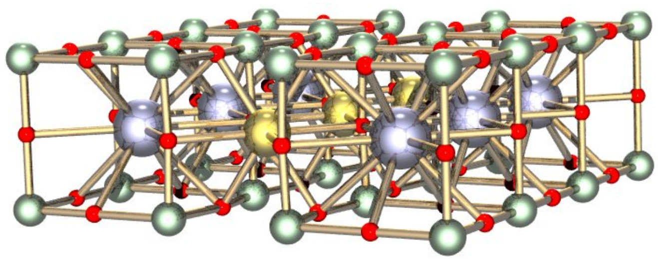
The computational difficulty of finding MPS ground states

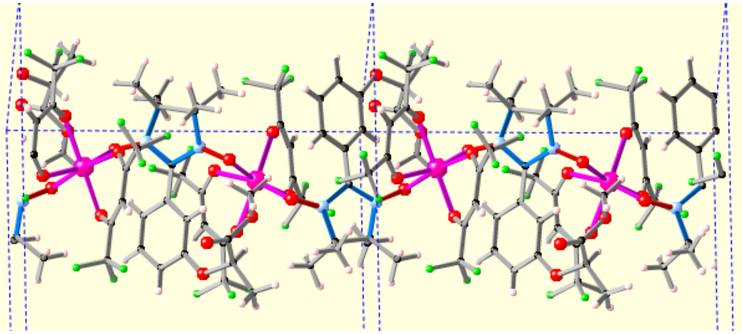
Norbert Schuch[1], Ignacio Cirac[1], and Frank Verstraete[2]

[1] Max-Planck-Institute for Quantum Optics, Garching, Germany
[2] University of Vienna, Vienna, Austria

Introduction

• Simulation of quantum spin lattices: central in condensed matter



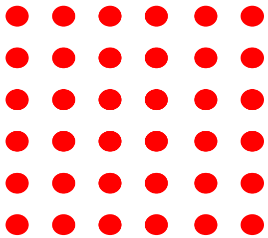


... e.g. understand the **ground state properties** of such systems

• Various successful algorithms, e.g.
  - Quantum Monte Carlo (QMC)
  - the Density Matrix Renormalization Group (DMRG) for 1D

• Want to understand (prove) range of applicability

One dimension is special



anything down
to 2D systems

- there exist problems
  where algorithms don't work
- *classical* 2D spin glasses **NP**-hard
  [Barahona '82]
- Quantum problem **QMA**-hard,
  even on *2D lattice of qubits*
  [Oliveira & Terhal '05]
- "physical" hard problems exist:
  simple spectrum & ground states

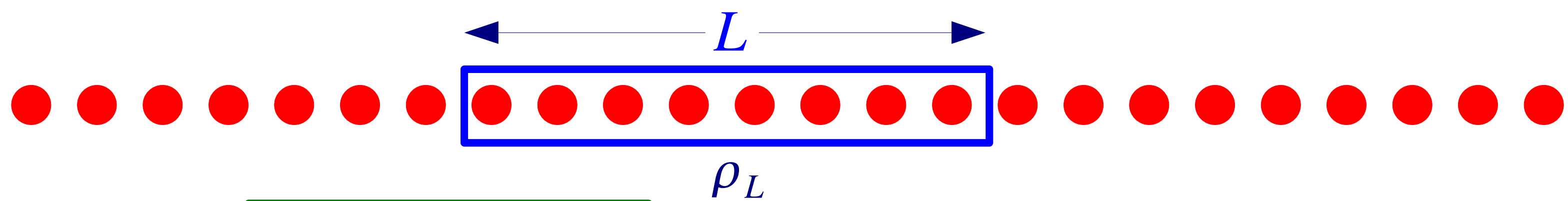
spin chains

- DMRG ess. always works in practice
- *classical* problem is easy
- **Quantum version QMA-hard !!**
  [Aharonov, Gottesman, Irani & Kempe '07]
- Hard instances have a **very complicated spectrum** and **highly entangled ground states**!

→ **unrealistic!**

DMRG

- Density Matrix Renormalization Group (DMRG): [White '92]
  Variational method over Matrix Product States (MPS)
- MPS have an efficient classical description
- Relevant property of MPS: Low amount of entanglement



$$S(\rho_L) \le \text{const.}$$ (*very* non-generic!)

⇒ ground states of gapped Hamiltonians well described by MPS [Hastings '08]

- Ground states of **QMA**-hard 1D systems are **highly entangled**
  ⇒ they cannot be described by MPS ⇒ **DMRG *cannot* work**!

Conjecture: DMRG works well on all "physical" systems, in particular those with low ground state entanglement.

However ...

Even under this assumption DMRG cannot always work.

- We construct a 1D Hamiltonian with:
  - **unique MPS ground states**
  - **nice spectral properties**, in part. a 1/poly(N) spectral gap
  - **it is frustration free**
    (≡ ground state already minimizes all local terms in the Hamiltonian)

  ... yet **finding its ground state is at least as hard as factoring!**

- Without uniqueness & frustration freeness, its **even NP-hard**.

  (cf. poster of Aharonov, Ben-Or, Brandao and Sattath:
  1D Hamiltonian with unique g.s. and 1/poly(N) gap is QCMA-hard)

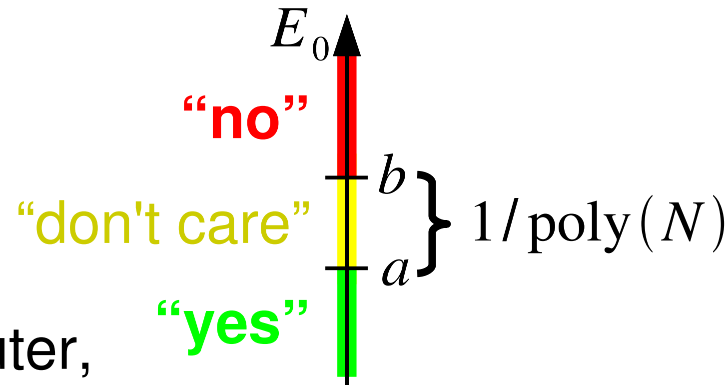
- ... and our results imply more limitations:
  - the success of **DMRG cannot even be certified**
  - **DMRG can't even work on frustration free systems**

QMA and ground state problems

- QMA: The **quantum version of NP** – the class of problems where "yes" instances have a **quantum proof** which can be **efficiently checked by a quantum computer**

- How does this relate to the complexity of "finding ground states"?

- Decision problem: Given $H = \sum h_i$,
  determine if $E_0(H) < a$ or $E_0(H) > b$
  (≈ compute E_0 with poly. accuracy)



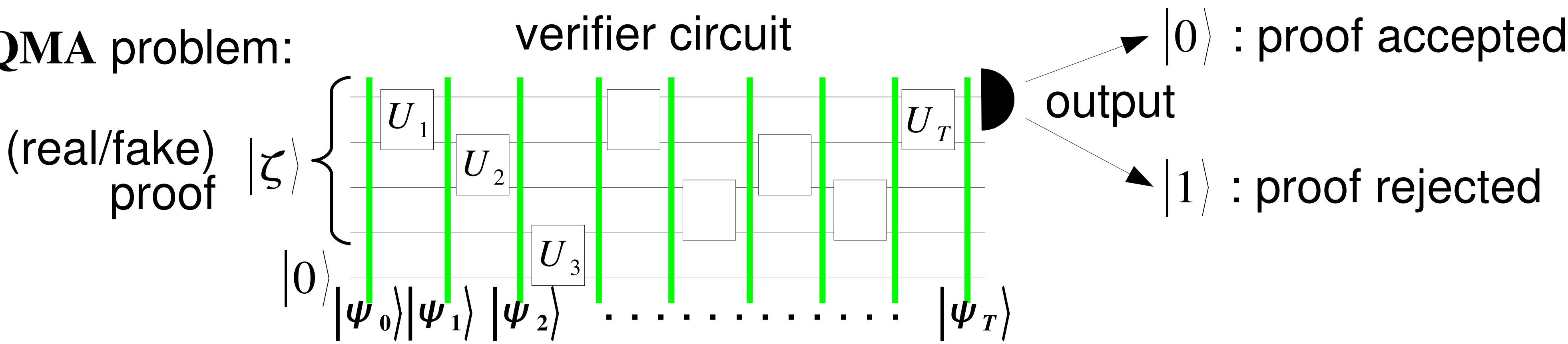
- This problem is inside **QMA**:
  The proof is $|\psi_0\rangle^{\otimes N}$ – using a quantum computer,
  $E(|\psi_0\rangle)$ can be estimated with polynomial accuracy.

- Can we, conversely, take any problem in **QMA**
  – i.e. anything which can be proven to a quantum computer –
  and rephrase it as a ground state problem?

Kitaev's QMA-hardness construction

Arbitrary problem in **QMA**: Can it be rewritten as a g.s. problem?

- **QMA** problem:



$\Rightarrow |\chi\rangle = \sum_{t=0}^{T} |\psi_t\rangle \otimes |t\rangle$ encodes the "proof history"

- construct Hamiltonian with valid history as ground state (if it exists!)

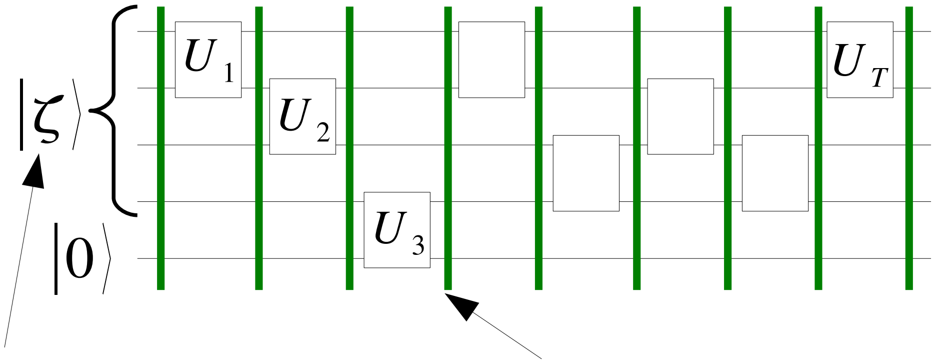
$$H = H_{\text{init}} + H_{\text{evol}} + H_{\text{final}}$$

Ham. penalizes:	wrong ancillas	wrong transitions	proof rejected

- "no" instances have to violate some of these terms:
  $\Rightarrow$ their g.s. energy is by 1/poly(N) above "yes" instances ("promise gap")

How to get rid of the entanglement

- "Problem": QMA problems yield highly entangled ground states!



$$|\chi\rangle = \sum_{t=0}^{T} |\psi_t\rangle \otimes |t\rangle$$

highly ent. arbitrary quantum circuit: highly entangling!

- Less entangled ground states $\rightarrow$ Restrict proof & verifier!

- Our choice: **Classical proofs** and **classical verifier** circuits

  $\Leftrightarrow$ restriction to **problems in NP**

- $|\chi\rangle = \sum_{t=0}^{T} |\psi_t\rangle \otimes |t\rangle$ superposition of $T = \mathrm{poly}(N)$ classical states, thus only weakly entangled ($\rightarrow$ MPS structure in 1D)

  (With two-qubit gates only, each timeslice can be slightly entangled)

The structure of the Hamiltonian

- QMA problems: Spectrum complicated
  (many proofs with similar acceptance probablity)

- classical **deterministic** verifiers: deterministic acceptance/rejection

- For any classical input $|\boldsymbol{a}\rangle$ to the verifier (incl. ancillas!), define

$$\mathscr{H}_{\boldsymbol{a}} = \mathrm{span}\left\{ |\boldsymbol{a}\rangle, U_1|\boldsymbol{a}\rangle, \dots, U_T \cdots U_1 |\boldsymbol{a}\rangle \right\}$$

$\Rightarrow$ H acts *independently* on the $\mathscr{H}_{\boldsymbol{a}}$

$$H\big|_{\mathscr{H}_{\boldsymbol{a}}} = \begin{pmatrix} TA+1 & -1 & & & \\ -1 & 2 & -1 & & \\ & \ddots & \ddots & \ddots & \\ & & -1 & 2 & -1 \\ & & & -1 & B+1 \end{pmatrix}$$

H_{init}

$H_{trans} = \sum_t \begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix}_{t,t+1}$

H_{final}

- $A = 0,1,2,\dots$: number of wrongly initialized ancillas
- $B = 0,1$: proof accepted/rejected

- This is a quantum random walk, techniques & solutions exist

Analyzing the spectrum

! We are interested in the **spectral gap** for each instance independently, not in the **promise gap** between "yes" and "no" instances.

"yes" instances

- $\exists\ |\boldsymbol{a}_0\rangle$ s.th. $A=0, \boldsymbol{B=0}$ in $\mathscr{H}_{\boldsymbol{a}_0}$
- ground state: $E_0=0$ in $\mathscr{H}_{\boldsymbol{a}_0}$ (frustration free!)
- gap: i) Within $\mathscr{H}_{\boldsymbol{a}_0}$: $E_1=\Omega(1/T^2)$
  ii) To g.s. of other $\mathscr{H}_{\boldsymbol{a}}$:
  $E\geq E_0(A=0,B=1)=\Omega(1/T^2)$

"no" instances

- $\nexists\ |\boldsymbol{a}_0\rangle$ s.th. $A=0, B=0$
- ground state for $A=0, \boldsymbol{B=1}$
- gap: i) within this subspace: $\Omega(1/T^2)$
  ii) to subsp. with $A>0$: $\Omega(1/T^2)$
  using Lemma on $\lambda_{\text{min}}(P+Q)\geq\ldots$

- spectral gap $\Omega(1/T^2)$
- "yes" instances frustration free
- excited states also have simple ent. structure

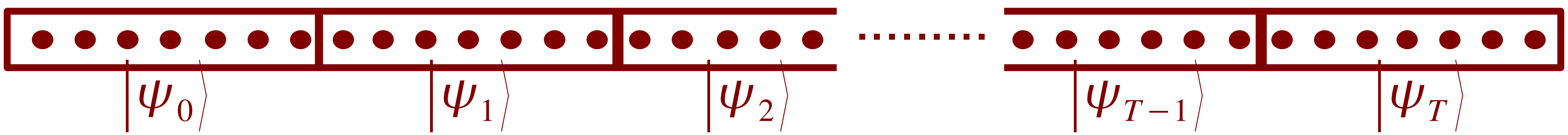
One-dimensionalizing the problem

- Problem in 1D: How to make time register locally accessible?

$$\left|\chi\right\rangle = \sum_{t=0}^{T} \left|\psi_t\right\rangle \otimes \left|t\right\rangle$$

[Aharonov, Gottesman, Irani & Kempe '07]

- Encode time in spatial location of qubits!

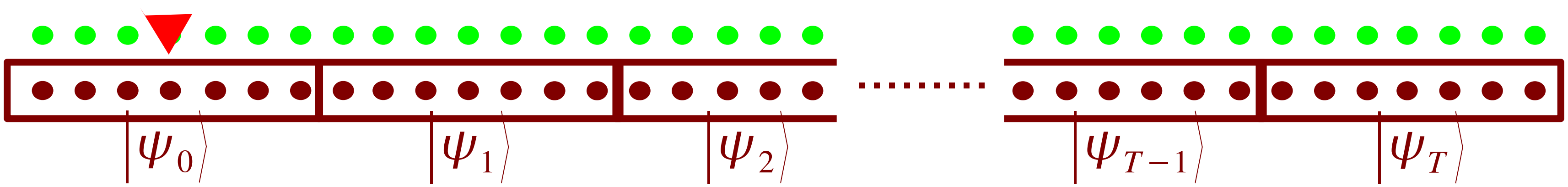


$$\left|\tilde{\chi}\right\rangle = \left|\psi_0\right|\emptyset\left|\emptyset\right|\emptyset\cdots\rangle + \left|\emptyset\right|\psi_1\left|\emptyset\right|\emptyset\cdots\rangle + \left|\emptyset\right|\emptyset\left|\psi_2\right|\emptyset\cdots\rangle + \ldots$$

- But how to implement H?

One-dimensionalizing the problem

- Realization of H: add control register;
  implement “head” propagating qubits and implementing circuit



- Extra term H_{penalty} penalizes illegal control register states

- “Clairvoyance lemma”: State space splits into
  - i) **one subspace** with **valid** control register configurations
  - ii) subspaces with only invalid configurations

  $\Rightarrow$ Any subspace ii) has energy at least $\Omega(1/T)$ (boosted).

$\Rightarrow$ Low-energy sector in subspace i) – same result as before.

Implications for DMRG

- apply to verifier circuit with **exactly one** satisfying assignment
  $\rightarrow$ e.g. prime factor decomposition

  (problems in $\mathbf{NP} \cap \mathbf{coNP}$ with unique proofs, or unique $\mathbf{TFNP}$)

The resulting Hamiltonian
- has a **unique MPS ground state**
- with a $1/\mathrm{poly}(N)$ **spectral gap** above
- low-energy eigenstates are MPS
- is **frustration free** (there are only "yes" instances)

But finding its ground state is at least as hard as factoring.

Notes: i) Ground state energy is always zero (decision problem trivial)!
ii) Solution can be read off the ground state ($\Rightarrow$ harder than decision problem!)

NP-hard instances

- What happens if we take an **NP**-complete problem?
- There are “yes” and “no” instances $\Rightarrow$
  - not frustration free (for “no” instances)
  - ground state not unique (at least for “no” instances)

The resulting Hamiltonian
- has **MPS ground states**
- a $\mathbf{1/\mathrm{poly}(N)}$ **spectral gap** above ground states
- low-lying eigenstates are MPS

Finding the ground state (energy) is NP-hard.

Notes: i) Ground state energy answers NP problem.
ii) “yes” instance: ground state contains solution ($\Rightarrow$ harder than decision problem!)

More implications

- **DMRG (probably) cannot be *certifyable*!**

> **Certifyability:** We cannot guarantee that DMRG converges, but **if it converges, it returns a certificate** proving it worked.

- Proof: - Take Hamiltonian encoding an NP problem
  - Assume DMRG certifyable $\Rightarrow$ "no" instances can be disproven

$$\Rightarrow \mathbf{NP} = \mathbf{coNP}$$

- **DMRG cannot even provably work for frustration free systems!**

- Proof: - Take Hamiltonian H encoding an NP-complete problem
  - Let DMRG algorithm run on H and check g.s. energy
  - "yes" instance $\Leftrightarrow$ frust. free $\Leftrightarrow$ DMRG works $\Leftrightarrow$ $E_0 = 0$
  - "no instance $\Leftrightarrow$ $E_0 > 1/\mathrm{poly}(N)$

$\Rightarrow$ Could be used to solve $\mathbf{NP}$-complete problems!

Summary

• apply Kitaev's QMA construction (and 1D version) to NP problems

⇒ class of Hamiltonians with:

unique MPS ground state, frustration free, 1/poly(N) gap

which is **at least as hard as factoring**

⇒ class of Hamiltonians with

MPS ground states, 1/poly(N) gap

which is **NP-hard**

("classical" version of 1D problem)

⇒ **no certifyable DMRG** can exist

⇒ no provable **DRMG for frustration free systems**

? What requirements do we need to prove that DMRG works? ?