\varphi_i^{\mathrm{A}}\rangle \otimes |\varphi_i^{\mathrm{B}}\rangle.$$

- $|\varphi_i^{\mathrm{A}}\rangle$ and $|\varphi_i^{\mathrm{B}}\rangle$ are orthogonal, $\langle\varphi_i^{\mathrm{A}}|\varphi_j^{\mathrm{A}}\rangle = \delta_{ij}$
- λ_i are eigenvalues $\rho_{\mathrm{A}} = \mathrm{tr}|\psi\rangle\langle\psi|$
- von Neumann entropy is a simple measure of total pure-state entanglement:

$$S(|\psi\rangle) = -\mathrm{tr}(\rho_{\mathrm{A}} \log_2 \rho_{\mathrm{A}}) = \sum_i -\lambda_i \log_2 \lambda_i.$$

Necessary $D \sim 2^{S(\psi)}$. Small $S(\psi) \Longleftrightarrow$ MPS efficient

MPS for GHZ state

State: $|\psi\rangle = \frac{1}{\sqrt{2}}(|0\ldots0\rangle + |1\ldots1\rangle)$.

- Schmidt decomposition :

$$|\psi\rangle = \sqrt{\tfrac{1}{2}}|0\ldots0\rangle \otimes |0\ldots0\rangle + \sqrt{\tfrac{1}{2}}|1\ldots1\rangle \otimes |1\ldots1\rangle.$$

- 2 nonzero $\lambda_i = \frac{1}{2} \quad \Longrightarrow D = 2$.

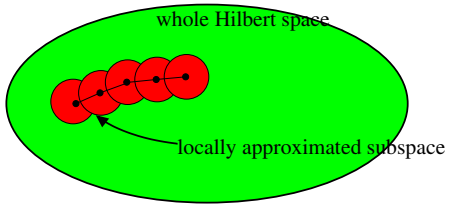
$$A^{s_1=0} = \begin{pmatrix} \frac{1}{\sqrt{2}} & 0 \\ 0 & 0 \end{pmatrix}, \quad A^{s_i=0} = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}, \quad A^{s_n=0} = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}$$

$$A^{s_1=1} = \begin{pmatrix} 0 & \frac{1}{\sqrt{2}} \\ 0 & 0 \end{pmatrix}, \quad A^{s_i=1} = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}, \quad A^{s_n=1} = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}$$

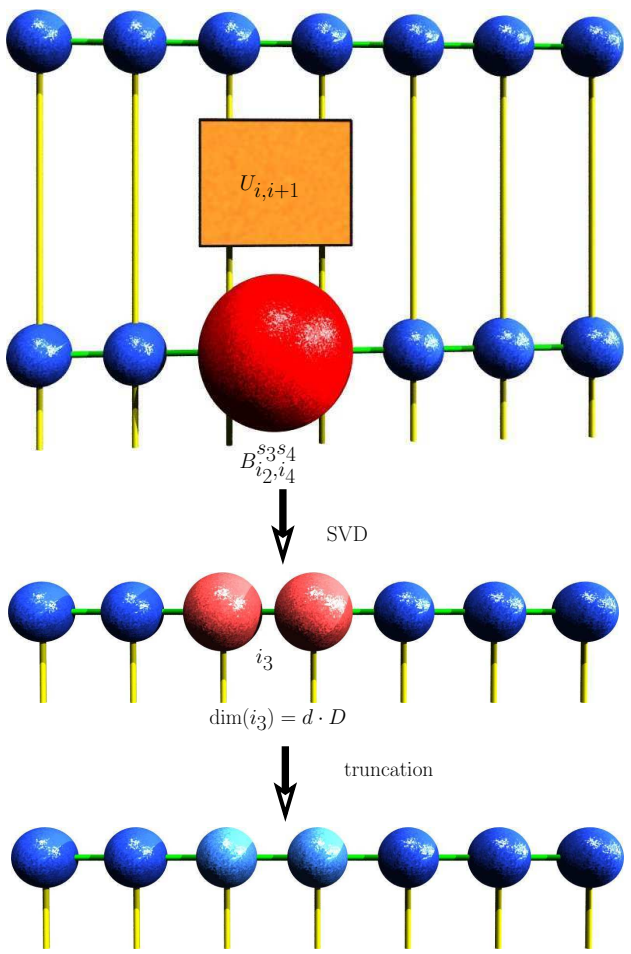
$$|\psi\rangle = \sum c_{s_1\ldots s_n}|s_1\ldots s_n\rangle, \qquad c_{s_1\ldots s_n} = \mathrm{tr}[A^{s_1}A^{s_2}\cdots A^{s_n}].$$

Numerical methods

- NRG (Wilson '75)
  - always keep states with the lowest energy
  - works if energy scales are well separated (e.g. impurities)
- DMRG (White '92)
  - for subsystems choose not the lowest energies but such states that $|\rho_{\mathrm{DMRG}} - \rho_{\mathrm{exact}}|$ is minimal!
  - *eigenvectors of ρ with the largest eigenvalues*
- t-DMRG (Vidal '03)
  - Can do time evolution of $\psi(t) = U\psi(0)$.



t-DMRG algorithm (*Vidal, PRL '03*)



- We write state in an MPS form
  $|\rho\rangle = \sum_{s_i} \mathrm{tr}[A_1^{s_1} \cdots A_n^{s_n}] |\rho_1^{s_1} \ldots \rho_n^{s_n}\rangle.$
- Do transformation U on two neighboring spins.
- We get $|\rho'\rangle =$
  $\sum_{s_i} \mathrm{tr}[A_1^{s_1} \cdots A_{j-1}^{s_{j-1}} \cdot B \cdot A_{j+2}^{s_{j+2}} \cdots A_n^{s_n}] |\rho_1^{s_1} \ldots \rho$
- Instead of two $D \times D$ matrices $A_j^{s_j} A_{j+1}^{s_{j+1}}$ we get one $2D \times 2D$ matrix B.
- We rewrite B as a product of two matrices by using SVD; keeping only D largest singular values (truncation!),
  $(B)_{is_j, ks_{j+1}} = (\tilde{A}_j^{s_j} \tilde{A}_{j+1}^{s_{j+1}})_{ik}$.

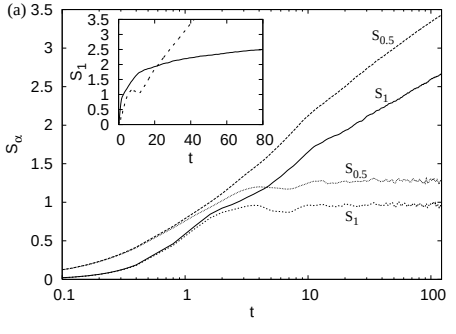
$|\psi(t)\rangle$ *with t-DMRG?*

t-DMRG will be efficient only if $S(t)$ grows slowly enough!

- From quantum chaos (and random circuits) we know that chaotic systems generate entropy efficiently. $S(t) \sim t$, in 1D it saturates at $S \sim n$ after time $t \sim n$.
- But even for integrable systems (e.g. transversal Ising, $H = \sum \sigma_i^x \sigma_{i+1}^x + \sigma_i^z$; Calabrese & Cardy '05) again $S(t) \sim t$.

$|\psi(t)\rangle$ in general never works (in time)!

(Except for MBL; Žnidarič, Prelovšek & Prosen, PRB 2008.)



(or special states, e.g., close to ground state; cond-mat)

Why the failure

- generic (random) $|\psi\rangle$ will indeed have a lot of entanglement.
- mostly in nonlocal DOF.
- we do not care about “strange” nonlocal observables.
- most of information in $|\psi(t)\rangle$ is non-physical (unobservable)

We are trying to calculate too much!

How about Heisenberg picture, operator $O(t)$?

- For integrable systems evolution of local operators can be efficient, even if evolution of ψ is not (Prosen & Žnidarič, PRE 2007).
- Still, for generic systems it does not work!

Density operators

Description by $\rho(t)$ might be better (e.g., due to environment)!

pure states ("singular") vs. density operators ("smooth")

Example:

random high-energy $|\psi\rangle$ well describes local expectations at $T = \infty$, i.e., the same as $\rho \sim \mathbb{1}$.

- But $|\psi\rangle$ is complicated and highly entangled.
- While $\rho \sim \mathbb{1} = \mathbb{1}_1 \otimes \mathbb{1}_2 \cdots \otimes \mathbb{1}_n$ is simple and separable (in operator space).

Indeed: DMRG works for ground states
($S \sim \log n$ in critical or const. in gapped, Vidal, Latorre, Rico & Kitaev 2003),
and thermal states (imaginary time evolution).

Lindblad equation *(Lindblad; Gorini,Kossakowski,Sudarshan '76)*

$$\frac{\mathrm{d}}{\mathrm{d}t}\rho(t) = \mathcal{L}(\rho(t)) = \mathrm{i}[\rho(t), H] + \mathcal{L}^{\mathrm{diss}}(\rho(t)),$$

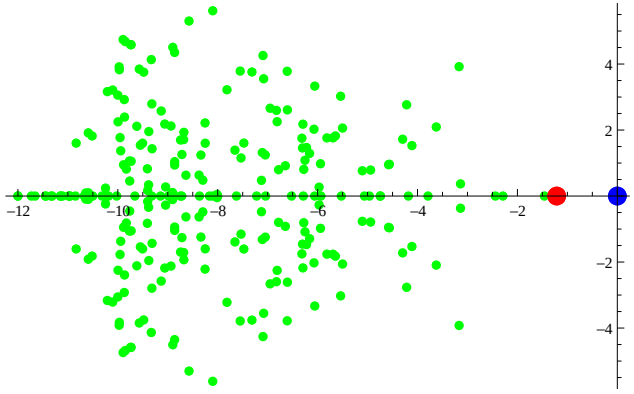
$$\mathcal{L}^{\mathrm{diss}}(\rho) = \sum_j [L_j\,\rho, L_j^\dagger] + [L_j, \rho\,L_j^\dagger].$$

- The generator $\mathcal{L}$ (the Liouvillian) is non-hermitean.

Brouwer's fixed-point theorem:

always a fixed point ρ_∞,

steady state $\rho_\infty = \mathrm{e}^{\mathcal{L}\cdot(\,t\to\infty)}\rho(0)$.

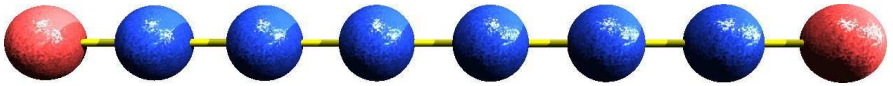


- Depending on L_j:
  - equilibrium steady state.
  - ρ_∞ is a nonequilibrium steady state (NESS).
- For small systems the choice of L_j can be important:

(F. Barra, Sci. Rep. **5**, 14873 (2015); E.Arrigoni et al. PRB **89**, 165105 (2014))

Transport

Transport can be studied via local L_j acting on the boundary.

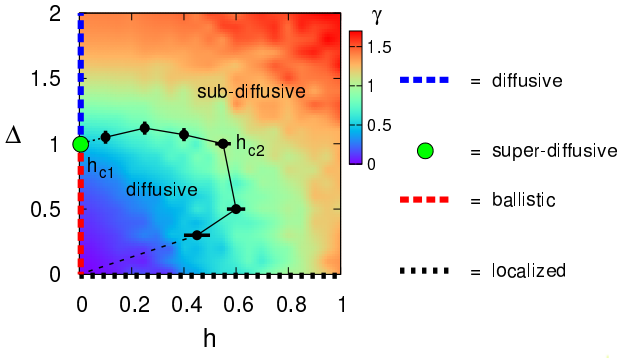


In the thermodynamic limit the choice of L_j should not matter.

Are there cases with low-rank MPO NESS? YES

- Exact NESS solutions:
  - fixed, e.g. $D = 4$ (driven XX chain, M.Ž. JPA , (2010)).
  - polynomial, e.g. $D \sim n^2$ (max. driven XXZ, Prosen PRL '11).
- Numerics (t-DMRG):
  - many works in last 8 years.
  - empirics: often works good at $T \gg 1$.
  - spin chains, ladders,...

M.Z., A.Scardicchio & V.K.Varma, PRL '16



Conclusions

Hard problems:

- Studying running time: measure does matter, especially for small problems.
- No real reason for a uniform measure (random 3-SAT).
- Single-solution instances having small m/n are hard.

Good classical algorithms:

- Pure states are frequently non-physical, $\longrightarrow$ hard to simulate.
- Think about relevant physics, observables,...$\longrightarrow \rho$.
- Lindblad master equation: equilibrium and nonequilibrium.
- Large systems in 1D and at high T.