The complexity of simulating strongly correlated quantum systems

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Overview

- Area laws
- Parameterizing ground states
- Complexity of finding ground states
- Dissipative quantum engineering and quantum computation

Hilbert space is a convenient illusion

- Let's investigate the features of the manifold of states that can be created under the evolution H(t) for times T polynomial in number of qubits N: $T = N^d$
  - Solovay-Kitaev: given a standard universal gate set on N spins (cN gates), then any 2-body unitary can be approximated with log(1/ε) standard gates such that $\| U - U_\varepsilon \| < \varepsilon$
  - Given any quantum circuit acting on pairs and of polynomial depth N^d, this can be reproduced up to error ε by using $N^d \log(N^d/\varepsilon)$ standard gates. The total number of states that can hence be created using that many gates scales as

$$(cN)^{N^d \log \frac{N^d}{\varepsilon}}$$

  - Consider however the D^N dimensional hypersphere; the number of points that are ε-far from each other scales doubly exponential in N:

$$\left(\frac{1}{\varepsilon}\right)^{D^N}$$

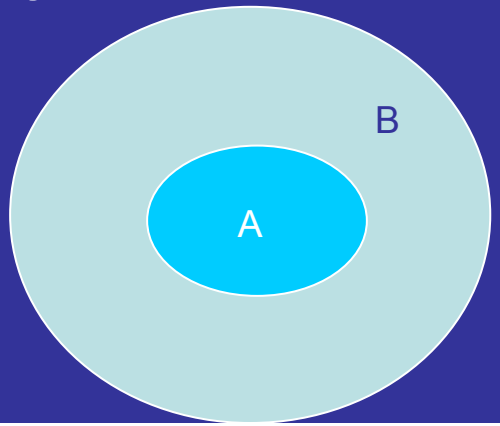
- Conclusion: all physical states live on a tiny submanifold in Hilbert space; there is no way random states (i.e. following the Haar measure) can be created in nature, even with a QC
- What about ground states?

Area laws, correlations, entanglement

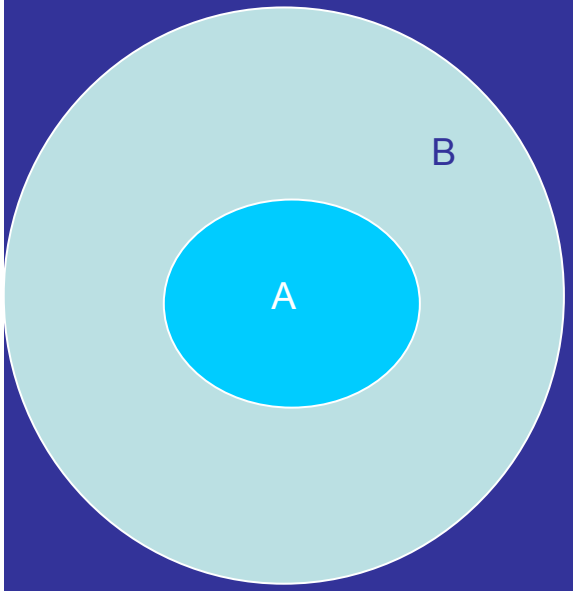
- Ground states and thermal states of local Hamiltonians have very special properties (both for classical and quantum), because the energy only depends on the local correlations
  - Thermal states: state with maximal local correlations compatible with symmetries (typically translational symmetry) *and* global entropy
  - GS: quantum fluctuations can decrease energy: entanglement

- Direct consequence: amount of correlations is small

  - Classical spin system: when looking at configuration of spins in a subregion, how much information does that give me about spins in complementary region?
    - Bounded by boundary between them, not by volume
  - Quantum case: same



Area laws



Quantifying the amount of correlations between A and B: mutual information

$$I_{AB} = S(\rho_A) + S(\rho_B) - S(\rho_{AB})$$

All thermal states exhibit an exact area law (as contrasted to volume law)

$$\rho_{AB} \approx \exp(-\beta H)$$

$$F(\rho_A \otimes \rho_B) = Tr(H\rho_A \otimes \rho_B) - \frac{S(\rho_A \otimes \rho_B)}{\beta} \geq Tr(H\rho_{AB}) - \frac{S(\rho_{AB})}{\beta}$$

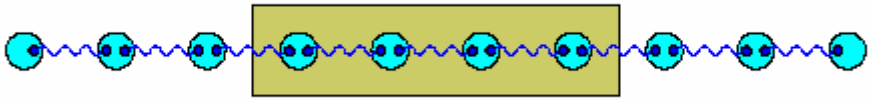
$$\Rightarrow I_{AB} \leq \beta\, Tr(H[\rho_A \otimes \rho_B - \rho_{AB}]) = \beta\, Tr(H_{AB}[\rho_A \otimes \rho_B - \rho_{AB}])$$

Cirac, Hastings, FV, Wolf

- All correlations are *localized* around the boundary, which is a big constraint
- What happens at zero temperature?
  - Classical: nothing
  - Quantum: gapped systems still seem to obey area law, critical systems might get a logarithmic correction (still exponentially smaller than what we get for random states)

Area laws

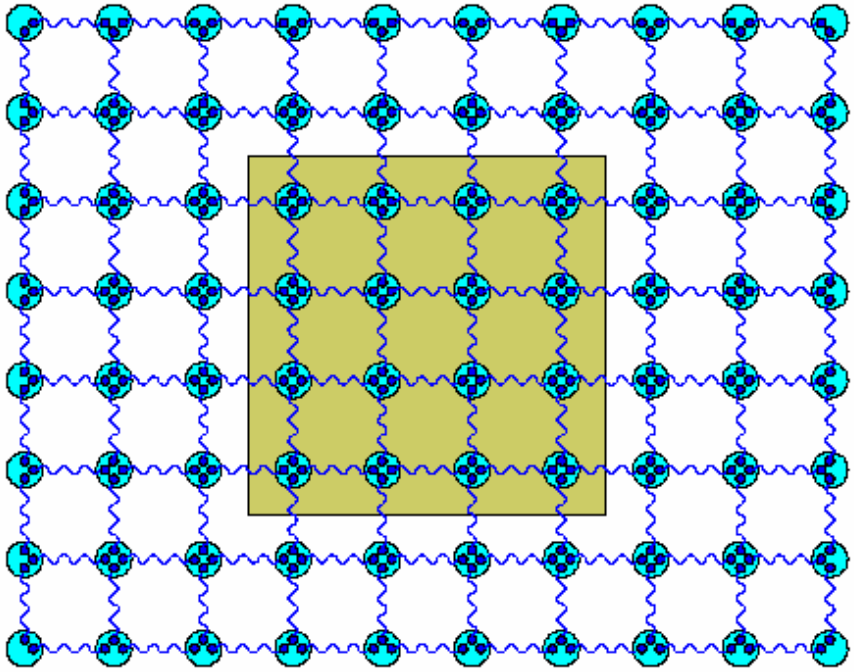
- Main picture: in case of ground states, entanglement is concentrated around the boundary



$$\text{Gapped:}\quad S(\rho_{1,2,\cdots,L}) \approx \frac{c+\bar{c}}{6}\ln(\xi)+\ldots$$

$$\text{Critical:}\quad S(\rho_{1,2,\cdots,L}) \approx \frac{c+\bar{c}}{6}\ln(L)+\ldots$$

Kitaev, Vidal, Cardy, Korepin, …



Gapped $S(\rho_{1,2,\cdots,L^2}) \approx a.\mathrm{L}+\cdots$

Critical

Free fermions $S(\rho_{1,2,\cdots,L^2}) \approx a.L\ln L+\ldots$ Wolf, Klich

Critical spin: $S(\rho_{1,2,\cdots,L^2}) \approx a.L+\ldots$ quant-ph/0601075

Topological entropy: detects topological quantum order locally!

$$S(\rho_{ABC})-S(\rho_{AB})-S(\rho_{AC})-S(\rho_{BC})+S(\rho_A)+S(\rho_B)+S(\rho_C)$$

Kitaev, Preskill, Levin, Wen

Stronger area laws using Renyi entropies

$$S_\alpha(\rho) = \frac{\log Tr \rho^\alpha}{1-\alpha}$$

$$S(\rho) = \lim_{\alpha \to 1} S_\alpha(\rho) \quad ; \quad S_{\alpha' \le \alpha}(\rho) \ge S_\alpha(\rho)$$

- Interpolates between von Neumann (a=1) to Schmidt number (a=0)
- Generic expected behaviour for local 1-D quantum spin systems:

$$\text{Gapped}: \quad S(\rho_{1,2,\cdots,L}) \approx \frac{\ln(\xi)}{\alpha} + \ldots$$

$$\text{Critical}: \quad S_\alpha(\rho_{1,2,\cdots,L}) \approx \frac{c+\bar{c}}{12}\left(1+\frac{1}{\alpha}\right)\ln(L) + \ldots$$

Korepin '05

- Proven rigorously in a model-independent way:

$$\text{Gapped 1D} \Rightarrow S_\alpha(\rho_{1,2,\cdots,L}) \approx \frac{\exp(\xi)}{\alpha} + \ldots$$

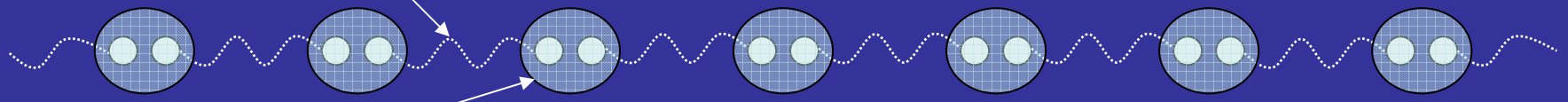
Hastings '07

Parametrizing ground states of quantum spin chains

- Search for class of wavefunctions that capture the properties of ground/thermal states

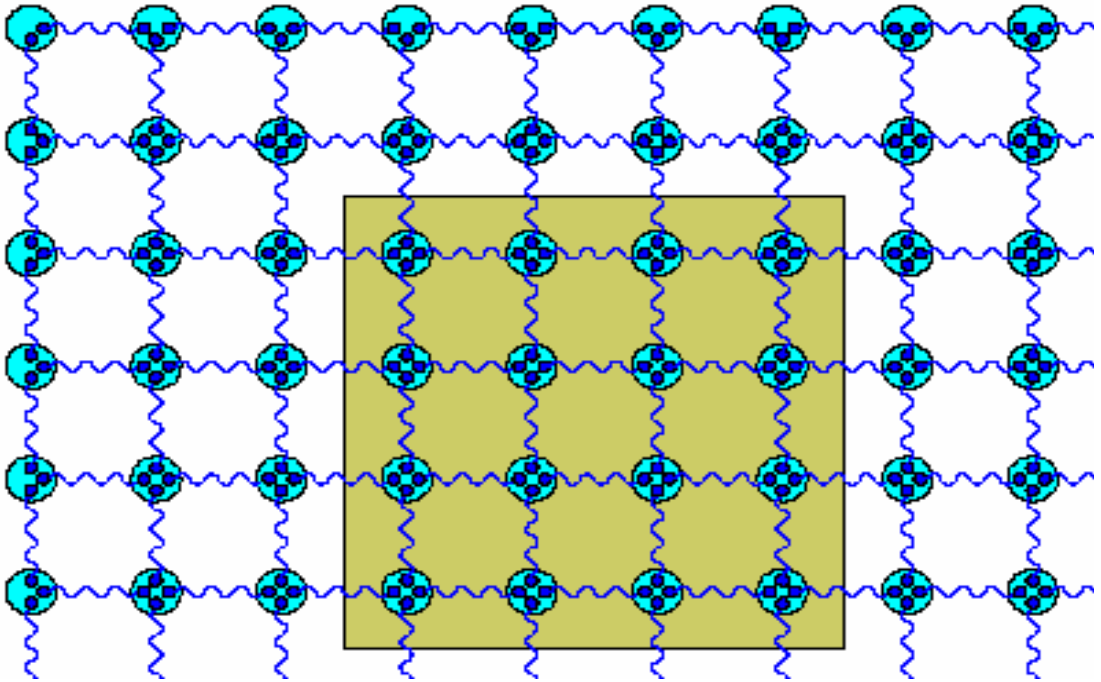
- In one dimension: AKLT/ Matrix Product States / Finitely Correlated States

$$|I\rangle = \sum_{i=1}^{D} |i\rangle|i\rangle$$



$$\text{Map P} : H^D \otimes H^D \rightarrow H^d$$

- In 2-D: AKLT / PEPS:



Efficiency of Parametrization

- So how good will MPS approximate ground states? We want find a bound on the scaling of D as a function of the precision desired and the number of spins N
  - We impose $\left\| \left|\psi_{ex}^{N}\right\rangle - \left|\psi_{D}^{N}\right\rangle \right\| \leq \varepsilon$ with ε independent of N,D
  - Because the scaling of the α-entropy of blocks of L spins in spin chains is bounded by

$$S_\alpha(\rho) = \frac{1}{1-\alpha}\ln\left(\mathrm{Tr}\,\rho^\alpha\right) = \frac{c+\bar{c}}{12}\left(1+\frac{1}{\alpha}\right)\ln(L)$$

    it follows that it is enough to choose $D_N \leq \frac{cst}{\varepsilon} N^{f(c)}$

  - It shows D only has to grow as a polynomial in the number of particles to obtain a given precision, even in the critical case! FV, Cirac, '06
- Hastings 2007: All ground states of gapped Hamiltonians obey area law
  - Similar proof in principle applies to the higher dimensional generalizations of MPS: PEPS
- MPS / PEPS are hence the ideal variational class of wavefunctions for simulating strongly correlated quantum spin systems; in other words: we have identified the right submanifold!

Complexity of finding MPS minimizing energy of a given local 1-D Hamiltonian

- In general: Aharonov/Kempe/Gottesman: no hope for finding GS of general 1-D Hamiltonians: problem is QMA-hard!

- In practice, very efficient method exists to find ground states of 1-D quantum spin systems: DMRG (variational method within the class of MPS)
  - Note: numerical RG of Wilson is also variational within class of MPS
  - How does it work?
    - Alternating least squares (ALS)
    - Complexity of ALS: NP-hard (Nermirovski, Eisert)

- Natural question to ask from the computational complexity point of view:

  - What power would it give me if I could find MPS that minimizes energy of a given 1-D Hamiltonian?

  .

Worst case is NP-complete

- Building upon QMA-constructions of Kitaev
  - Given a quantum circuit consisting of unitaries U_t , we can construct the *almost* frustration free Hamiltonian

$$H = H_0 + \sum_{t=0}^{T-1} H_t + H_f$$

$$H_0 = \left(\sum_{k=anc} |1\rangle_k \langle 1| \right) \otimes |0\rangle\langle 0| \qquad ; \qquad \mathrm{H_f} = |1\rangle_{res} \langle 1| \otimes |T\rangle\langle \mathrm{T}|$$

$$H_t = U_t \otimes |t+1\rangle\langle t| + U_t^{-1} \otimes |t\rangle\langle t+1|$$

whose ground state is

$$|\chi_0\rangle = \frac{1}{\sqrt{T+1}} \sum_{t=0}^{T} |\psi_t\rangle |t\rangle$$

- Kitaev, Kempe, Aharonov, Gottesman: this Hamiltonian can be made local and 1-D (hence deriving QMA-hardness result)
- Observation: if we choose all unitaries to be permutations, then $|\chi_0\rangle$ is a superposition of separable states and hence with all Renyi entropies bounded, but reversible computation has same power as Turing machine hence NP-hardness result
  - gap of Hamiltonian can even be calculated exactly: $\Delta \cong 1/\ poly(N)$
  - To prove that problem is inside NP: trivial

Further results on Quantum Merlin Arthur (QMA)

- Oliveira and Terhal (’04): nearest neighbour Hamiltonian of spin ½ on a square lattice: finding ground state is QMA-complete
  - Trick: use gadgets / perturbation theory to create effective many-body interactions
  - Catch (cfr. Talk of Bravyi): couplings have to scale with system size

- One can go further:
  - Hubbard model with local varying magnetic field: QMA-complete

$$H_{\text{Hubbard}} = -t \sum_{<i,j>,s} a^{\dagger}_{i,s} a_{j,s} + U \sum_{i} n_{i,\uparrow} n_{i,\downarrow} - \sum_{i} \vec{B}_i \cdot \vec{\sigma}_i$$

  - Similar: Heisenberg model with local varying magnetic field
  - Hubbard and Heisenberg model natural candidates for quantum spin glasses

  - Consequences for density functional theory:
    - if an efficient description exists for the universal functional, then QMA=NP !

What about complexity of preparing PEPS?

- At least as hard to find PEPS as it is to find MPS
- Problem is even not in NP:
  - Given a PEPS, calculate its energy is PP-hard problem

    This follows from the fact that the complexity of contracting a tensor network (like arising in classical partition functions) is PP
  - In practice: efficient ways of doing this (PEPS-algorithms exploiting area laws); cfr DMRG
- Important property of all MPS/PEPS: they are ground states of frustration free Hamiltonians

$$H = \sum_t P_t \quad ; \quad P_t \geq 0 \quad ; \quad P_t |\chi_0\rangle = 0$$

- Question: how to prepare “physical” PEPS using a quantum computer?

Dissipative quantum engineering

- Define a dissipative process (master equation) whose fixed point corresponds to ground state of the frustration-free Hamiltonian

$$\frac{d}{dt}\rho = \sum_i L_i \rho L_i^* - \frac{1}{2}\left(\sum_i L_i^* L_i \rho + \sum_i \rho L_i^* L_i \right) \qquad \rho(t) = \exp(Lt)\rho(0)$$

  - A sufficient condition for the ground state to be a fixed point:

$$\forall i: \quad L_i |\psi_0\rangle = 0$$

  - We want that only ground states are fixed points. This we can do by choosing

$$L_i = U_i P_i$$

    where the unitary rotates part of the “bad” subspace into the “good” one. It can be shown that this makes condition also necassary

- This is how to prepare MPS/PEPS

- How efficient? Central quantity of interest: the gap of the Liouvillian

$$\mathcal{L} = \sum_\alpha L_\alpha \otimes \bar{L}_\alpha - \frac{1}{2}\left(\sum_\alpha L_\alpha^\dagger L_\alpha \otimes I + I \otimes \sum_\alpha L_\alpha^\dagger L_\alpha\right)$$

  - Polynomially versus exponentially small in system size: P vs. NP
  - Gap of the Liouvillian quantifies complexity of simulating system on a quantum computer!
    - Gap of Hamiltonian: does not tell anything about computational complexity: Ising spin glasses have gap 1, but gap in Liouvillian should be exponentially small (has this been proven?)
    - Can one prove that this scaling is independent on actual choice of Lindblad operators?

- Note: given a CP-map with corresponding gap, this can always be turned into Liouvillian with same gap (cfr e.g. from Metropolis to Fokker-Planck)

$$\mathcal{L}(\rho) = N\left[\mathcal{T}(\rho) - \rho\right]$$

Examples of dissipative state engineering

- Case of Hamiltonian that only contains commuting terms: convergence after time O(log(N)) or O(N.log(N)) depending on nature of excitations (local vs. topological)
  - Special cases: cluster states, toric code state, …
  - Relevance of this class of states: fixed points of real-space RG transformations on the level of quantum states

- Case of MPS: seems to be efficient (for now, we can only prove that gap = exp(-(logN)^2) using previous Liouvillian, although we now how to do define other one with poly gap).

- General PEPS: no bounds known, as should be (if we could prepare any PEPS with small bond dimension, we could solve any problem in PP=postBQP). Philosophy: physical PEPS will correspond to fast convergence

- Finite-Temperature Gibbs states in case of commuting operators: OK using Metropolis-like ideas

Dissipatively driven quantum phase transitions

- Can a quantum phase transition be driven by dissipation?
- One can easily construct families of frustration free Hamiltonians that exhibit quantum phase transitions: "**Rokhsar-Kivelson"** Hamiltonians
  - Take any classical spin system exhibiting finite-T phase transition (e.g. Ising model)

$$Z = \sum_{s_1 s_2 \ldots} \exp\left(-\beta \sum_{\langle k,l \rangle} H(s_k, s_l) \right)$$

  - Define the quantum state which is coherent version of partition function:

$$|\Psi\rangle = \frac{1}{\sqrt{Z}} \sum_{s_1 s_2 \ldots} \exp\left(-\frac{\beta}{2} \sum_{\langle k,l \rangle} H(s_k, s_l) \right) |s_1\rangle |s_2\rangle |s_3\rangle \ldots$$

    - Has exactly the same correlation functions as classical one
    - Is ground state of local frustration-free Hamiltonian which depends on parameter beta : PEPS!
    - Obviously exhibits a quantum phase transition if parameter beta is varied

- Hence: zero-temperatuere quantum phase transitions can be driven by dissipative processes

Dissipative quantum computation

- What is the computational power of a purely dissipative quantum systems with local Lindblad operators and no coherent evolution?

$$\frac{d}{dt}\rho = \sum_i L_i \rho L_i^* - \frac{1}{2}\left(\sum_i L_i^* L_i \rho + \sum_i \rho L_i^* L_i \right)$$

  - BQP-complete: as powerful as a quantum computer!
  - Proof: use frustration-free Kitaev Hamiltonian where you add appropriate initialization conditions (cfr. Adiabatic QC), use Lindblad operators discussed before, and one can prove that gap of Liouvillian is poly(1/T)
    - gap independent of actual quantum computation done!
    - Defies some of DiVincenzo criteria for QC: no initialization, no unitaries
    - Robustness issues, fault tolerance, comparison with adiabatic QC?

- What about non-equilibrium quantum phase transitions: quantum traffic ?

Simulating general master equations with a QC

- Add qubit ancilla, and couple it via Hamiltonian $H = \Omega(\sigma_- \bar{L}^\dagger + \sigma_-^\dagger L)$ to the original many-body system. Then simulate dephasing channel $L_a = \sqrt{\Gamma}\sigma_-$ on that ancilla with a strength $\Gamma \gg \Omega$
- Second order perturbation theory yields desired master equation
- All gadget constructions can be generalized to this non-Hermitean setting

Conclusion

- Thinking about general structure of low-energy wavefunctions is fun and useful
- Thinking about area laws is fun and useful
- Thinking about computational complexity vs. many-body systems is fun and useful
- Thinking about dissipation is fun and useful
- Thinking about Ackerman numbers is fun and useful
- Thinking about Hamiltonian complexity is fun and useful
- Being in Santa Fe is fun