Efficient approximation of gapped spin chain ground states.

The unfrustrated case.

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Honours Talks
2014

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Ground state approximation
C. T. Chubb

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Conclusion

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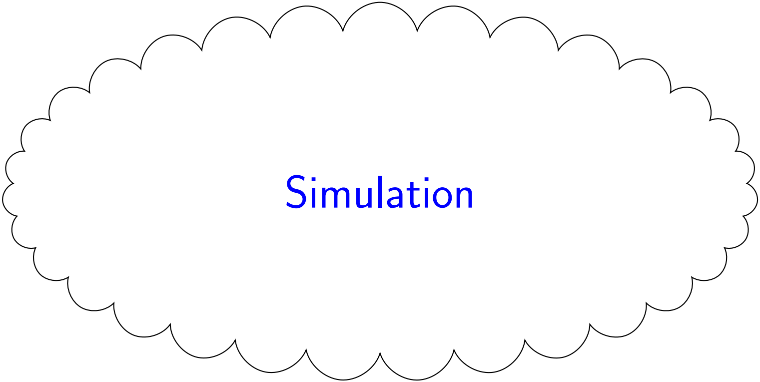

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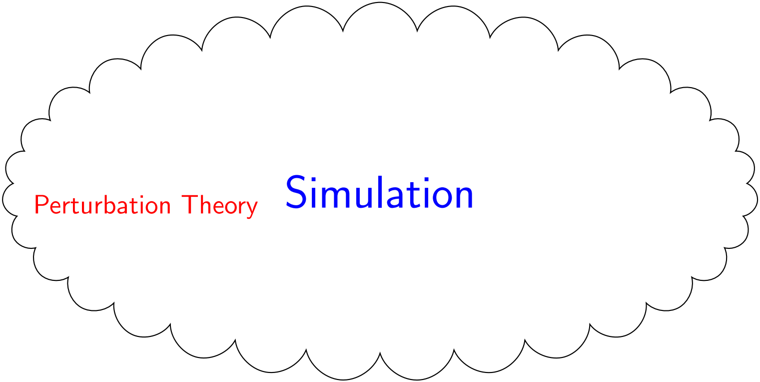

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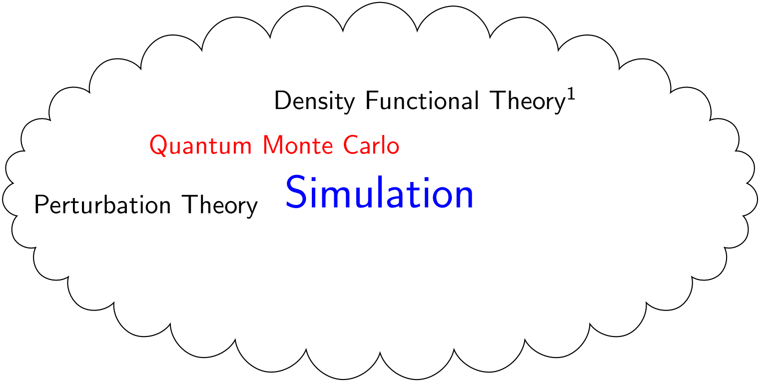

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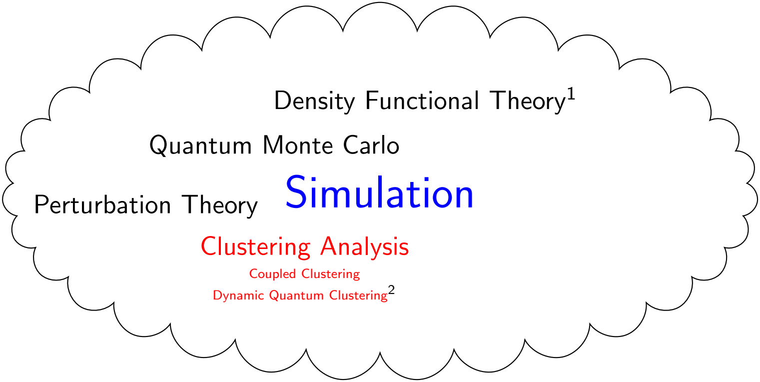

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- Dynamic Quantum Clustering[2]

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- Density Matrix Renormalisation Group[4]
- Time Dependent Variational Principle
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- The toy problem we are going to consider is ground state approximation of a spin system. This forms an important stepping-stone to more general low-temperature simulations.

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Question

Are there any non-trivial 'physically realistic' conditions under which 1D local systems can be simulated with provable efficiency?

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Role of entanglement

- One main limiting factor is entanglement.
- Classical states can be specified on each subsystem piecewise, quantum systems however can exhibit any linear combination of such a <u>product state</u> (c.f. tensor products).

$$\text{Variables in a classical state} \sim \text{poly(System size)}$$
$$\text{Variables in a quantum state} \sim \text{exp(System size)}$$

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Idea

A structural bound (limit on entanglement) implies a complexity bound (efficiency of approximation).

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- For a state $|\psi\rangle$, the full state and reduced state specified on a region A are given by

$$\rho = |\psi\rangle\langle\psi| \qquad\qquad \rho_A = \operatorname{Tr}_{\bar{A}} \rho$$

- The full state ρ is pure but ρ_A needn't be; the entropy of ρ_A is a measure of the entanglement between regions A and $\bar{A}$, e.g.:

$$R_\alpha(\rho_A) := \frac{\log \operatorname{Tr} \rho_A^\alpha}{1-\alpha} \qquad \text{(Rényi Entropy)}$$

$$R_1(\rho_A) = -\operatorname{Tr}(\rho_A \log \rho_A) = S(\rho_A) \qquad \text{(Entropy)}$$

$$R_0(\rho_A) = \log \operatorname{rank}(\rho_A) = \log B(\rho_A) \qquad \text{(Rank)}$$

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- Local systems exhibit a light-cone (up to exponential corrections) given by the Lieb-Robinson[1] velocity v_{LR}:

$$\left\|[A,B]\right\| \leq e^{-c(d-v_{LR}t)}\left\|A\right\|\left\|B\right\|$$

where d/t are the distance/time between observables A and B.

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Definition (Spectral gap/Gapped Hamiltonian)

The **spectral gap** ΔE of a Hamiltonian is the difference between the ground and first excited energy. **Gapped Hamiltonians** are those for which the spectral gap is lower bounded by a constant $\Delta E = \Omega(1)$.

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- Ground states exhibit exponential decay of correlations[2] with characteristic length ξ:

$$|\langle AB\rangle - \langle A\rangle\langle B\rangle| \leq e^{-d/\xi}\,\|A\|\,\|B\| \qquad \xi := \frac{2v_{LR}}{\Delta E}$$

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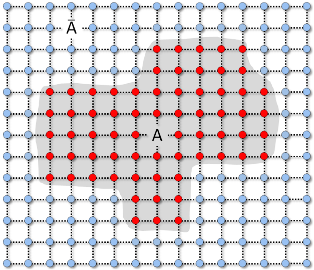

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$$S = \mathcal{O}(|A|)$$

[1] Number of spins contained within.

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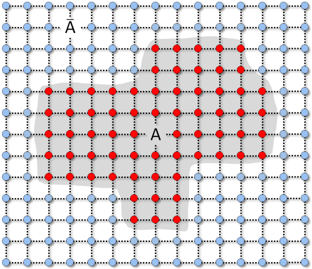

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Is this typical of ground states? The two previous notions of locality seem to suggest otherwise.

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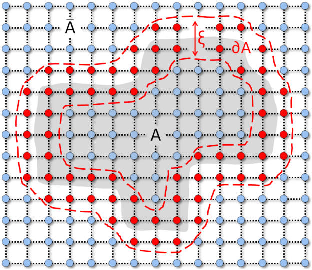

We might suspect $S(\rho_A) \lesssim \xi\,|\partial A|$.

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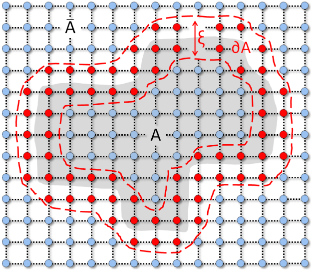

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Conjecture (Area Law of entanglement entropy)

Ground states of local and gapped systems obey an 'are'[1] law

$$S(\rho_A) = \mathcal{O}(|\partial A|)$$

[1] Number of spins along the boundary.

Proofs of the 1D area law

- For 1D local states with a gap lower bounded by ϵ:

Year	**Result**	**Notes**
2007[1]	$S \leq e^{\mathcal{O}(\epsilon^{-1})}$	Combinatorial
2012[2]	$S \leq \tilde{\mathcal{O}}(\epsilon^{-3})$	Unfrustrated only
2013[3]	$S \leq \tilde{\mathcal{O}}(\epsilon^{-3/2})$	Frustrated
2014[4]	$R_\alpha \leq \tilde{\mathcal{O}}(\alpha^{-3}\epsilon^{-1})$	One ground of a degen. system

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- For our purposes we are going to assume an area law for <u>all</u> degenerate ground states.

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Matrix Product States

- One consequence of the area law is the existence of a $1/\text{poly}(n)$-accurate approximate ground state with entanglement rank bounded

$$B \leq \exp\left(\mathcal{O}\left(\epsilon^{-1/4}\log^{3/4} n\right)\right) = n^{o(1)}$$

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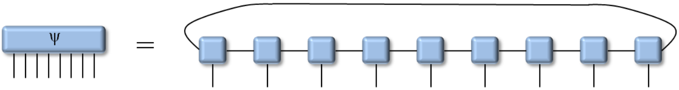
- As such we can utilise the Matrix Product State ansatz



- This ansatz allows for any state with the given entanglement rank to be represented by $n^{o(1)}$ complex numbers; efficient representation.

The Viable Set

Our algorithm is based on the unique ground state algorithm of Landau, Vazirani and Vidick. This class of ground state algorithms works by constructing viable sets.

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- The cardinality of this set is s.

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If we can construct a $(n, \mathrm{poly}(n), \eta)$-viable, then by minimise the Hamiltonian on this set we can efficiently find a state with $1-\eta$ ground state overlap.

Procedure

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- Each step alters one of the viability parameters in turn.

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- Firstly we want to increment the number of spins. Take S_{i-1} to be the viable set on $i-1$ spins.

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- Construct $S_i^{(1)}$ by:

Algorithm Step 1: Extension

Taking $\{|j\rangle\}$ to be the computational basis on the ith spin

$$\text{Return } S_i^{(1)} := \left\{ |s\rangle \otimes |j\rangle \,\middle|\, |s\rangle \in S_{i-1},\ 1 \leq j \leq d \right\}.$$

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- This will send a $(i-1, s, \delta)$-viable set to a (i, ds, δ)-viable set, where d is the local dimension of each spin.
- Extension alone will tend to exponentially grow the cardinality, so the next step is to trim the cardinality back down.

Size trimming

Algorithm Step 2: Size Trimming

Take σ to be a density matrix supported on $\mathrm{Span}\left(S_i^{(1)}\right)\otimes\mathbb{C}^B$ given as the solution to the size-trimming convex program:

$$\begin{aligned} \text{min} \qquad & \sum_{j=1}^{i-1} \mathrm{Tr}(H_j\sigma) \\ \text{such that} \qquad & \mathrm{Tr}(\sigma)=1, \quad \sigma\geq 0 \end{aligned}$$

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Take $|u\rangle$ to be the highest eigenvector of σ, and decompose this state as $|u\rangle = \sum_{j=1}^{B} |u_j\rangle |j\rangle$.

$$\text{Return } S_i^{(2)} := \{|u_j\rangle \mid \forall j\}.$$

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- This sends a $(i, ds, \delta = c\epsilon^2/n)$-viable set to a $(i, p_1, 1/12)$-viable set, where $p_1 = n^{2^{\mathcal{O}(1/\epsilon)}}$ is the number of optimisations.

Error reduction

- The main idea here is to use approximate ground state projectors (AGSP).

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- An AGSP P is an operator for which
  - For any ground state $|\Gamma\rangle$, $P|\Gamma\rangle = |\Gamma\rangle$.
  - For any state $|\Gamma^\perp\rangle$ orthogonal to the ground, $\left\|P\left|\Gamma^\perp\right\rangle\right\|$ is small.
  - The entanglement P generates is not too large.

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Algorithm Step 4: Error Reduction

Take the decomposition of the approximate AGSP $K = \sum_k A_j \otimes B_j$.

$$\text{Return } S_i^{(4)} := \left\{ A_j |s\rangle \middle| \forall j,\ |s\rangle \in S_i^{(3)} \right\}.$$

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- This sends a $(i, p_1, 1/2)$-viable set to a $(i, pp_1, c\epsilon^2/n)$-viable set, where $p = n^{\mathcal{O}(1)}$ is related to the entanglement rank of the AGSP.

Parameter table

Stage	i	s	B	δ
Iteration 0	0	1	0	0
	$\vdots$	$\vdots$	$\vdots$	$\vdots$
Iteration $i-1$	$i-1$	pp_1	pp_2	$c\epsilon^2/n$
Iteration i:				
Extension	$\mathbf{i}$	dpp_1	pp_2	$c\epsilon^2/n$
Size Trimming	i	$\mathbf{p_1}$	$dp^2p_1p_2$	$1/12$
Bond Trimming	i	p_1	$\mathbf{p_2}$	$1/2$
Error Reduction	i	pp_1	pp_2	$\mathbf{c\epsilon^2/n}$
Iteration $i+1$	$i+1$	pp_1	pp_2	$c\epsilon^2/n$
	$\vdots$	$\vdots$	$\vdots$	$\vdots$
Iteration $n-1$	n	pp_1	pp_2	$c\epsilon^2/n$
Final iteration	n	p_0p_1	p_0p_2	η

All the parameters are poly(n) (ignoring ϵ-dependence) and each step run in poly(n) time. The final run-time of this algorithm is

$$T = n^{2^{\mathcal{O}(1/\epsilon)}} \cdot \mathrm{poly}(n/\eta)$$

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  - ~~The local energy contributions may not be minimal (frustration) and they may not be identical for different ground states.~~ Assume Hamiltonian is unfrustrated.
  - The optimisations are only guaranteed to give a single witness state.

Left-distinguishability

- Whilst the two ground states are orthogonal on the whole system, their components on the first i spins need not be.

Left-distinguishability

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  so any set which is $(1,s,\delta)$-viable for Γ_1 is $(1,s,\delta)$-viable for Γ_2 also.

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  - On the first two spins however the states 'look' orthogonal

$$|\Gamma_1\rangle = |00{*}\rangle \qquad |\Gamma_2\rangle = |01{*}\rangle$$

    so viability for Γ_1 doesn't imply any viability for Γ_2.

Left-distinguishability

The non-degenerate optimisation gives the first witness state. We then measure the magnitude of the second state captured by the first optimisation by:

Definition (Left-Distinguishability)

We define the **left-distinguishability** to be $D = 1 - \mathrm{Tr}(\rho_L P)$ where ρ_L is the left-reduced density operator of the desired second witness, and P is the projection onto the span of the current viable vectors.

$D = 0$ corresponds to entirely indistinguishable.

$D = 1$ corresponds to entirely distinguishable.

Degenerate Size-Trimming: Low D Case

- In this case a viable set for the first witness is also a viable set for the second witness.
- As D grows the error of the second witness grows.

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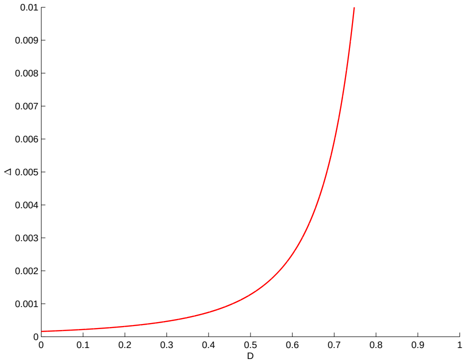


Degenerate Size-Trimming: High D Case

In this case we want to 'project away' from the current viable set.

Algorithm Step 2.2: Degenerate Size Trimming

Take σ_2 supported on Span $\left(S_i^{(1)}\right) \otimes \mathbb{C}^B$ given as the solution to the degenerate size-trimming convex program:

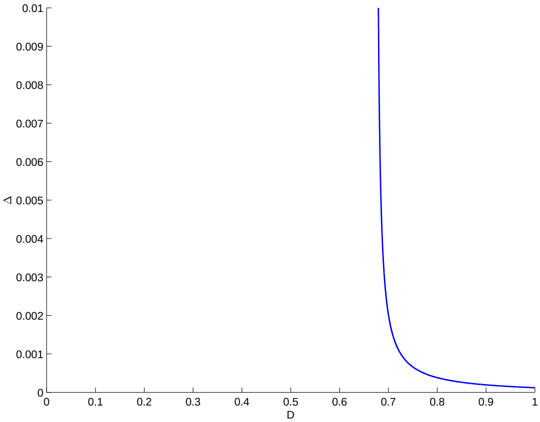
$$\begin{aligned} \min \quad & \mathrm{Tr}(\sigma_2 P) \\ \text{such that} \quad & \sum_{j=1}^{i-1} \mathrm{Tr}(H_j \sigma) \leq \sqrt{c}\epsilon \\ & \mathrm{Tr}(\sigma) = 1, \quad \sigma \geq 0 \end{aligned}$$

Again taking $|u_2\rangle \sum_{j=1}^{B} |u_{2,j}\rangle |j\rangle$ to be the highest eigenvector of σ_2.

$$S_i^{(2,2)} := \{|u_{2,j}\rangle \mid \forall j\}$$

$$\text{Return } S_i^{(2)} := S_i^{(2,1)} \cup S_i^{(2,1)}$$

Degenerate Size-Trimming: High D



Degenerate Size-Trimming: All D

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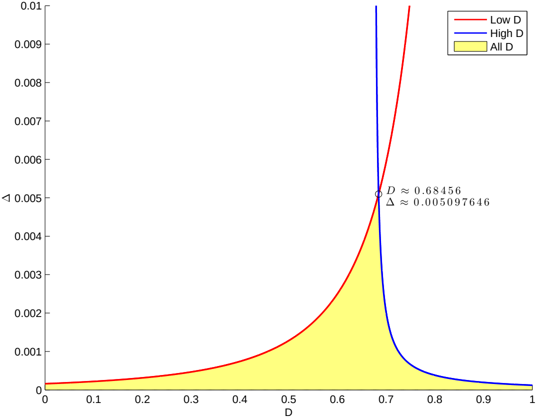

Combining the two bounds gives a D-independent bound on the error

$$\Delta < 1/100$$

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Size Trimming	i	$\mathbf{p_1}$	$dp^2p_1p_2$	$1/100$	–
Bond Trimming	i	p_1	$\mathbf{p_2}$	$1/4$	–
Error Reduction	i	pp_1	pp_2	–	$\mathbf{c\epsilon^3}$
Iteration $i+1$	$i+1$	pp_1	pp_2	–	$c\epsilon^3$
	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$
Iteration $n-1$	n	pp_1	pp_2	–	$c\epsilon^3$
Final iteration	n	p_0p_1	p_0p_2	η	η

Run-time improved to

$$T = \begin{cases} \mathrm{poly}(n/\eta) \cdot n^{\mathcal{O}(\epsilon^{-1})} & \text{for } \eta^{-1} = \mathrm{poly}(n) \\ \mathrm{poly}(n/\eta) & \text{for } \eta^{-1} = 2^{o(\log n)} \end{cases}$$

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  - Could boost heuristic methods such as DMRG.

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- Gives example of Structural Complexity implying Computational Complexity.
- More general area laws, higher dimensions or different conditions.

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All D
Parameter table

Conclusion

Conclusion

- Gives example of Structural Complexity implying Computational Complexity.
- More general area laws, higher dimensions or different conditions.
- More general forms of simulation e.g. time-evolution.