Title: Quantum spin Hamiltonian problems and Interactive Proofs

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Abstract: Complexity class MA is a class of yes/no problems for which the answer `yes\' has a short certificate that can be efficiently checked by a classical randomized algorithm. We prove that MA has a natural complete
problem: stoquastic k-SAT. This is a quantum-mechanical analogue of the satisfiability problem such that k-bit clauses are replaced by k-qubit projectors with non-negative matrix elements. Complexity class AM is a generalization of MA in which the certificate may include a short conversation between Prover and Verifier. We prove that AM also has a natural complete problem: stoquastic Local Hamiltonian with a quenched disorder. The problem is to evaluate expectation value of the ground state energy of disordered local Hamiltonian with non-positive matrix elements.

Quantum spin Hamiltonian problems

and

Interactive Proofs

Sergey Bravyi, David DiVincenzo, Barbara Terhal

IBM Watson Research Center

Perimeter Institute
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Introduction

Given a system of $n \gg 1$ interacting quantum spins (qubits) with a Hamiltonian H. One needs to compute the ground state energy of H.

H is $2^n \times 2^n$ matrix. It is practically impossible to compute the ground state energy by the standard linear algebra methods.

Deterministic algorithms (Mean Field Theory, DMRG, Perturbation Theory Expansion): use simple, depending on $poly(n)$ parameters, variational states to approximate the actual ground state.

Randomized algorithms (Green's Function Monte Carlo): a random walk on the set of 2^n basis vectors gives us information about the whole Hilbert space by visiting only $poly(n)$ basis vectors.

Goal: Identify a class of quantum systems that can be simulated using randomized algorithms.

Outline:

- Stoquastic k-SAT problem
- Random walk algorithm for stoquastic k-SAT
- Stoquastic Hamiltonians and Interactive Proofs

Classical 3-SAT

$$\text{Input:} \quad \begin{cases} n = \#\ \text{bits}, \\ M = \#\ \text{clauses}, \\ \text{3-bit clauses } C_1, \ldots, C_M : \{0,1\}^n \to \{0,1\} \end{cases}$$

$$\text{Example:} \quad \begin{cases} x = (x_1, x_2, \ldots, x_n), \\ C_\alpha(x) = x_1 \vee x_3 \vee (\neg x_8), \\ C_\alpha(x) = 1 \text{ unless } x_1 = 0,\ x_3 = 0,\ x_8 = 1 \end{cases}$$

$$\text{Assignment } x \left\{ \begin{array}{c} \text{satisfies} \\ \text{violates} \end{array} \right\} \text{clause } C_\alpha \text{ iff } \left\{ \begin{array}{c} C_\alpha(x) = 1 \\ C_\alpha(x) = 0 \end{array} \right\}$$

$$\text{yes-instance:} \quad \begin{cases} \exists\, x \in \{0,1\}^n : C_\alpha(x) = 1 \quad \text{for all } \alpha \\ \text{(there exists assignment satisfying all clauses)} \end{cases}$$

$$\text{no-instance:} \quad \begin{cases} \forall\, x \in \{0,1\}^n \quad \exists \alpha : C_\alpha(x) = 0 \\ \text{(any assignment violates at least one clause)} \end{cases}$$

Quantum 3-SAT

Input: $\begin{cases} n = \#\ \text{qubits}, \\ M = \#\ \text{clauses}, \\ \epsilon \geq 1/poly(n) = \text{precision parameter}, \\ \text{3-qubit projectors (clauses) } \Pi_1, \ldots, \Pi_M : (\mathbb{C}^2)^{\otimes n} \to (\mathbb{C}^2)^{\otimes n} \end{cases}$

$\Pi_\alpha^\dagger = \Pi_\alpha$, $\Pi_\alpha^2 = \Pi_\alpha$, but in general $\Pi_\alpha \Pi_\beta \neq \Pi_\beta \Pi_\alpha$.

Assignment $|\theta\rangle \in (\mathbb{C}^2)^{\otimes n} \begin{Bmatrix} \text{satisfies} \\ \text{violates} \end{Bmatrix}$ clause Π_α iff $\begin{Bmatrix} \Pi_\alpha |\theta\rangle = |\theta\rangle \\ \langle\theta|\Pi_\alpha|\theta\rangle \leq 1 - \epsilon \end{Bmatrix}$

yes-instance: $\begin{cases} \exists |\theta\rangle \in (\mathbb{C}^2)^{\otimes n} : \Pi_\alpha |\theta\rangle = |\theta\rangle \quad \text{for all} \quad \alpha. \\ \text{(There exists assignment satisfying all clauses)} \end{cases}$

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Comment 1: If all projectors Π_α are diagonal in the computational basis, quantum 3-SAT reduces to classical 3-SAT.

Comment 2: Given an instance of quantum 3-SAT $(n, M, \epsilon, \Pi_1, \ldots, \Pi_M)$ one can define a 3-local Hamiltonian

$$H = -\sum_{\alpha=1}^{M} \Pi_\alpha.$$

Let E_0 be the ground state energy of H. Then

$$\text{yes-instance:} \quad E_0 = -M,$$

$$\text{no-instance:} \quad E_0 \geq -M + \epsilon.$$

Stoquastic 3-SAT

Definition 1. *Stoquastic 3-SAT is a special case of quantum 3-SAT such that all projectors Π_α have real non-negative matrix elements in the computational basis:*

$$\langle x|\Pi_\alpha|y\rangle \geq 0 \quad \textit{for all } x, y \in \{0,1\}^n.$$

Randomized algorithm for stoquastic 3-SAT

Keep in mind that stoquastic 3-SAT is NP-hard.
Let's set a realistic objective:

Problem 1: Given an instance of stoquastic 3-SAT $(n, M, \epsilon, \Pi_1, \ldots, \Pi_M)$, a basis vector $w \in \{0,1\}^n$, and an accuracy $\delta > 0$.

yes-instance: $\exists\, |\theta\rangle \,:\, \Pi_\alpha |\theta\rangle = |\theta\rangle$ for all α and $|\langle w|\theta\rangle| \ge \delta$.

no-instance: $\forall\, |\theta\rangle \quad \exists\, \alpha \,:\, \langle\theta|\Pi_\alpha|\theta\rangle \le 1-\epsilon$.

Theorem 1: Problem 1 can be solved by a randomized algorithm with a running time $T = poly(n, \epsilon^{-1}, \log(\delta^{-1}))$.

Comment: if a satisfying assignment $|\theta\rangle$ exists, it has overlap $\delta \ge 2^{-n/2}$ with at least one basis vector w. Thus a description of w provides a classical proof that a satisfying assignment exists.

Non-negative projectors: some properties

(1) Intersection of non-negative projectors is a non-negative projector
$\Pi_1 \cap \Pi_2 = \{|\psi\rangle \,:\, \Pi_1|\psi\rangle = |\psi\rangle, \quad \Pi_2|\psi\rangle = |\psi\rangle\}$

(2) A satisfying assignment can always be chosen as a non-negative vector: $\Pi|\theta\rangle = |\theta\rangle$ implies $\Pi|\tilde{\theta}\rangle = |\tilde{\theta}\rangle$, where $|\tilde{\theta}\rangle = \sum_x |\langle x|\theta\rangle|\,|x\rangle$.

(3) Any non-negative projector can be written as $\Pi = \sum_{j=1}^{r} |\psi_j\rangle\langle\psi_j|$, where $r = \mathrm{Rk}(\Pi)$, and $\{|\psi_j\rangle\}$ are pairwise orthogonal non-negative states.

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Randomized algorithm for stoquastic 3-SAT

Let $(n, M, \epsilon, \Pi_1, \ldots, \Pi_M)$ be an instance of stoquastic 3-SAT. Define an operator

$$G = \frac{1}{M} \sum_{\alpha=1}^{M} \Pi_\alpha.$$

It has non-negative matrix elements $G_{x,y} = \langle x|G|y\rangle$.

yes-instance : the largest eigenvalue of G is 1

no-instance : the largest eigenvalue of G is $\leq 1 - \epsilon/M$

$$G = \frac{1}{M} \sum_{\alpha=1}^{M} \Pi_\alpha$$

covariant derivative.

Randomized algorithm for stoquastic 3-SAT

Let $|\theta\rangle$ be a sat. assignment supported on a set of basis vectors S:

$$\Pi_\alpha |\theta\rangle = |\theta\rangle \text{ for all } \alpha, \quad |\theta\rangle = \sum_{x\in S} \theta_x |x\rangle, \quad \theta_x > 0, \quad S \subseteq \{0,1\}^n.$$

Then

$$G|\theta\rangle = |\theta\rangle.$$

One can define a random walk on S with transition probabilities

$$P_{x\to y} = \left(\frac{\theta_y}{\theta_x}\right) G_{x,y}.$$

Indeed, $P_{x\to y} \geq 0$, $\sum_{y\in S} P_{x\to y} = \theta_x^{-1} \sum_y G_{x,y}\,\theta_y = 1$ for all $x \in S$.

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Lemma: Suppose Π is a non-negative projector and $\Pi|\theta\rangle = |\theta\rangle$ for some $|\theta\rangle = \sum_{x\in S} \theta_x |x\rangle$, $\theta_x > 0$. Then

(1) $\langle x|\Pi|x\rangle > 0$ for all $x \in S$.

(2) If $\langle x|\Pi|y\rangle > 0$ for some $x, y \in S$, then

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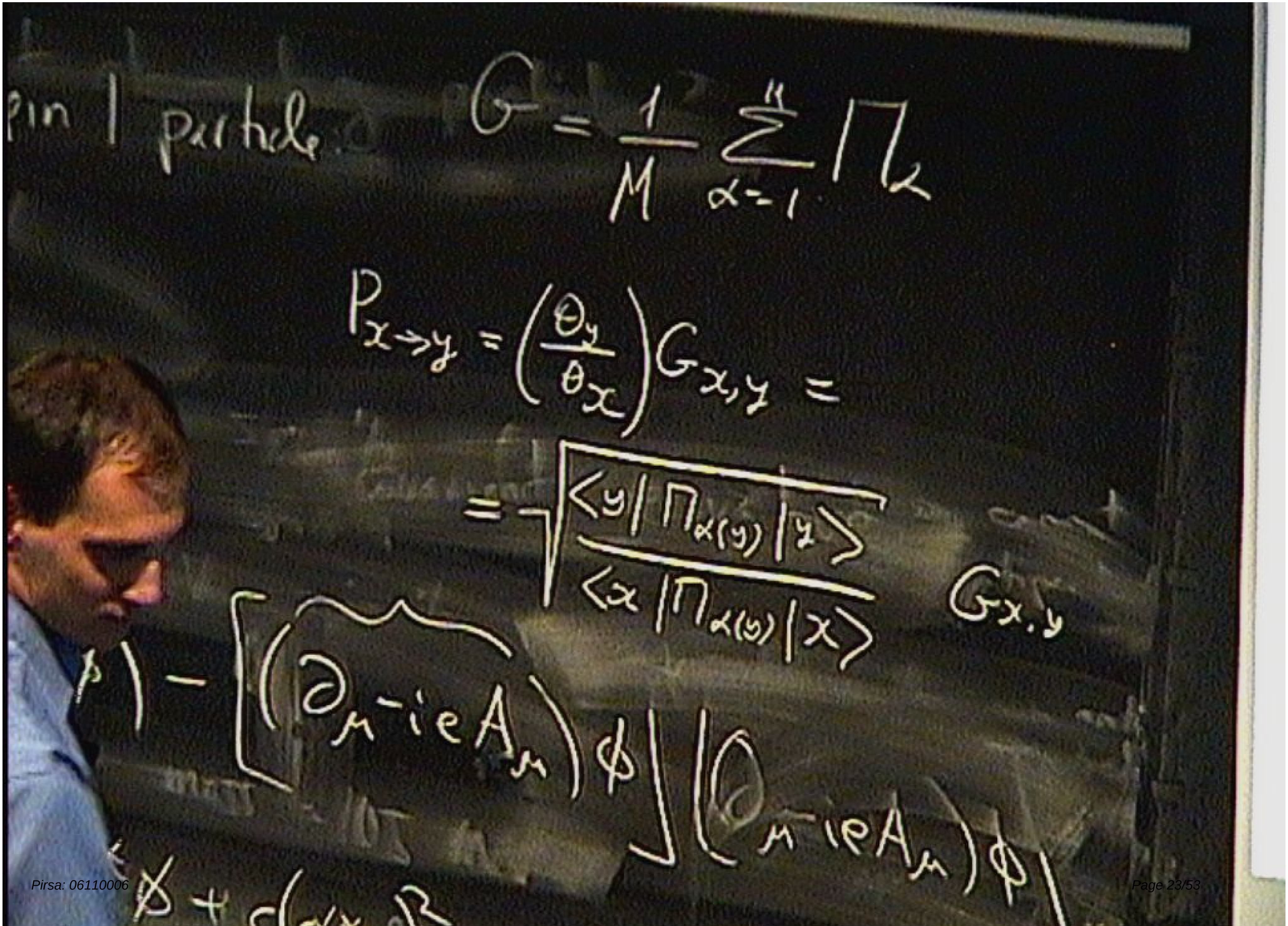
pin | particle
G = 1/M Σ_{α=1}^{M} Π_α
P_{x→y} = (θ_y / θ_x) G_{x,y} =
= -√(<y|Π_{α(y)}|y> / <x|Π_{α(y)}|x>) G_{x,y}
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If a sat. assignment $|\theta\rangle$ does not exist, this definition can produce unnormalized transition probabilities $P_{x\to y}$. Before making each step of the random walk one has to verify that $\sum_y P_{x\to y} = 1$.

It can be done efficiently because G is a sparse matrix.

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Since for no-instances the largest eigenvalue of G is at most $1 - \epsilon/M$, $\mathbf{Pr}$(RW makes L steps) decreases exponentially with L. The prefactor depends only on n and δ.

Randomized algorithm for stoquastic 3-SAT

Step 1: Suppose current state of RW is x_j. Verify $\langle x_j|\Pi_\alpha|x_j\rangle > 0$ for all α.
Step 2: Find a set $N(x_j) = \{y : G_{x_j,y} > 0\}$.
Step 3: For every $y \in N(x_j)$ choose any α_y such that $\langle y|\Pi_{\alpha_y}|x_j\rangle > 0$.

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If $j+1 < L$, goto Step 1.

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Step 9: Decide that the answer is 'yes'.

Lemma: Suppose Π is a non-negative projector and $\Pi|\theta\rangle = |\theta\rangle$ for some $|\theta\rangle = \sum_{x\in S} \theta_x |x\rangle$, $\theta_x > 0$. Then
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n | particle:

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$\phi) - \left[\left(\partial_\mu - ieA_\mu \right) \phi \right| \ldots$

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Problem 1: Given an instance of stoquastic 3-SAT $(n, M, \epsilon, \Pi_1, \ldots, \Pi_M)$, a basis vector $w \in \{0,1\}^n$, and an accuracy $\delta > 0$.

yes-instance: $\exists\, |\theta\rangle\,:\, \Pi_\alpha |\theta\rangle = |\theta\rangle$ for all α and $|\langle w|\theta\rangle| \geq \delta$.

no-instance: $\forall\, |\theta\rangle \quad \exists\, \alpha\,:\, \langle\theta|\Pi_\alpha|\theta\rangle \leq 1 - \epsilon$.

Suppose the number of steps L in the random walk is chosen such that

$$2^{n/2}\,\delta^{-1}\,(1 - \frac{\epsilon}{M})^L \leq \frac{1}{3},$$

which can be done with $L = poly(n, \epsilon^{-1}, \log(\delta^{-1}))$. Then the algorithm above solves Problem 1 with error probability 1/3.

See quant-ph/0611021 for details.

Complexity class MA (Merlin-Arthur games)

MA is a class of decision problems for which 'yes'-instances have a proof that can be efficiently verified by a classical randomized algorithm. Here a proof is a bit string that is given to the verifier (Arthur) capable of doing poly-time probabilistic computation by the prover (Merlin) with unlimited computational power.

Completeness: for yes-instances Merlin can find a proof that convinces Arthur

Soundness: for no-instances Arthur will reject any proof w.h.p.

A decision problem is called MA-complete iff it belongs to MA and any other problem in MA can be reduced to it.

Theorem 1. *Stoquastic k-SAT belongs to* MA *for any $k = O(1)$.*

Indeed, in order to prove that a satisfying assignment $|\theta\rangle$ exists Merlin can send Arthur a basis vector w such that $\langle\theta|w\rangle \geq 2^{-n/2}$.

Theorem 2. *Stoquastic k-SAT is* MA*-complete for any $k \geq 6$.*

See quant-ph/0611021 for details.

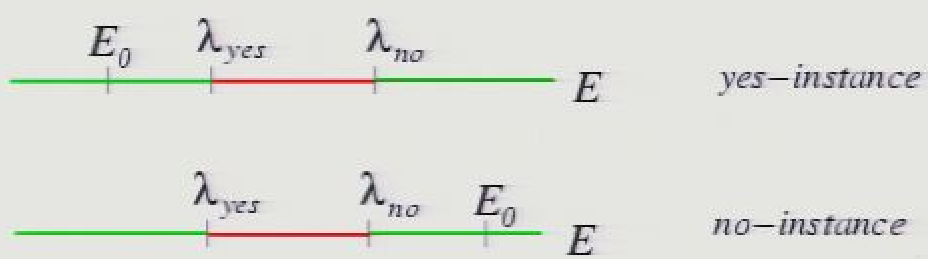
Minimum eigenvalue problem for local Hamiltonians (LH-MIN)

Input:
$$\begin{cases} n = \#\text{ qubits}, \\ k\text{-local Hamiltonian } H = \sum_{\alpha=1}^{M} H_\alpha \text{ on } n \text{ qubits}, \\ \text{lower/upper thresholds } \lambda_{\text{yes}} < \lambda_{\text{no}} \end{cases}$$

Constraints: $\|H_\alpha\| \le poly(n), \quad \lambda_{\text{no}} - \lambda_{\text{yes}} \ge 1/poly(n).$

yes-instance:
$$\begin{cases} \exists\,|\theta\rangle \,:\, \langle\theta|H|\theta\rangle \le \lambda_{\text{yes}}, \\ \text{(the smallest eigenvalue of } H \text{ is } \le \lambda_{\text{yes}}) \end{cases}$$

no-instance:
$$\begin{cases} \forall\,|\theta\rangle \quad \langle\theta|H|\theta\rangle \ge \lambda_{\text{no}}, \\ \text{(the smallest eigenvalue of } H \text{ is } \ge \lambda_{\text{no}}) \end{cases}$$



Theorem: LH-MIN is QMA-complete for $k \geq 2$
[Kitaev 99, Kempe, Kitaev, Regev 04]

QMA (Quantum Merlin-Arthur games) is a class of decision problems for which yes-instances have a proof that can be efficiently verified by a quantum algorithm. Here a proof is a quantum state that is given to the verifier (Arthur) capable of doing poly-time quantum computation by the prover (Merlin) with unlimited computational power.

Completeness: for yes-instances Merlin can find a proof that convinces Arthur w.h.p.

Soundness: for no-instances Arthur will reject any proof w.h.p.

Is there any special class of local Hamiltonians for which LH-MIN is MA-complete?

Stoquastic Hamiltonians

Def: Let $H = \sum_\alpha H_\alpha$ be a k-local Hamiltonian acting on n qubits.
H is called stoquastic iff
$\langle x|H_\alpha|y\rangle \leq 0$ for all basis vector $x \neq y$, and for all α.

(1) Stoquastic Hamiltonians have no "phase frustrations", i.e., ground state can be chosen as a real non-negative vector.

(2) Any classical (diagonal) Hamiltonian is stoquastic.

(3) Gibbs operator $e^{-\beta H}$ has non-negative matrix elements

(4) A property of being stoquastic can be efficiently verified.

Stoquastic Hamiltonians: examples

(1) Ising model with transverse field

(2) Heisenberg ferromagnetic model

(3) Heisenberg anti-ferromagnetic model on a bipartite graph

(4) Hamiltonians for adiabatic evolution algorithm [Farhi et all. 00]

Beyond qubits:

(5) Interacting bosons (Hubbard model, ^{4}He, Bose-Einstein condensates)

(6) Jaynes-Cummings model and spin-boson model

Typically Hamiltonian is not stoquastic only if fermionic degrees of freedom are present.

Theorem 3. *Complexity of stoquastic LH-MIN does not depend on k as long as $k \geq 2$.*

Theorem 4. *Stoquastic LH-MIN is hard for* MA.

Theorem 5. *Stoquastic LH-MIN belongs to the complexity class* AM *(Arthur-Merlin games)*

See quant-ph/0606140 for the proof

AM is a class of decision problems for which yes-instances have a proof that can be efficiently verified by a classical randomized algorithm. Here a proof may include a conversation between Arthur and Merlin with a constant number of communication rounds. Arthur can generate his questions using randomness. By definition, MA $\subseteq$ AM.

Corollary: Stoquastic LH-MIN is not QMA-complete unless QMA $\subseteq$ AM

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Example: Ising model in the transverse field

Let $G = (V, E)$ be a graph with n vertices. Qubits live at vertices. Let A be adjacency matrix of G. Consider stoquastic 2-local Hamiltonian

$$H(h) = \frac{1}{2} \sum_{u,v=1}^{n} A_{u,v} (Z_u Z_v - I) - h \sum_{u=1}^{n} X_u, \quad h \geq 0,$$

Let $\lambda(h)$ be the smallest eigenvalue of $H(h)$.

$$\lambda(0) = -(\text{the maximum weight of a cut of } G).$$

Thus evaluating $\lambda(0)$ is NP-hard. Since

$$|\lambda(h) - \lambda(0)| \leq ||H(h) - H(0)|| \leq n\, h,$$

Stoquastic LH-MIN for $H(h)$ is NP-hard if $nh \leq 1/3$.

One can show that the ground state $|\theta\rangle$ of $H(h)$ obeys $\theta_x \geq 2^{-poly(n)}$ for all basis vectors x. Thus Merlin's proof can not be just a basis vector having large overlap with $|\theta\rangle$.

Open problems:

- Adiabatic q. computation with stoquastic Hamiltonians
- Perturbation theory gadgets for quantum and stoquastic k-SAT problems
- Identify "easy" 1D cases of stoquastic LHP
- Connect to empirical Green's Function Monte Carlo method

Randomized algorithm for stoquastic 3-SAT

Step 1: Suppose current state of RW is x_j. Verify $\langle x_j|\Pi_\alpha|x_j\rangle > 0$ for all α.
Step 2: Find a set $N(x_j) = \{y : G_{x_j,y} > 0\}$.
Step 3: For every $y \in N(x_j)$ choose any α_y such that $\langle y|\Pi_{\alpha_y}|x_j\rangle > 0$.

Step 4: For every $y \in N(x_j)$ compute number $P_{x_j \to y} = G_{x_j,y} \sqrt{\frac{\langle y|\Pi_{\alpha_y}|y\rangle}{\langle x_j|\Pi_{\alpha_y}|x_j\rangle}}$.
Step 5: Verify $\sum_{y \in N(x_j)} P_{x_j \to y} = 1$.
Step 6: Generate $x_{j+1} \in N(x_j)$ according to $P_{x_j \to y}$.

Step 7: Compute and store a number $r_{j+1} = \frac{P_{x_j \to x_{j+1}}}{G_{x_j,x_{j+1}}}$.
If $j+1 < L$, goto Step 1.

Step 8: Verify $\prod_{j=1}^{L} r_j \leq 1/\delta$.

Step 9: Decide that the answer is 'yes'.

Randomized algorithm for stoquastic 3-SAT

$$P_{x\to y} = \left(\frac{\theta_y}{\theta_x}\right) G_{x,y} = \begin{cases} \sqrt{\frac{\langle y|\Pi_{\alpha(y)}|y\rangle}{\langle x|\Pi_{\alpha(y)}|x\rangle}} G_{x,y}, & \text{if } G_{x,y} > 0 \\ 0, & \text{if } G_{x,y} = 0 \end{cases}$$

Consider the probability for the random walk to make L steps:

$$\mathbf{Pr}(\text{RW makes } L \text{ steps}) = \begin{cases} 1 & \text{for yes-instances,} \\ \sim \sum_{x_L} (G^L)_{x_0,x_L} & \text{for no-instances} \end{cases}$$

Since for no-instances the largest eigenvalue of G is at most $1 - \epsilon/M$, $\mathbf{Pr}$(RW makes L steps) decreases exponentially with L. The prefactor depends only on n and δ.

Randomized algorithm for stoquastic 3-SAT

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If a sat. assignment $|\theta\rangle$ does not exist, this definition can produce unnormalized transition probabilities $P_{x\to y}$. Before making each step of the random walk one has to verify that $\sum_y P_{x\to y} = 1$.

It can be done efficiently because G is a sparse matrix.

Randomized algorithm for stoquastic 3-SAT

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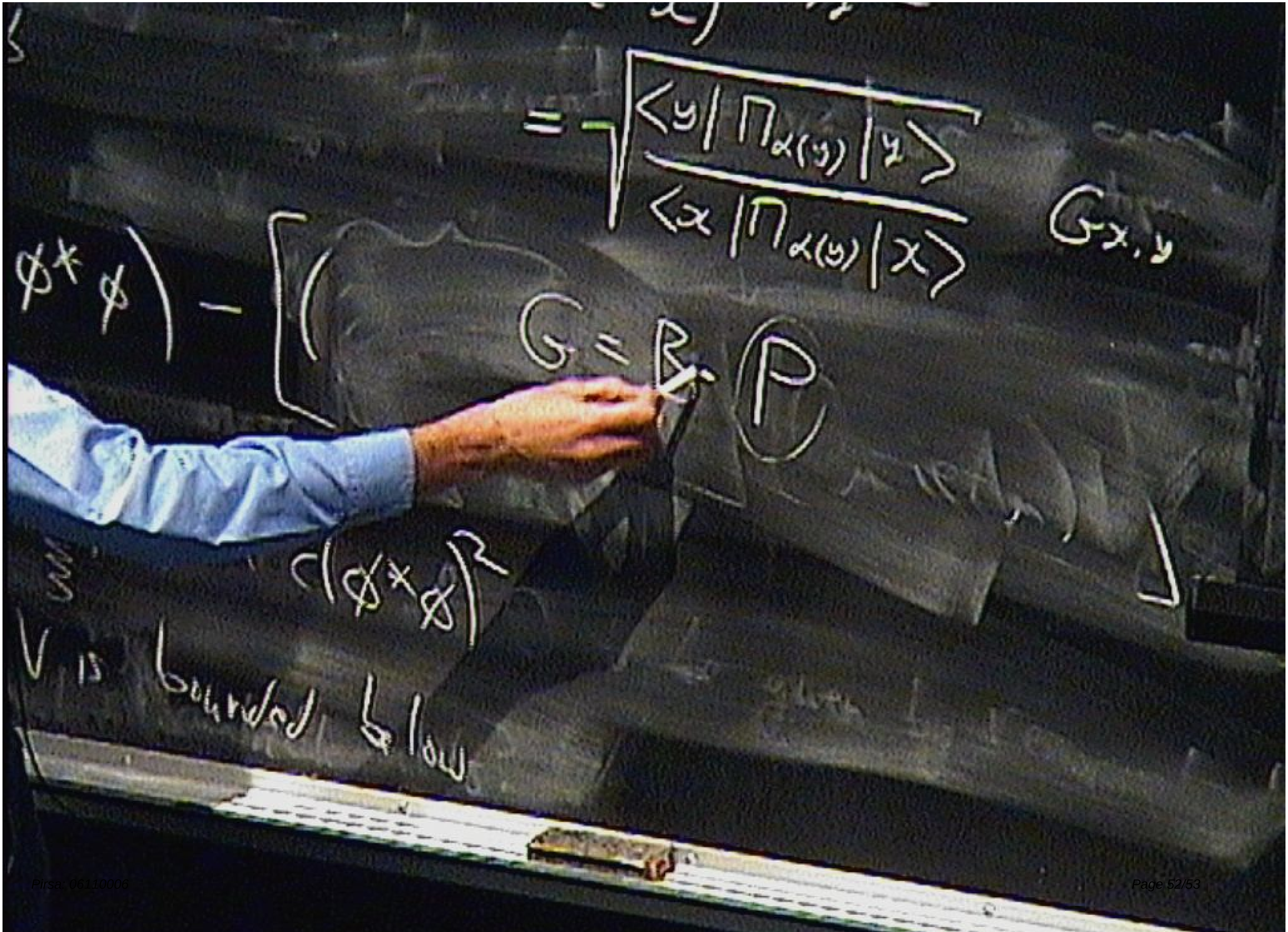
= −√(⟨y| Π_α(y) |y⟩ / ⟨x| Π_α(y) |x⟩)   G_x,y
φ* φ) −
G = B (P)
c(φ* φ)^R
V is bounded below

$$= \sqrt{\frac{\langle y | \Pi_{\alpha(y)} | y \rangle}{\langle x | \Pi_{\alpha(y)} | x \rangle}} \; G_{x,y}$$

$$\phi^* \phi) - \Big[\big(\qquad \big) \Big]$$

$$G = B \cdot P$$

$$b \phi^* \phi + c(\phi^* \phi)^2$$

V is bounded below