Title: Classifying Hamiltonians in terms of computational complexity

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Abstract: <p>Quantum many-body systems ranging from a many-electron atom to a solid material are described by effective Hamiltonians which are obtained from more accurate Hamiltonians by neglecting or treating weak interactions perturbatively. Quantum complexity theory asks about the quantum computational power of such quantum many-body models for both practical as well as fundamental purposes. Three distinct computational classes have emerged within this framework: namely (1) classical Hamiltonians such as the Ising model, (2) sign-free or stoquastic Hamiltonians such as the transverse field Ising model, and (3) fully quantum Hamiltonians such as the Heisenberg model. Each class can be characterized by certain prototype universal Hamiltonians which can encode the physics of any other Hamiltonian in that class. We will show how this encoding is established through the use of perturbation theory via perturbative gadgets. We will discuss the technical expression of this classification in terms of the complexity classes NP, Stoquastic MA and QMA and the power of these Hamiltonians for performing quantum adiabatic computation.</p>

Classifying Hamiltonians in terms of their computational complexity

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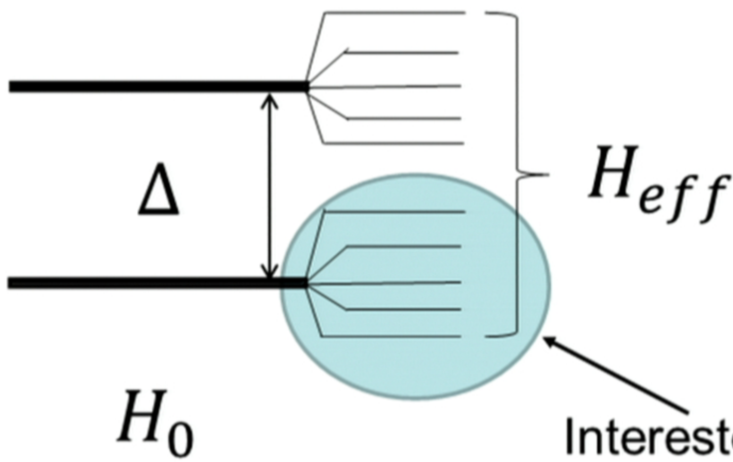
Tools

We can relate the low-energy physics of two Hamiltonians by using degenerate perturbation theory. Let $H = H_0 + V$ where V is a perturbation with $\Delta \gg ||V||$.



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$$\varphi_0(H) \approx \varphi_0(H_{eff})$$

Interested in the lower part of the spectrum & eigenstates

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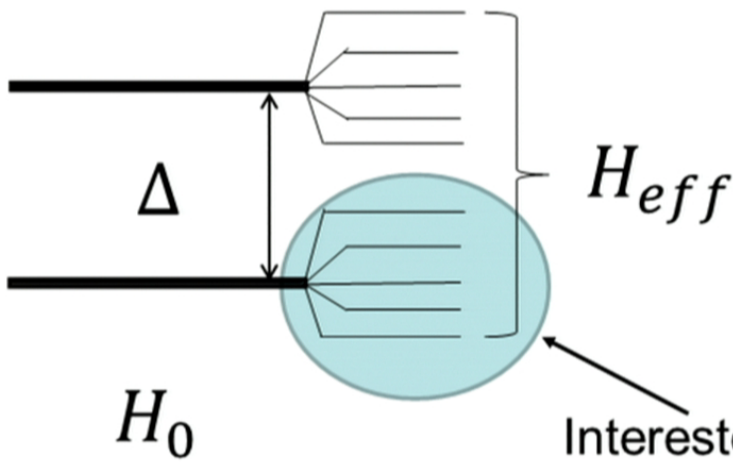

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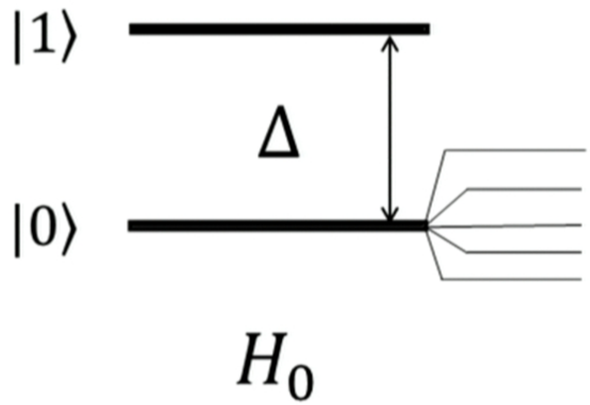
Off-resonant atom-photon interaction

Jaynes-Cummings model

$$H = \omega_r\left(a^\dagger a\right) - \frac{\omega_q}{2}Z + \frac{\Omega}{2}\left(a^\dagger\sigma_- + a\sigma_+\right)$$

with detuning $\Delta = \omega_q - \omega_r \gg \Omega$. In interaction frame at frequency ω_r one has

$$H' = -\frac{\Delta}{2}Z + \frac{\Omega}{2}\left(a^\dagger\sigma_- + a\sigma_+\right) = H_0 + V$$

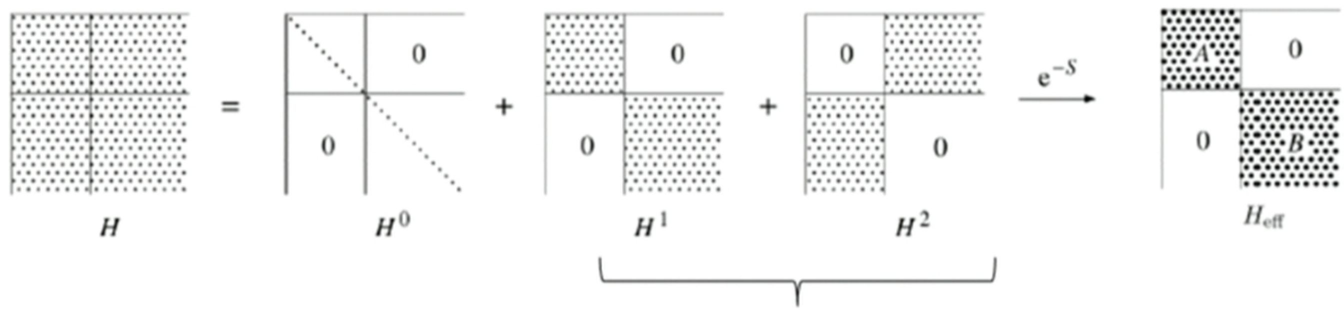


$$H_{eff} = \left(\omega_r - \frac{g^2}{\Delta}Z\right)a^\dagger a - \frac{1}{2}\left(\omega_q + \frac{g^2}{\Delta}\right)Z$$

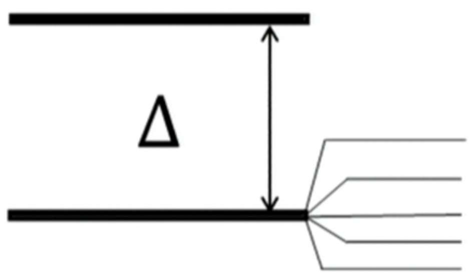
AC-Stark shift and Lamb shift

Schrieffer-Wolff Perturbation Theory

$$H = H_0 + V$$



V



H_0

$$H_{eff} = e^{S} H e^{-S} \approx H + [S, H] + \frac{[S,[S,H]]}{2} + \ldots$$

$S = -S^{\dagger}$, block-off diagonal and is perturbatively generated

Reverse Engineering

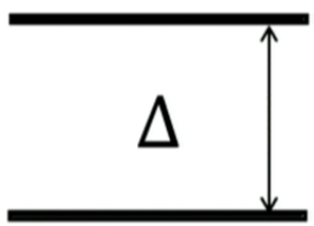
We have H_{target} which is complicated….

We want to construct $H = H_0 + V$ such that $H_{target} = P_0 H_{eff} P_{0.}$

$$H_{eff} = e^S H e^{-S} \approx H + [S,H] + \frac{[S,[S,H]]}{2} + ..$$

Perturbation Gadget

$S = -S^\dagger$, block-off diagonal and is perturbatively generated



H_0

Kempe, Kitaev, Regev 2004;
Terhal, Oliveira 2005;
Bravyi, DiVincenzo, Loss, Terhal 2008
and many more papers

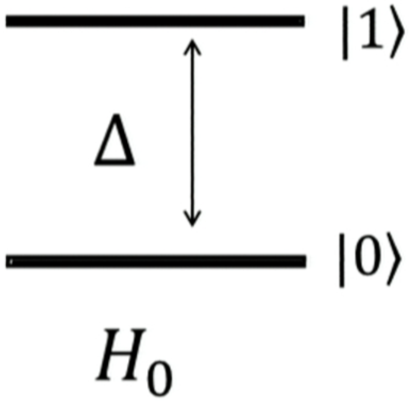
Example: subdivision gadget

We have $H_{target} = A \otimes B$ and take a mediator qubit m.

Take $H_0 = \Delta|1\rangle\langle 1|_m$ and $\mathrm{V} = \sqrt{\Delta/2}\, X_m \otimes (-A + B) + V_{exta}$

with $V_{extra} = \frac{1}{2}(A^2 + B^2)$.

In 2nd order perturbation theory in $\varepsilon = 1/\sqrt{\Delta}$



$$H_{target} = P_0 e^S H e^{-S} P_0 \approx A \otimes B + O(\varepsilon)$$

$$S = -i\sqrt{{}^{1}/_{2\Delta}}\, Y_m \otimes (-A + B) + ..$$

Upshot: k-body interaction is replaced by (1+k/2)-body interaction.

Games

Merlin

Unlimited computational power,
can help Arthur, but is possibly evil.

Arthur

Earthling with limited
computational power,
has to solve problem with
help of Arthur

Problems

- Given integers N, p < N in log N bits.

Does N have a prime factor less than p?

- Given n bits $x_1 \dots x_n$ and constraints C_i on these bits of the form, e.g. $C_1 = x_1 OR \overline{x_{10}} OR x_8$

Can one find $x_1 .. x_n$ which satisfy all constraints?

- Let $H = \sum_i H_i$ be a Hamiltonian on n qubits.

H_i acts on O(1) qubits. Given a bound *E*.

All described by poly(n) bits.

Does H have a state with energy less than *E*?

Arthur

Help from Arthur has to be complete and sound

Classical Arthur
Computation is a poly(n)-sized classical circuit.

NP

Probabilistic Classical Arthur
Computation by Arthur is a poly(n)-sized classical circuit which uses random bits.

MA

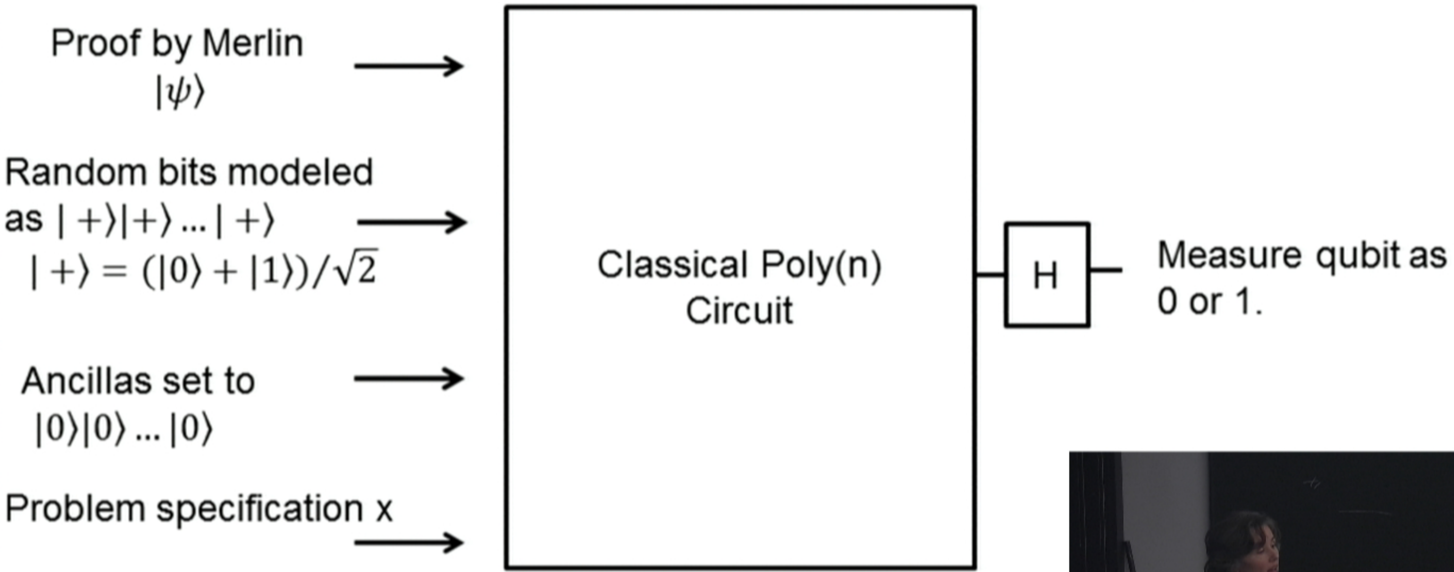
Stoquastic Arthur

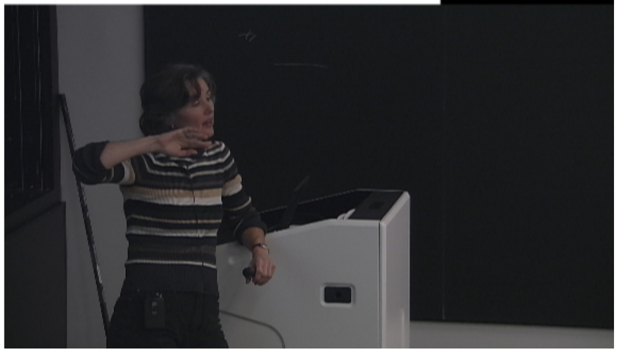
StoqMA

Quantum Arthur
Computation by Arthur is a poly(n)-sized quantum circuit.

QMA

Stoquastic Arthur





Stoquastic Arthur

Proof by Merlin $|\psi\rangle$ →

Random bits modeled as $|+\rangle|+\rangle \dots |+\rangle$ →
$|+\rangle = (|0\rangle + |1\rangle)/\sqrt{2}$

Ancillas set to $|0\rangle|0\rangle \dots |0\rangle$ →

Problem specification x →

Classical Poly(n) Circuit — H — Measure qubit as 0 or 1.

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Problem specification x →

Classical Poly(n)
Circuit V

No amplification!

Measure qubit as
$|\pm\rangle = |0\rangle \pm |1\rangle/\sqrt{2}$

Given $\varepsilon_{yes}, \varepsilon_{no}, |\varepsilon_{yes} - \varepsilon_{no}| \geq 1/poly(n)$.

YES: $\Pr(+) = \Pr(V; x, \psi) \geq \varepsilon_{yes}$. **NO:** $\Pr(+) = \Pr(V; x, \psi) \leq \varepsilon_{no}$

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Proof by Merlin $|\psi\rangle$ $\longrightarrow$

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Hamiltonians and Computational Complexity

NP

Classical Hamiltonians.
Ising model spin glass $H = \sum_{ij} J_{ij} Z_i Z_j + \sum_i J_i Z_i$

StoqMA

Sign-free Hamiltonians.
Transverse field Ising model

$$H = \sum_{ij} J_{ij} Z_i Z_j + \sum_i J_i X_i$$

QMA

Quantum Hamiltonians.
Heisenberg model $H = \sum_{ij} J_{ij} (Z_i Z_j + X_i X_j + Y_i Y_j)$

Barahona 1982; Bravyi, Hastings 2014; Montanaro, Cubitt 2013 and many earlier results

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More examples of stoquastic Hamiltonians

- Quantum transverse Ising model $H = H_{ising}(Z) - \Gamma \sum_i X_i$
- Jaynes-Cummings Hamiltonian
- Spin-boson model
- Josephson-junction flux qubits Hamiltonians (Hamiltonians engineered by company D-wave for AQC).

Stoquastic Hamiltonians are quite ubiquitous.

Non-stoquastic are typically fermionic systems, charged particles in a magnetic field.

Note: we are interested in ground-state properties of these Hamiltonians.

Stoquastic Hamiltonias

General definition: stoquastic Hamiltonians are real and have non-positive off-diagonal elements in some standard basis |i>.

Then G=I-t H is a nonnegative matrix (in this basis) for suff. small real t.
The Gibbs matrix G=exp(- β H) is a nonnegative matrix.

Perron-Frobenius Theorem:

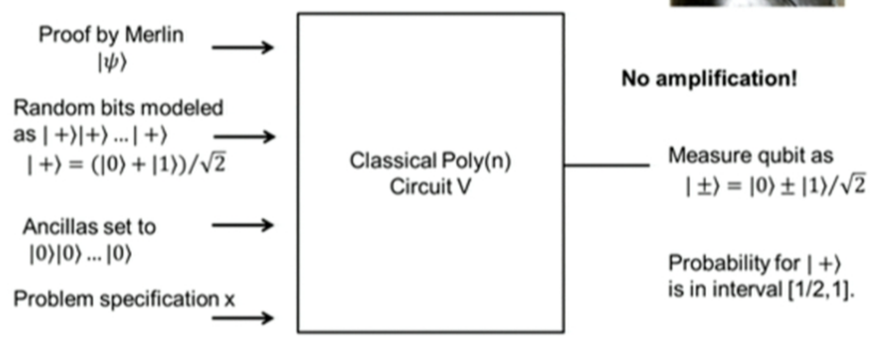
Eigenvector with largest eigenvalue of G (groundstate of H) is a nonnegative vector, i.e. $|\varphi\rangle = \sum_i \alpha_i \, |i\rangle$ with $\alpha_i \geq 0.$

Term-wise stoquastic

Stoquastic Hamiltonians and verifiers (technical)

Why can a stoquastic Arthur decide whether a stoquastic Hamiltonian has a state with energy less than *a* or all states have energy larger than *a+1/poly(n)*?

Stoquastic Arthur



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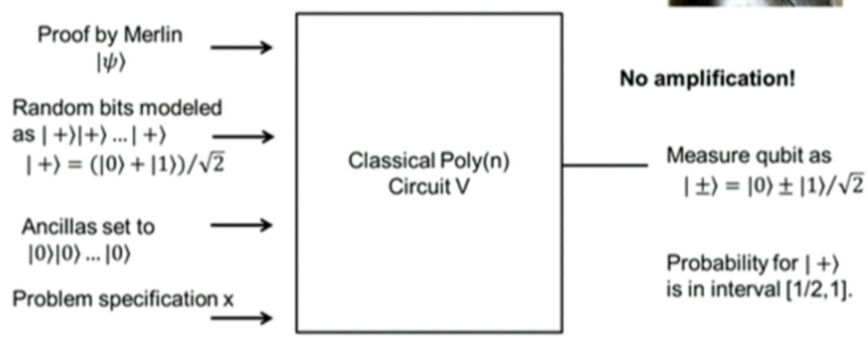

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Stoquastic Hamiltonians and verifiers (technical)

Lemma 2. *Let H be k-local stoquastic Hamiltonian on n qubits. There exist constants $\gamma > 0$ and β such that*

$$\gamma H + \beta I = \sum_j p_j U_j H_j U_j^\dagger, \tag{10}$$

where $p_j \geq 0$, $\sum_j p_j = 1$, U_j is a quantum circuit on n qubits with X and CNOT gates. The stoquastic term H_j is either $-|0\rangle\langle 0|^{\otimes k}$ or $-X \otimes |0\rangle\langle 0|^{\otimes k-1}$. All terms in the decomposition Eq. (10) can be found efficiently.

Any k-qubit Hermitian operator R with non-positive matrix elements can be written as

$$R = \frac{1}{2} \sum_{x,y \in \Sigma^k} R_{x,y} \left(|x\rangle\langle y| + |y\rangle\langle x| \right), \quad R_{x,y} \leq 0.$$

CNOT gates such that $|x\rangle = U_{x,y}|0^k\rangle$, $|y\rangle = U_{x,y}|10^{k-1}\rangle$. Thus we get

$$R = \sum_{x \in \Sigma^k} R_{x,x} U_x \left(|0\rangle\langle 0|^{\otimes k} \right) U_x^\dagger + \frac{1}{2} \sum_{x \neq y \in \Sigma^k} R_{x,y} U_{x,y} \left(X \otimes |0\rangle\langle 0|^{k-1} \right) U_{x,y}^\dagger.$$

Using X measurement

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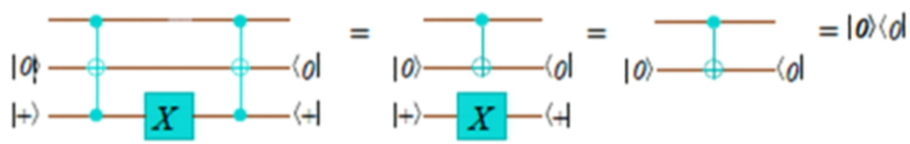

Figure 2: How to simulate measurement of $|0\rangle\langle 0|$ by measurement of X.

We can measure $P_0 = |0\rangle\langle 0|$ on a state ψ by having two ancillas $|0\rangle$ *and* $|+\rangle$ and a Toffoli gate, and measure X on $|+\rangle$.

$$Prob(+) = \mathrm{Tr}(|+\rangle\langle +|\varrho) = \mathrm{Tr}(\rho(I+X)/2)$$

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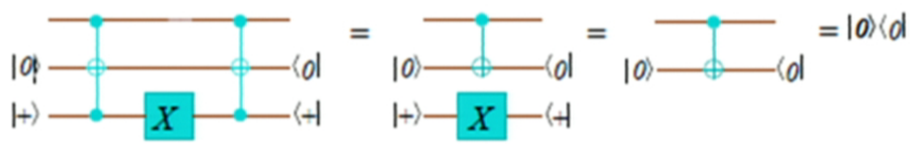

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Fault-tolerant perturbation gadgets?

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