The Complexity of Hamiltonian Problems

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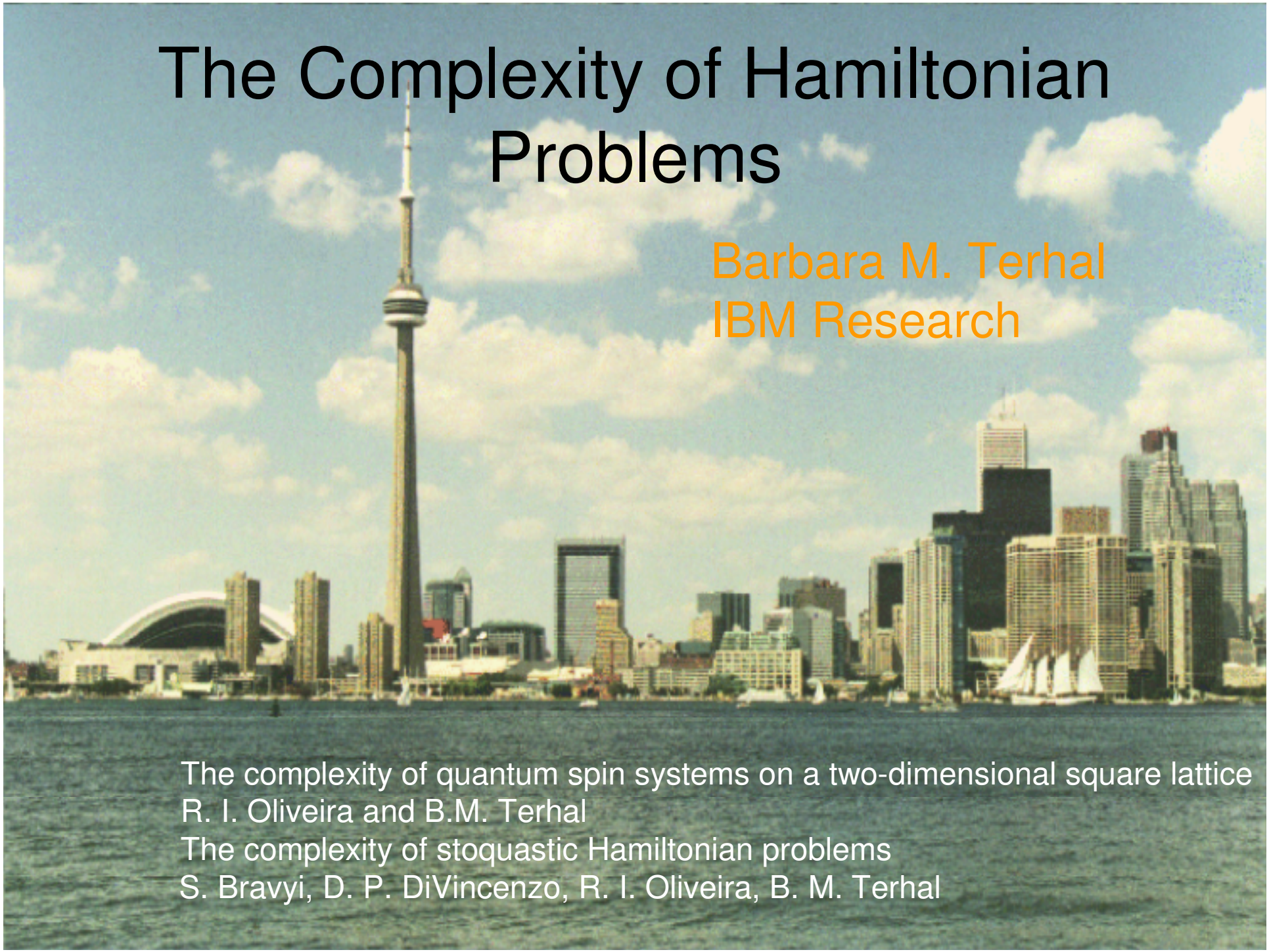


The complexity of quantum spin systems on a two-dimensional square lattice
R. I. Oliveira and B.M. Terhal
The complexity of stoquastic Hamiltonian problems
S. Bravyi, D. P. DiVincenzo, R. I. Oliveira, B. M. Terhal

Computational Complexity of Decision Problems

Merlin.
The all-powerful prover which cannot necessarily be trusted. The goal of Merlin is to prove to Arthur that the answer to his decision problem is YES. If this can be achieved the proof is complete. If the answer is NO, Merlin can still try to convince Arthur that the answer is yes. The proof is sound if Arthur cannot be convinced.

Arthur.
A mere mortal who can run polynomial time algorithms only. Wants to solve the decision problem by possible interaction(s) with Merlin.

Computational Complexity

	Interaction between Arthur and Merlin	Arthur runs	Arthur outputs A_x
P	none	p(olynomial)time algorithm in size of input x	If Y(es), $A_x=1$ If N(o), $A_x=0$
BPP	none	ptime probabilistic algorithm	If Y, $P(A_x=1) \geq 2/3$ If N, $P(A_x=0) \geq 2/3$
NP	Proof y by Merlin	ptime algorithm with input y	If Y, $\exists$ y, $A_x(y)=1$ If N, $\forall$ y $A_x(y)=0$
MA	Proof y by Merlin	ptime probabilistic algorithm with input y	If Y, $\exists$ y $P(A_x(y)=1) \geq 2/3$ If N, $\forall$ y $P(A_x(y)=0) \geq 2/3$

Computational Complexity

	Interaction between Arthur and Merlin	Arthur runs	Arthur outputs A_x
AM	Arthur gives Merlin random r. Merlin returns random proof y_r	ptime probabilistic algorithm	If Y, $P(A_x(r,y_r)=1) \geq 2/3$ If N, $P(A_x(r,y_r)=0) \geq 2/3$
BQP	None	ptime quantum algorithm	If Y, $P(A_x=1) \geq 2/3$ If N, $P(A_x=0) \geq 2/3$
QMA	Quantum proof ξ by Merlin	ptime quantum algorithm	If Y, $\exists\ \xi\ P(A_x(\xi)=1) \geq 2/3$ If N, $\forall\ \xi\ P(A_x(\xi)=0) \geq 2/3$
PostBPP	None	ptime probabilistic algorithm,post-selection on a bit b=1	If Y, $P(A_x=1\|b=1) \geq 2/3$ If N, $P(A_x=0\|b=1) \geq 2/3$

Classical Spin Glass is NP-complete

A decision problem L is NP-complete when

- The problem L is in NP.
- Any problem in NP can be mapped onto L so that solving L efficiently implies solving any problem in NP efficiently.

An example, Barahona '82:

Definition 3 (ISING SPIN GLASS) *Given is an interaction graph* $G = (V, E)$ *with Hamiltonian*

$$H_G = \sum_{i,j \in E} J_{ij} Z_i \otimes Z_j + \sum_{i \in V} \Gamma_i Z_i. \qquad (1)$$

Here the couplings $J_{ij} \in \{-1, 0, 1\}$ *and* $\Gamma_i \in \{-1, 0, 1\}$ *and* $Z = |0\rangle\langle 0| - |1\rangle\langle 1|$ *is the Pauli* Z *operator. Decision Problem: is* $\lambda(H_G) \leq \alpha$*?*

λ(H) is the ground-state energy.

Is there a similar result for quantum spin glasses?

Local Hamiltonian Problems (LH-MIN)

Given is a k-local Hamiltonian H. Either the ground-state energy $\lambda(H) \leq \alpha$ or $\lambda(H) \geq \beta$ for two given constants $\alpha < \beta$ (with $|\beta-\alpha| \geq 1/\text{poly}(n)$)
k-local means that the Hamiltonian is a sum of interactions and each interaction is between at most k qubits.

Kitaev: 5-local LH-MIN is QMA-complete.

Further results:
Kempe, Kitaev, Regev: 2-local Hamiltonian is QMA-complete.
Aharonov *et al.*: 2-local Hamiltonian using 6-dimensional particles on a 2D lattice is QMA-complete.
Oliveira, Terhal: 2-local Hamiltonian on qubits on a 2D lattice is QMA-complete.
Quantum counterpart of the classical result. Uses perturbation theory.

Our starting point and our goal

A 5-local Hamiltonian with the following structure.
Each qubits is involved in a constant number of 5-local interactions.
Each 5-local interaction involves only qubits in each other's neighborhood when we represents the qubits on a 2D plane.

Goal: find a 2-local Hamiltonian with approximately the same lowest ground-state energy as the 5-local Hamiltonian and the following structure

1. Each qubit is involved in at most 4 interactions and each interaction is a simple tensorproduct of two Pauli operators.
2. The 2-local (2-qubit) interactions occur between nearest neighbor qubits in a plane (there are no crossing interaction edges) or on a 2D lattice.

This can all be accomplished using perturbation theory based on mediator qubits.

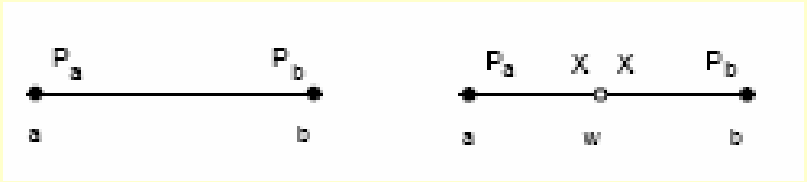
- Any k-local Hamiltonian can be treated this way.
- Perturbation method can also reproduce ground-states (and gaps) approximately.

Novel use of perturbation theory

In physics we usually have Hamiltonian in which the strength of different interactions or fields vary widely. We use perturbation theory to understand the effective behavior of such Hamiltonian. Example: two spin ½ particles interacting weakly with a photon mode; this can generate an effective interaction between the spin ½ particles.

Here, the opposite approach. We have a target interaction which may involve several qubits and we want to generate it effectively by choosing a Hamiltonian with a large term and a small perturbation.

Perturbatively mediated interactions



Consider k-local interaction $H_{target}=A\mathbb{1}\quad B$ where A and B are k/2-local operators on sets of qubits a and b.

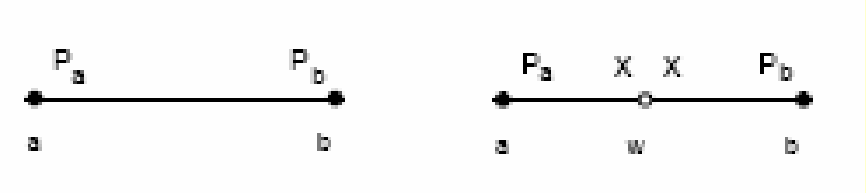
Define a new qubit w, the mediator qubit and a new hamiltonian $\hat{H}=H+V$. The mediator qubit interacts with the set a and the set b in V and mediates the interaction between a and b.

|1> ——— ≡≡≡ $H=\Delta\,|1\rangle\langle 1|_w$ with large Δ

|0> ——— ≡≡≡ $V=(\Delta/2)^{1/2}\,(-A+B)\mathbb{1}\quad X_w$ where $||V|| < \Delta/2$

Here X_w is the Pauli X operator on the mediator qubit.
In the unperturbed groundstate the mediator qubit is set to |0>. V is a small perturbation that gives a correction to this ground-state and its energy.

Perturbatively mediated interactions



$\hat{H}=H+V$ where $H=\Delta\,|1\rangle\langle 1|_w$ with large Δ

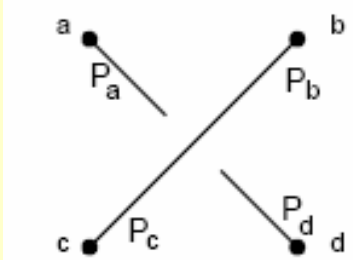
$V=(\Delta/2)^{1/2}\,(-A+B)\mathbb{1}\quad X_w$ where $||V|| < \Delta/2$

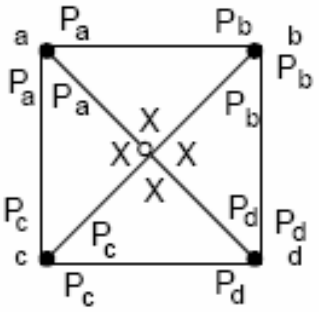
This correction can be estimated by evaluating the self-energy up to lowest relevant order in perturbation theory. Second order processes involves flipping the mediator qubit by interaction (with V) and flipping it back: This generates an effective interaction approximately equal to

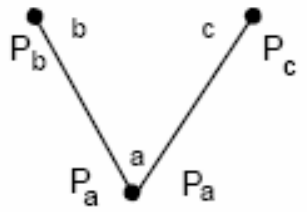
$H_{eff}\mathbb{1}\ (-(\Delta/2)\,(-A+B)^2/\Delta)\mathbb{1}\quad |0\rangle\langle 0|_w=(H_{target}+A^2/2+B^2/2)\mathbb{1}\quad |0\rangle\langle 0|_w$

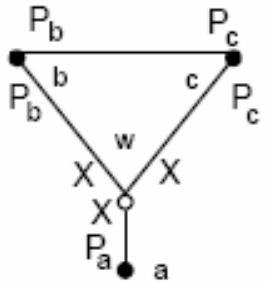
One can prove a rigorous theorem showing that $\lambda(\hat{H})\ \mathbb{1}\ \lambda(H_{eff})$
Repeated (serial) application of this trick gives 3-local terms. Kempe *et al.* has a 3 to 2-local gadget (or one can use an alternative mediator qubit gadget)

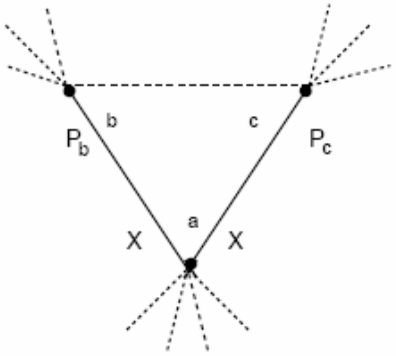
Applications of mediator qubits

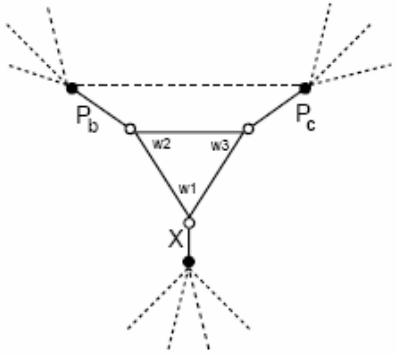












Cross Gadget: removing a cross in the interaction graph. All qubits a,b,c,d can flip the mediator qubit.

Fork Gadget:
Qubit a interacts with b and c with (Pauli) operator P_a.

`Degree reduction': First we put mediator qubits on the edges ab and ac. Then we apply the Fork gadget.

Parallel and serial application of these gadgets

We can show that the ground state energy of our 5-local Hamiltonian can be approximated by the ground state energy of a 2-local Hamiltonian on a 2D lattice by applying the perturbation gadgets in parallel and in series.

In parallel: O(n) interactions are generated by introducing a new Hamiltonian with O(n) mediator qubits and O(n) perturbations V_i.
To 2^{nd} order in perturbation theory these gadgets act independently.
But Δ for each mediator qubit has to be larger than $2 \Sigma_i ||V_i||$=poly(n), polynomial in the total number of qubits n.

Final 2-local interaction has large fields that are poly(n) in strength and small interactions that are constant (as a function of n) in strength.

In series: the total number of these parallel applications will be constant, since fields scale approximately as n^c after c applications.

More general use of perturbation theory

Let's say we have an `interesting' space or state that is the ground-space of a k-local Hamiltonian with some spatial structure (every qubit interacts with a set of `neighbors').

Using perturbation theory one can show that there exists a 2-local Hamiltonian on a 2D lattice whose ground-space is approximately the same as the ground-space of the k-local Hamiltonian (and the corresponding eigenvalues are also approx. the same). The gap above the ground-space is also approx. preserved.

Example: toric code space.

Explicitly proved in Oliveira & Terhal.

Stoquastic Hamiltonians

Not all quantum systems are created equal, some quantum systems are more quantum than others.

Stoquastic k-local Hamiltonians are

1. k-local Hamiltonians which are real

2. The off-diagonal elements $i \neq j$ $\langle i|H|j\rangle \leq 0$ where $|i\rangle$ is some (standard) basis. This implies that for all i,j $\langle i| e^{-\beta H} |j\rangle \geq 0$.

Why is the ground-state energy problem for these Hamiltonians special?

Ground-state $|\varphi\rangle = \Sigma_i \alpha_i |i\rangle$ where $\alpha_i \geq 0$.

$P(i) = \alpha_i / \Sigma_i \alpha_i$ is a probability distribution. How `quantum' is the lowest-eigenvalue problem for this class?

Examples of Stoquastic Hamiltonians

- Nonrelativistic particles in a potential, H=K+V. Potential term V is diagonal in the position basis, i.e. for $x \neq y$ $\langle x|V|y\rangle = 0$.
Kinetic energy $K = -\Sigma_i \Delta_i^2/2m_i$, which is off-diagonal in the position basis and non-positive.
- Hamiltonians with generalized conjugate variables such as many Josephson-junction Hamiltonians (with charge & flux degrees of freedom) or spin-less bosons.
- Bosonic Hubbard model (in the number basis)
- Ferromagnetic Heisenberg models (and some antiferromagnetic models)
- Quantum transverse Ising model.

Note that this class includes all classical systems for which the ground-state problem can be NP-complete!

Typical examples of non-stoquastic systems are fermionic systems or charged particles in a magnetic field.

A Largest Eigenvalue Problem

Consider $G=(I-s\,H)/2 \geq 0$ for some small enough parameter s.

Largest eigenvalue μ problem of a nonnegative (sparse) matrix G

$$\mu(G)=(1-s\,\lambda(H))/2$$

Determine this largest eigenvalue μ by estimating $Tr(G^L)$ for large enough L=poly(n).

Yes: If $\lambda(H) \leq 0$, $\mu(G) \geq ½$ and $Tr(G^L) \geq 2^{-L}$

No: If $\lambda(H) \geq 1/poly(n)$, $\mu(G) \leq (1-1/poly(n))/2$, $Tr(G^L) \leq 2^{-L}\, 2^{n-L/poly(n)}$

How does one estimate $Tr(G^L)$?

What physicists know

For stoquastic Hamiltonians in d spatial dimensions one can express $Tr(G^L)$ as the partition function of a classical system in d+1 dimensions with periodic boundary conditions.
Heuristic strategy: estimate this partition function using Monte Carlo sampling or estimate the expectation value of an observable M in the ground-state as $Tr(M\, G^L)/Tr(G^L)$.

How hard is this really?

Our result: LH-MIN for stoquastic Hamiltonians is a problem in the complexity class AM.

Classical but not easy.

Another ‘physics’ approach

G is almost a stochastic matrix except the entries in each row do not add up to 1. Rescale G such that all row entries add to less than 1, i.e. $b_j=\Sigma_i G_{i,j} \leq 1$, or

G=PB where P is stochastic and B is diagonal matrix with weight b_j.

Stochastic single walker process:
An input i to G is kept `alive’ with probability $b_i$. With probability $1-b_i$ the walker `dies’. If it is alive, it is mapped on bitstring j with probability according the matrix P.

What is the probability to obtain an output k after L steps, conditioned on the walker not dying? We assume a random input i.

$P(k)=\Sigma_i \langle k| G^L |i\rangle/(\Sigma_{i,k} \langle k| G^L |i\rangle)$

Analysis of walker process

But G^L is close to $\mu^L |\varphi\rangle\langle\varphi|$ for large enough L (assuming a 1/poly(n) gap in the eigenvalue spectrum).

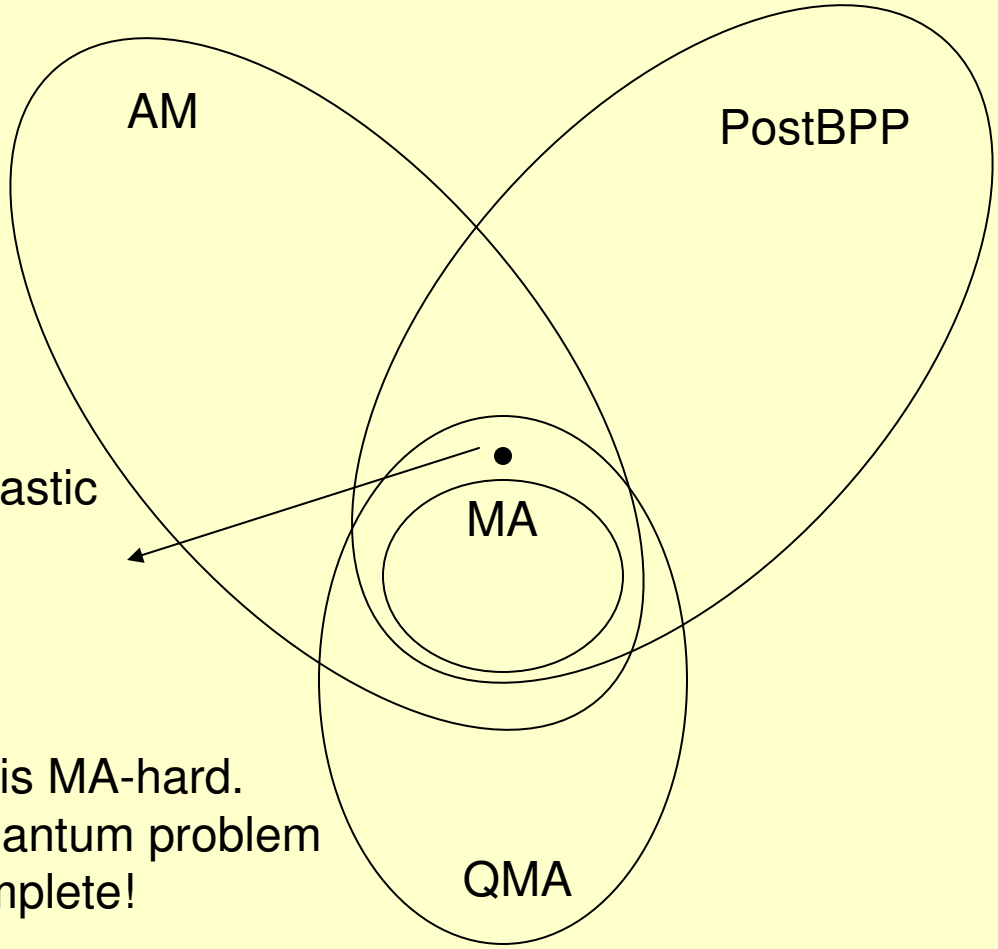
This implies that for large enough L, P(k) is close to the ground-state probability distribution.

One can estimate the largest eigenvalue as $\mu=\Sigma_k P(k) b_k$
(and we also obtain the ground-state approximately)

Remember that we conditioned on the walker not dying…
Multiple walkers? How efficient can this process be? Green's function Monte Carlo technique.

Our result: LH-MIN for stoquastic Hamiltonians
with a 1/poly(n) gap is a problem in the complexity class PostBPP.

An overview of complexity



LH-MIN for stoquastic Hamiltonians

Is it in MA?

One can prove it is MA-hard.
If it is in MA, a quantum problem would be MA-complete!

The Stoquastic Computer

Adiabatic evolution with general (local) Hamiltonians is universal for quantum computation.

What is the power of adiabatic quantum computation with stoquastic (local) Hamiltonians?
Define a complexity class: BSP

Bounded-error Stoquastic Polynomial time (sits between BPP and BQP).

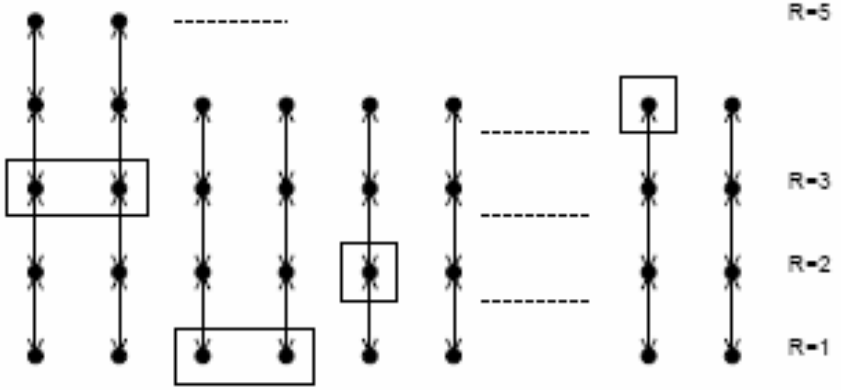
Similarly we can define SMA: stoquastic Merlin-Arthur (between MA and QMA)
What problems sit in BSP? Factoring (no…)?
What problems are BSP-complete?
Stoquastic LH-MIN is SMA-complete. Adiabatic evolution with stoquastic Hamiltonians is universal for the stoquastic computer….

Is it easier to build a stoquastic computer than a quantum computer? To what extent is this model physical and not artificial?

A modified 5-local Hamiltonian

We need the following starting point: a k-local Hamiltonian in which every qubit interacts with a constant number of other qubits in its neighborhood (in a 2 dimensional plane).

Lay-out of the circuit A. Every qubit is acted on by a constant number of gates and time evolves locally.



$$H_{\text{in}} = \sum_{q \notin Q_{\text{in}}} |1\rangle\langle 1|_q \otimes |100\rangle\langle 100|_{c_{f_q-1} c_{f_q} c_{f_q+1}},$$

All qubits except those given by Merlin are constrained to be in the zero state right before they are acted upon by the first gate

Figure 1: Two-dimensional spatial layout of the computational qubits. A qubit is indicated by a •. One and two-qubit gates are indicated by boxes. Swap operations between qubits are indicated with arrows. The order in which the swap and gate operations are executed is as follows. The single gate in the first row $R = 1$ is executed, then the first row of qubits is swapped with the second row, starting with the qubit on the right. Then the gate on the second row of qubits is executed following by swapping the qubits in row $R = 2$ and $R = 3$ starting with the qubit on the left.

Kempe, Kitaev, Regev, SIAM Journal of Computing 35 (5), 2006

Perturbation Theorem

More accurately, we have a Hilbert space $\mathcal{L} = \mathcal{L}_+ \oplus \mathcal{L}_-$ where $\mathcal{L}_-$ is the ground-space of H. Let $\Pi_\pm$ be the projectors on $\mathcal{L}_\pm$ and we can define for some operator X, $X_{\pm\mp} = \Pi_\pm X \Pi_\mp$ and $X_+ \equiv X_{++}$. In order to calculate the perturbed eigenvalues, one introduces the self-energy operator $\Sigma_-(z)$ for real-valued z

$$\Sigma_-(z) = H_- + V_{--} + V_{-+} G_+ (I - V_{++} G_+)^{-1} V_{+-}, \tag{9}$$

where we can perturbatively expand

$$(I - V_{++} G_+)^{-1} = I + V_{++} G_+ + V_{++} G_+ V_{++} G_+ + \ldots. \tag{10}$$

Here G_+, called the unperturbed Green's function (or resolvent) in physics literature, is defined by

$$G_+^{-1} = z I_+ - H_+. \tag{11}$$

In Ref. [1] the following theorem is proved (here we state the case where the ground-space of H has eigenvalue 0 and H has a spectral gap Δ above the ground-space)

Theorem 7 *([1]) Let $||V|| \leq \Delta/2$ where Δ is the spectral gap of H. Let $\tilde{H}|_{<\Delta/2}$ be the restriction to the space of eigenstates with eigenvalues less than $\Delta/2$. Let there be an effective Hamiltonian H_{eff} with $\text{Spec}(H_{\text{eff}}) \subseteq [a, b]$. If the self-energy $\Sigma_-(z)$ for all $z \in [a-\epsilon, b+\epsilon]$ where $a < b < \Delta/2 - \epsilon$ for some $\epsilon > 0$, has the property that*

$$||\Sigma_-(z) - H_{\text{eff}}|| \leq \epsilon, \tag{12}$$

then each eigenvalue $\tilde{\lambda}_j$ of $\tilde{H}|_{<\Delta/2}$ is ϵ-close to the jth eigenvalue of H_{eff}. In particular

$$|\lambda(H_{\text{eff}}) - \lambda(\tilde{H})| \leq \epsilon. \tag{13}$$

Local NGM Hamiltonian is MA-hard

MA. Represent Arthur's verification circuit quantumly. The circuit takes |+> states for randomness, ancillary |00..0> and Merlin's proof y as inputs. The circuit consists of reversible classical computation and at the end a single qubit is measured in the Z-basis.
One can show that Merlin cannot cheat by giving quantum inputs instead of bit strings y.

What problem is hard for this formulation of MA, i.e. do Kitaev's circuit-to-Hamiltonian mapping.

Theorem: 2-local NGM Hamiltonian is MA-hard.

Proof idea: 5-local NGM Hamiltonian is MA-hard by inspection.
Reduction to 2-local via NGM-form preserving perturbation gadgets.