

### Many-body physics from the point of view of quantum information theory

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#### Setting

- Hilbert space of N particles/spins/modes/qubits: exponentially big
- Central question in QIT: what can I do <u>more efficiently</u> with N qubits than with bits?
  - IT tasks: Quantum Computing, Quantum Cryptography
  - Physics tasks: Quantum Simulation (condensed matter systems, quantum chemistry, ...)
- Central theoretical problems (not mentioning experimental related ones):
  - What are the minimal requirements to be able to do universal quantum computation?
  - What is the role of entanglement?
  - Can coherence be preserved in arbitrary large systems for arbitrary long times? (quantum fault tolerance)
  - What is the complexity of simulating quantum systems?
    - What computational power would it give me if I could e.g. find the ground state of a certain class of Hamiltonians

#### Topics

- Hilbert space is a convenient illusion
- Computational complexity of simulating strongly correlated quantum systems
- Entanglement structure of ground states of many-body Hamiltonians on the lattice
- Quantum circuits for simulating quantum Hamiltonians

#### Accessibility of full Hilbert space is an illusion

- Size of Hilbert space of system of N particles / modes / ... scales exponentially with N.
  - What is the fraction of states that are physical, i.e. can be created as by a quantum computer in a time that scales polynomially with the systems size?
     Exponentially small : A quantum computer cannot explore the full Hilbert space



A. Qarry, FV '09

- All physical states live on a tiny submanifold: this opens up the possibility of parameterizing this corner in Hilbert space (opens door for variational methods)
- Lots of work on random states: e.g. Popescu, Winter et al.: take a random state with a given energy, and look at a small subsystem: looks like  $\rho^{-\beta H}$

## Quantum simulation from the computer science point of view

• What is the computational complexity of finding ground states of general local Hamiltonians (e.g. nearest neighbour interactions on a square lattice)?



- P: class of problems that can be solved efficiently using classical computer
- BQP: class of problems that can be solved efficiently using quantum computer
- NP: class of problems whose solution can be checked efficiently using classical computer
- QMA: class of problems whose solution can be checked efficiently using quantum computer
- Kitaev/Aharonov/Kempe/Terhal/Irani/Gottesman/...: QMA-hard as a function of N for local lattice Hamiltonians in any dimension!

- What about reasonable Hamiltonians?
  - Take e.g. the problem of estimating the ground state energy of a system of N electrons interacting via the Coulomb force in an external potential (input variables = external potential): QMA-hard

N. Schuch, FV '08

- Direct implications:
  - An efficient specification of the universal density functional as used in density functional theory would imply QMA=P
  - Hubbard model with constant t and U but varying onsite magnetic fields: QMA-complete

- Central problem in field of quantum chemistry: N-representability
  - Is there a N-particle quantum state compatible with the 2-particle density operator  $\langle a_i^* a_j^* a_k a_l \rangle$ ?
    - Problem is intractable: QMA-complete!

Liu, Christandl, FV, PRL '07

- But: it is not because ground states are hard to find, that there is no simple parameterization of them: they might have a very simple structure (cfr. Spin glasses)
- Can we identify the corner in Hilbert space that corresponds to ground states of local many-body quantum Hamiltonians?
  - Is so: this would lead to a systematic way of coming up with variational ansatze
    - Cfr. some of the biggest breakthroughs in condensed matter physics involved guessing the right wave function (BCS, Laughlin, ...)
  - What is the structure of entanglement in those systems?

#### Entanglement structure of relevant states: 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)

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

$$F(\rho_{A} \otimes \rho_{B}) = Tr(H\rho_{A} \otimes \rho_{B}) - \frac{S(\rho_{A} \otimes \rho_{B})}{\beta} \ge Tr(H\rho_{AB}) - \frac{S(\rho_{AB})}{\beta}$$
$$\Rightarrow I_{AB} \le \beta Tr(H[\rho_{A} \otimes \rho_{B} - \rho_{AB}]) = \beta Tr(H_{AB}[\rho_{A} \otimes \rho_{B} - \rho_{AB}])$$

Cirac, Hastings, Wolf, FV '08

- 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)
     Kitaev, Vidal, Wolf, Korepin, ...
  - Gapped 1-D quantum spin systems: always obey strict area law!

Hastings '08

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#### Matrix Product States

- If an area law applies, then a state can efficiently be parameterized by a socalled matrix product state (MPS) / valence bond state / finitely correlated state
  - MPS: most general state in 1-D that obeys a strict area law by construction: rank of reduced density operators is cst (D<sup>2</sup>)

 We want to bound the cost of approximating state that obeys area law with a MPS for given precision as a function of number of spins:

$$\left\|\psi_{ex}^{N}\right\rangle - \left|\psi_{D}^{N}\right\rangle\right\| \leq \varepsilon \qquad \qquad D_{N} \leq \frac{CSt}{\varepsilon} N^{f}$$

- Breaking of exponential wall: polynomial vs. exponential complexity
- Complete identification of manifold of ground states of gapped quantum spin systems
  - DMRG, MPS-based algorithms: variational methods within this class of states!

#### Projected Entangled Pair States (PEPS) / Tensor Product States (TPS)



- Natural generalization of MPS to higher dimensions
- Obeys area laws, ... : parameterization of every GS of gapped 2-D quantum Hamiltonian (Hastings)
- Can be generalized to fermionic systems without sign problem
- What is best way of doing variational calculations with those states?

FV, Cirac '04

#### Quantum simulators for finding ground states: adiabatic time evolution

Farhi et al.'00



Adiabatically following the ground state of a Hamiltonian; adiabatic condition:

$$T >> \min_{s} \frac{\Gamma(s)}{\Delta(s)^{2}}$$
  $\Gamma(s) = \left\langle \left(\frac{dH}{ds}\right)^{2} \right\rangle - \left\langle \frac{dH}{ds} \right\rangle^{2}$ 

- That means: we can prepare ground state in phases different from the one we start from on a QC if no level crosssing and/or gap scales polynomial in system size
- This suggests that a very good way of representing ground states can be found using a quantum circuit!

#### **Quantum Circuits**

Quantum circuit is a representation of every possible Hamiltonian evolution



- What kind of quantum circuits are needed to prepare ground states of general Hamiltonians?
  - Find inspiration in field of renormalization group methods and perturbation theory

#### RG-methods as quantum circuits

• Numerical renormalization group:





Class of states generated like this:

Matrix Product States

Virtue: possible to calculate any tensor product expectation value efficiently -> quantum circuit that can be simulated efficiently on a classical computer

#### RG quantum circuit in the lab

- Class of D-dim. MPS gives a complete characterization of all N-particle states that can be created by sequential generation through coupling to a D-level ancillary system (Markov chain)
  - Photonic qubits generated by a cavity QED source
  - Quantum dot coupled to a microcavity
  - Interaction of ions with phonons in ion trap

#### 0 0 D

- 1-to-1 correspondence between maps P and unitaries occurring in "cavity"
  - Constructive: MPS-structure automatically yields description of how to generate states
- Example for D=2: GHZ-, cluster-, W- states

- Other RG schemes: Ma-Dasgupta-Fisher renormalization group
  - Random Heisenberg model



$$\begin{bmatrix} -\varepsilon^2 A B^{-1} A^* & O(\varepsilon^3) \\ O(\varepsilon^3) & Q \end{bmatrix} = \begin{bmatrix} I & \varepsilon X \\ -\varepsilon X^* & I \end{bmatrix} \begin{bmatrix} 0 & \varepsilon A \\ \varepsilon A^* & B \end{bmatrix} \begin{bmatrix} I & -\varepsilon X \\ \varepsilon X^* & I \end{bmatrix}$$

 The class of wavefunctions obtained like this coincide with the Multiscale entanglement renormalization ansatz (MERA) of G. Vidal

# Vidal '06 MERA: coarse-graining of lattice

• What about scale-invariant states for fermions: OK

Corboz, Evenbly, FV, Vidal '09

• PS: all MERA states obey strict area law in dimensions>1

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# What happens for non-equilibrium systems?

- Quantum circuits with CP-maps instead of unitaries
- Can again be very well described by MPS; figure of merit is the entanglement of purification



Mutual information and entropy cost / entanglement of purification as a function of lpha , eta

#### Quantum circuits for diagonalizing Hamiltonians

- One can in principle go further and try to diagonalize a complete Hamiltonian using a quantum circuit (cfr. Original approach of Wilson)
  - Possible because all low-energy states are "special" (effective lowenergy Hamiltonians can e.g. be theories of quasi-free particles)

 $UHU^* = H_{coarse-grained}$ 

- For 1-D Ising model in transverse field:  $H_{eff} = UH_{XY}U^* = \sum_i \omega_i \sigma_i^z$
- Can be done for e.g. perturbed Kitaev model



Kitaev's toric code Hamiltonian is a fixed point of such a coarse-graining transformation; local perturbations can be proven to be irrelevant perturbations (become smaller and smaller)

Classification of fixed points leads to a classification of topological theories

Coarse-graining at finite T: temperature goes up!

Veznik, Rico, Schuch, FV

#### Conclusion

- Quantum information theory offers new look at the many-body quantum problem
  - Motivation: what can we do more efficiently with qubits than with bits
  - What are fundamental limits of DFT, ...
- Insights into the entanglement structure lead to novel simulation methods : MPS, PEPS, MERA