Title: Quantum Simulations of Quantum and Classical Systems

Date: Jan 22, 2007 04:00 PM

URL: http://pirsa.org/07010006

Abstract: If a large quantum computer (QC) existed today, what type of physical problems could we efficiently simulate on it that we could not simulate on a conventional computer? In this talk, I argue that a QC could solve some relevant physical "questions" more efficiently. First, I will focus on the quantum simulation of quantum systems satisfying different particle statistics (e.g., anyons), using a QC made of two-level physical systems or qubits. The existence of one-to-one mappings between different algebras of observables or between different Hilbert spaces allow us to represent and imitate any physical system by any other one (e.g., a bosonic system by a spin-1/2 system). We explain how these mappings can be performed showing quantum networks useful for the efficient evaluation of some physical properties, such as correlation functions and energy spectra. Second, I will focus on the quantum simulation of classical systems. Interestingly, the thermodynamic properties of any d-dimensional classical system can be obtained by studying the zero-temperature properties of an associated d-dimensional quantum system. This classical-quantum correspondence allows us to understand classical annealing procedures as slow (adiabatic) evolutions of the lowest-energy state of the corresponding quantum system. Since many of these problems are NP-hard and therefore difficult to solve, is worth investigating if a QC would be a better device to find the corresponding solutions.

Quantum Simulations of Quantum and Classical Systems

Rolando D. Somma, P-21 LANL

G. Ortiz, M. Knill, R. Laflamme, C. Batista, D. Berkeland, J. Chiaverini, W. Lybarger…

Perimeter Institute
January 22nd, 2007

Los Alamos NATIONAL LABORATORY

Quantum Institute

Quantum Simulations of Quantum and Classical Systems

Rolando D. Somma, P-21 LANL

(G. Ortiz, M. Knill, R. Laflamme, C. Batista, D. Berkeland, J. Chiaverini, W. Lybarger…

Perimeter Institute
January 22nd, 2007

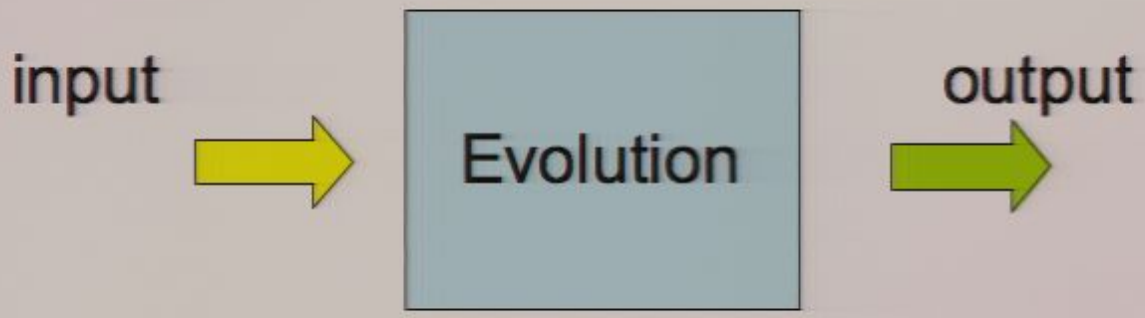
-Conventional Computers $\rightarrow \mathcal{O}(2^N)$

N-qubit systems

$$H = \begin{pmatrix} h_{11} & h_{12} & \cdots & & h_{12^N} \\ h_{21} & h_{22} & \cdots & & h_{22^N} \\ \vdots & \vdots & \ddots & & \vdots \\ & & & \ddots & \\ h_{2^N 1} & h_{2^N 2} & \cdots & & h_{2^N 2^N} \end{pmatrix}$$

-Quantum Computers

Quantum Physical Process $\Longleftrightarrow$ Quantum Information Process



Quantum Simulation: imitate the physical process

If we had a large QC… what type of physical processes could we simulate?

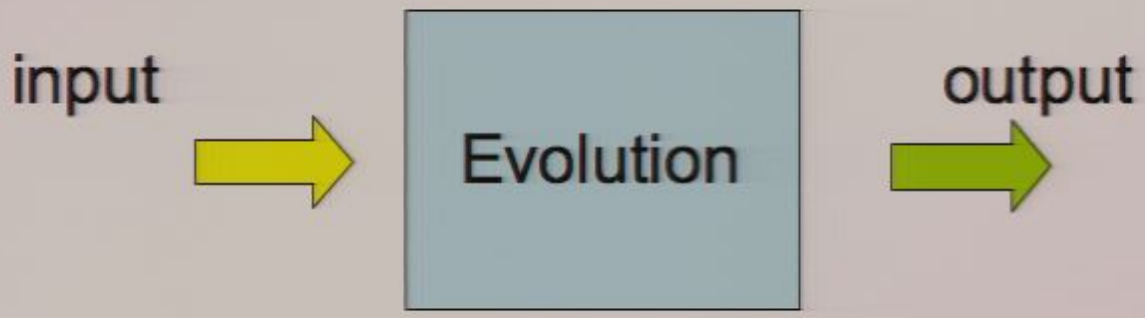
-Conventional Computers $\rightarrow \mathcal{O}(2^N)$

N-qubit systems

$$H = \begin{pmatrix} h_{11} & h_{12} & \cdots & & h_{12^N} \\ h_{21} & h_{22} & \cdots & & h_{22^N} \\ \vdots & \vdots & \ddots & & \vdots \\ & & & \ddots & \\ h_{2^N 1} & h_{2^N 2} & \cdots & & h_{2^N 2^N} \end{pmatrix}$$

-Quantum Computers

Quantum Physical Process $\Longleftrightarrow$ Quantum Information Process



Quantum Simulation: imitate the physical process

If we had a large QC… what type of physical processes could we simulate?

Outline

-Standard Model of Quantum Computation

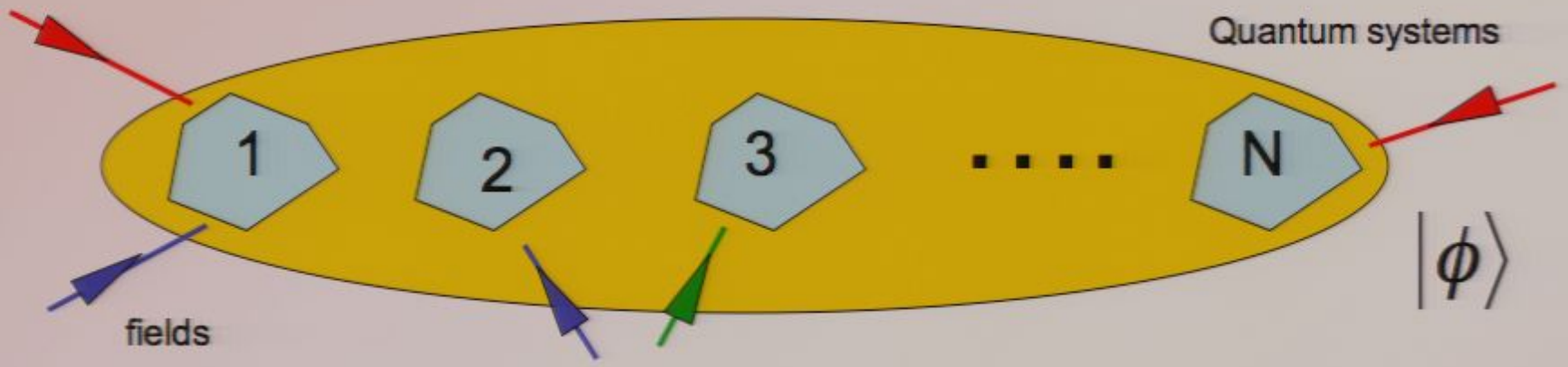
-Efficient Quantum Simulations of Spin Systems

-Adiabatic Quantum Computation?

-Quantum Simulations of Bosonic and Fermionic Systems

-Quantum Simulations of Classical Systems

Deterministic Quantum Algorithms



1- Preparation of an initial (pseudo) pure state $\rightarrow |\phi\rangle$

2- Unitary Evolution $\rightarrow U_P ... U_1 |\phi\rangle$ (e.g., external fields)

3- Measurement of Observable (after *n* repetitions)

$$\rightarrow \langle\sigma\rangle = \langle\phi|U_1^\dagger \cdots U_P^\dagger \sigma U_P \cdots U_1|\phi\rangle$$

Encoded Result $\boxed{\langle\sigma\rangle_{exact} = \langle\sigma\rangle_{meas} \pm 1/\sqrt{n}}$

Algorithm: Errors & Efficiency

In reality $\boxed{\langle \sigma \rangle_{exact} = \langle \sigma \rangle_{meas} \pm \varepsilon}$

Some reasons…

The algorithm is performed a finite # of times (proj. measur.)

Gate imperfections (cont. parameter; will not discuss)

Approximation of Evolution

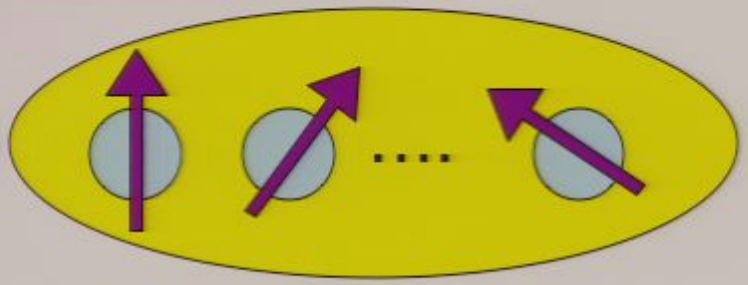
Decoherence (will not discuss)

Def.: an algorithm is efficient with respect to N (problem size) if the amount of resources needed (# of bits and operations) scales at most as poly(N) and poly($1/\varepsilon$).

Algorithms in the Standard Model of QC

-QC is made of qubits

$$|\psi(t)\rangle = a_0|0...0\rangle + a_1|0..1\rangle + ...+ a_{2^N-1}|1..1\rangle$$

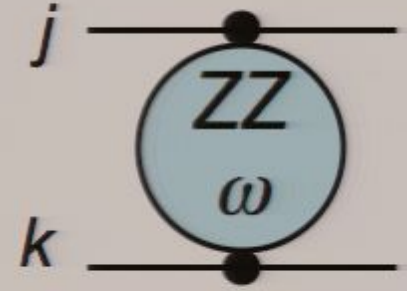


-Language given by the Pauli Algebra

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \; ; \; \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \; ; \; \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

-Possible elementary gates: single qubit rotations + two-qubit interactions

$$R_\mu(\vartheta) = e^{-i\vartheta\sigma_\mu/2}$$



$$R_{jk}(\omega) = e^{-i\omega\sigma_z^j\sigma_z^k/2}$$

Universal control

$$U = \prod_j U_j$$

-Measurement: Projection onto an eigenstate of $\prod_{j,\mu} \sigma_j^\mu$

Algorithms in the Standard Model of QC

Resources:

-Number of qubits $\longrightarrow \mathcal{O}(N)$

-Number of single and two-qubit gates $\longrightarrow \mathcal{O}(N^p)$

- Number of repetitions $\longrightarrow \mathcal{O}(1/\epsilon^2)$

-Time required to prepare desired initial state $\longrightarrow \mathcal{O}(??)$

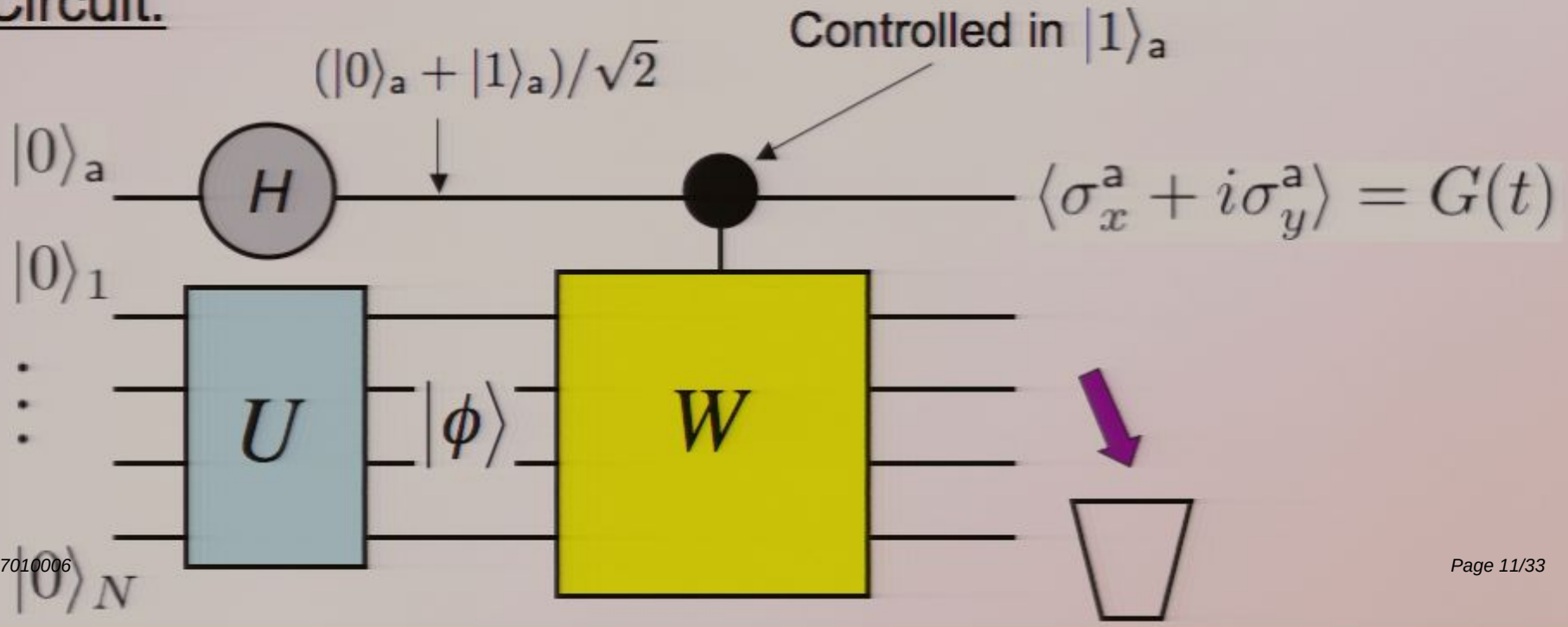
N is the volume of the system to be simulated

Quantum Simulations: Computation of Correlation Functions

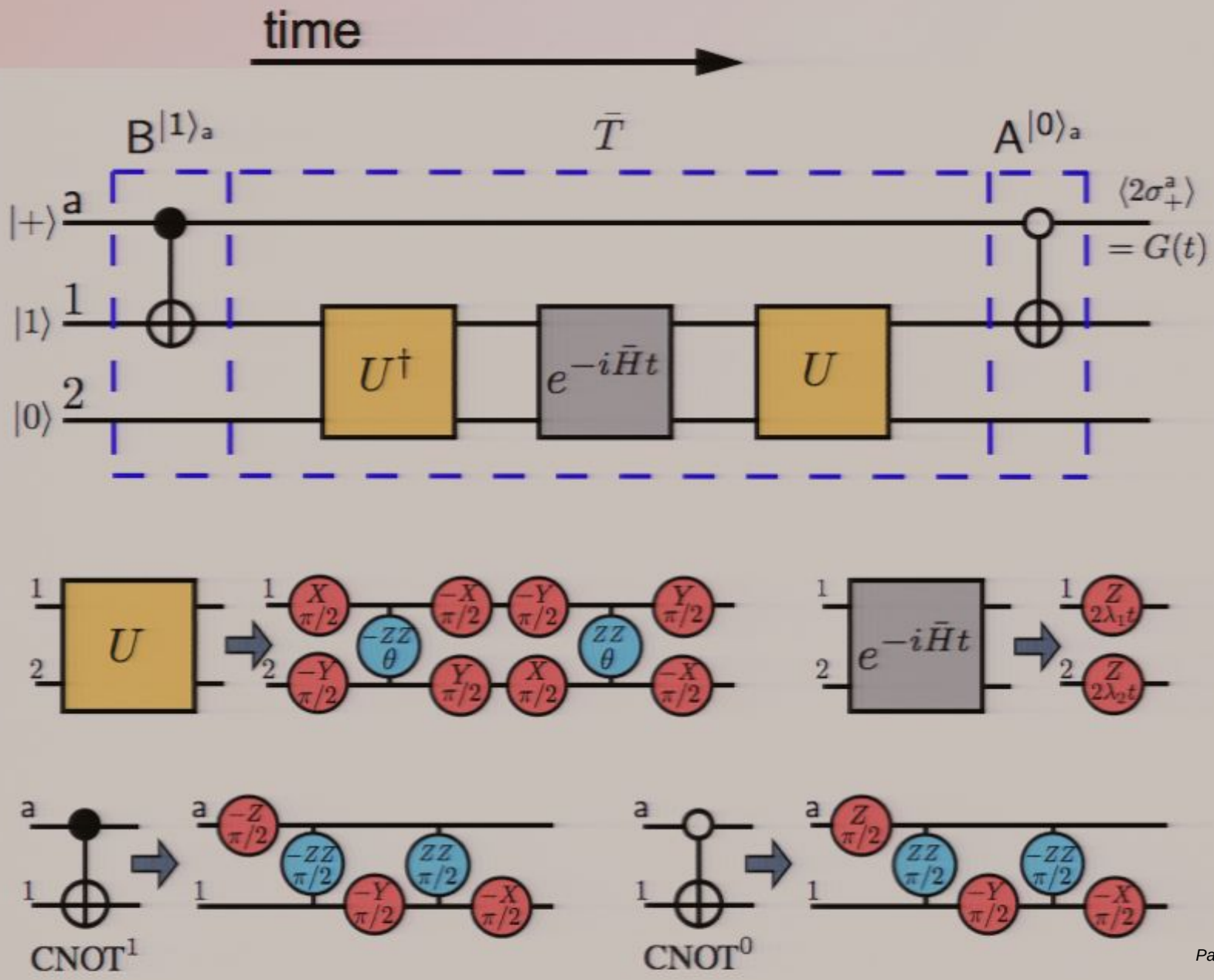
$$G(t) = \langle \phi | W | \phi \rangle; |\phi\rangle = U|0_1 ... 0_N\rangle; W^+ = W^{-1}; U^+ = U^{-1}$$

N = Size of quantum system to be simulated…. Can we obtain *G* efficiently (poly (*N*))?

Circuit:



Example of a Quantum Circuit

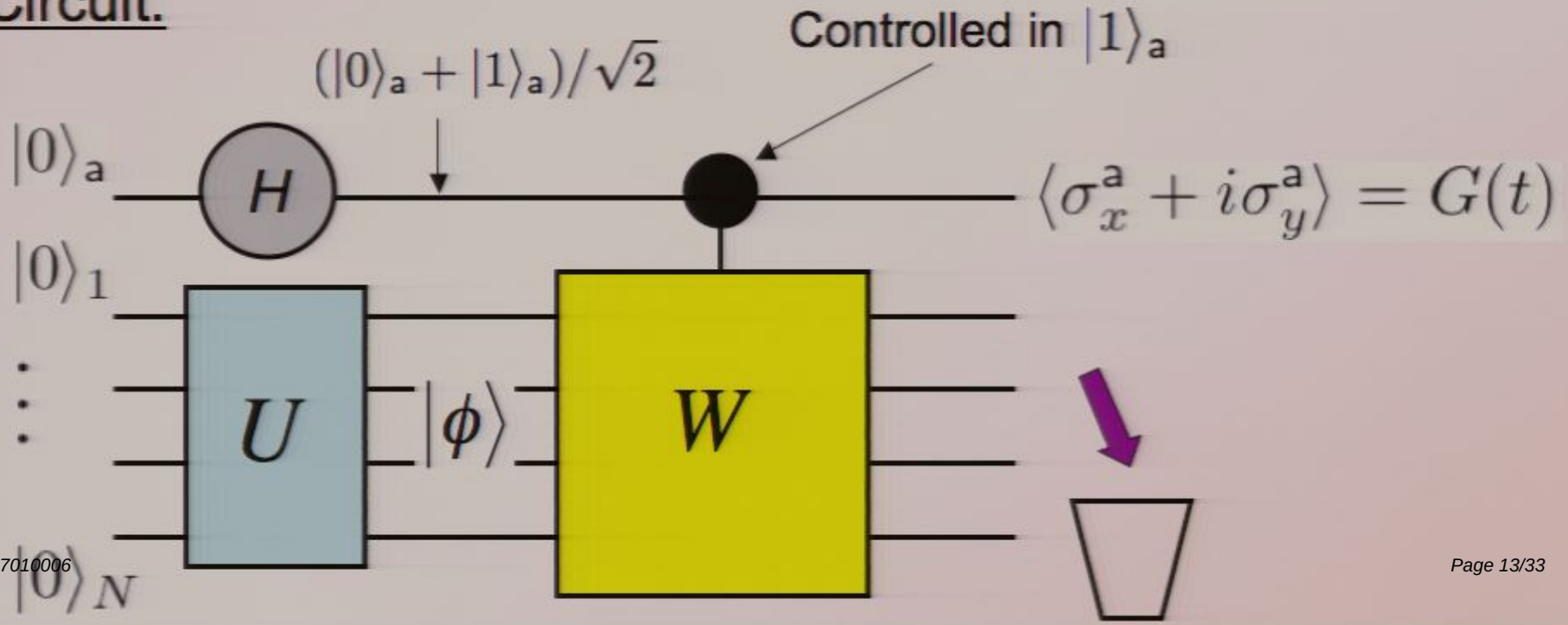


Quantum Simulations: Computation of Correlation Functions

$$G(t) = \langle \phi | W | \phi \rangle; |\phi\rangle = U|0_1 ... 0_N\rangle; W^+ = W^{-1}; U^+ = U^{-1}$$

N = Size of quantum system to be simulated…. Can we obtain *G* efficiently (poly (*N*))?

Circuit:



Quantum Simulations: Computation of Correlation Functions

1- # of qubits is $N+1$

2- Assume $U = \prod_{j=1}^{P \leq \mathrm{poly}(N)} U_j$ (product of elementary gates: The initial state can be easily prepared)

3- Assume $W = e^{iHt} \rightarrow H = \sum_{j=1}^{\mathrm{poly}(N)} c_j H_j;\ H_j = \prod_{k,\mu} \sigma_\mu^k$ (Physical Hamiltonian)

$\rightarrow e^{iHt} \approx \prod_{j=1}^{\mathrm{poly}(N)} W_j$

4- Single qubit measurement (flipping coin)

A QC can obtain $G(t)$ efficiently (i.e., poly(N) resources)

It is not known, in general, how to compute $G(t)$ efficiently on a CC (2^N)

Exponential Speed-up

Quantum Simulations: Trotter Approximation

3- Assume $W = e^{iHt} \rightarrow H = \sum_{j=1}^{\mathrm{poly}(N)} c_j H_j;\ H_j = \prod_{k,\mu} \sigma_\mu^k$ (Physical Hamiltonian)

$$\rightarrow e^{iHt} \approx \prod_{j=1}^{\mathrm{poly}(N)} W_j$$

$$e^{iHt} = \prod e^{iH\Delta t}; e^{iH\Delta t} \approx e^{ic_1 H_1 \Delta t} .. e^{ic_P H_P \Delta t} \longrightarrow \varepsilon_{TA} \approx \|H\|^2 t\Delta t$$

Fixed error $\Rightarrow O(N^2)$

$$H_j = \sigma_x^1\sigma_z^2\sigma_x^3 \Rightarrow e^{ic_j H_j} = e^{-i\pi\sigma_y^2/4} e^{-i\pi\sigma_x^2\sigma_x^3/4} e^{-i\pi\sigma_y^1/4} e^{ic_j\sigma_z^1\sigma_z^2} e^{i\pi\sigma_y^1/4} e^{i\pi\sigma_x^2\sigma_x^3/4} e^{i\pi\sigma_y^2/4}$$

$$e^{i\pi\sigma_y^3/4} e^{i\pi\sigma_y^3/4} e^{-i\pi\sigma_z^2\sigma_z^3/4} e^{-i\pi\sigma_y^3/4} e^{-i\pi\sigma_y^3/4}$$

12 single qubit rotations + 3 phase gates

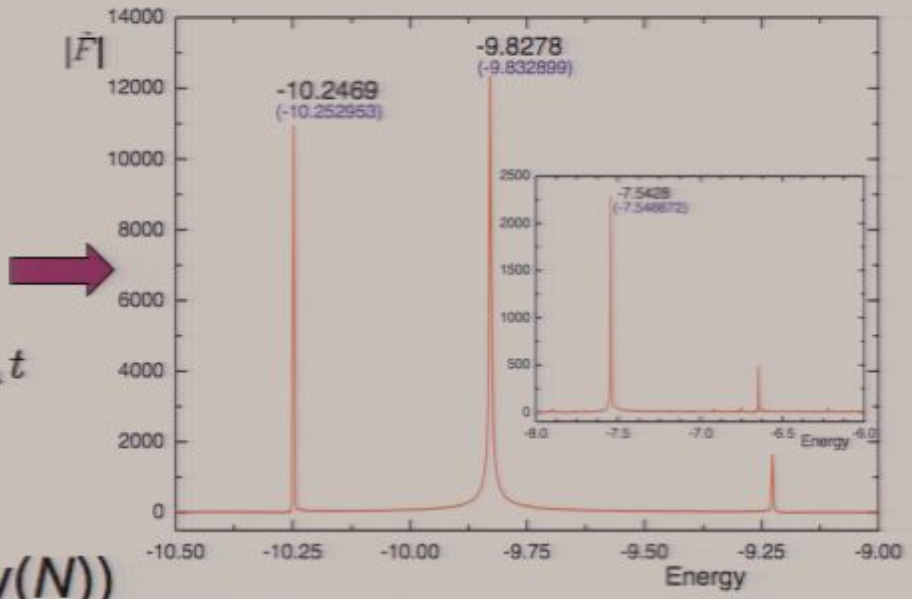
Quantum Simulations: Computation of Ground-State Properties

$H|n\rangle = E_n|n\rangle \quad n = 0 \rightarrow$ Ground state

→ Complex quantum Hamiltonian

$E_0 = ??$

Don't know how to prepare GS



$|\phi\rangle = \sum_n c_n|n\rangle \rightarrow G(t) = \sum_n |c_n|^2 e^{iE_n t}$

Some trial state; easy to prepare (poly(*N*))

$G(t) = \langle\phi|e^{iHt}|\phi\rangle \qquad G(t_1), G(t_2), ..., G(t_M)$

Fourier transform!

The method is efficient if c_0 is finite [i.e., $c_0 \neq \exp(-N)$]

Quantum Simulations: Computation of Ground-State Properties

-In general, it is exponentially hard to obtain the ground-state energy E_0

Why?

-We don't know how to prepare

$$|g\rangle = \prod_{j=1}^{\mathrm{poly}(N)} U_j |0_1 \cdots 0_N\rangle$$

Exactly solvable models
(no quantum advantage)

$$|\phi\rangle \ / \ \langle\phi|g\rangle \neq \exp(-aN)$$

Perform the algorithm exponentially many times

e.g., mean-field solution:

$H \rightarrow \underbrace{H_{MF}}$

Exactly solvable

That's true for simulating the water molecule…

P. Love, et.al

Quantum Simulations: Computation of Ground-State Properties

Also….

$$|\phi\rangle = c_0|g\rangle + c_1|1\rangle + \ldots$$

$$e^{-iHt}|\phi\rangle = c_0 e^{-iE_0 t}|g\rangle + c_1 e^{-i(E_0+\Delta)t}|1\rangle + \ldots$$

Energy gap

Sometimes we need to resolve both frequencies….

⇩

$\mathcal{O}(1/\Delta)$ repetitions for the DFT

How does the gap close with the system size?

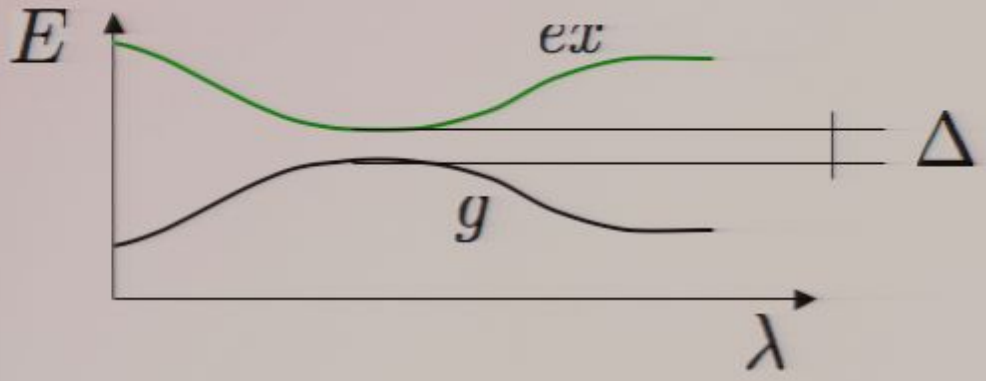
Computation of Ground-State Properties: Adiabatic QC

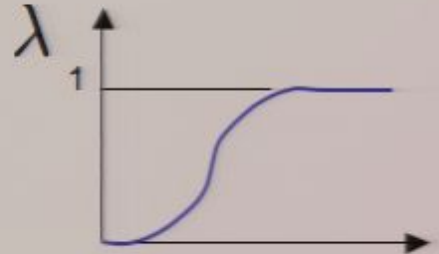
- The complexity relies on the preparation of a particular state (or a state close to it)

Adiabatic QC

Exactly solvable: we know how to prepare its ground state easily

$$H_\lambda = (1-\lambda)H_0 + \lambda H \; ; \; \lambda(0) = 0 \; ; \; \lambda(\infty) = 1$$





$$U \approx \prod_{j=1}^{M} e^{iH_{\lambda(t_j)}\Delta t_j}$$

$$|\langle g|U|0_1 \cdots 0_N\rangle| \to 1$$

$M \propto \Delta^{-2}$

If the gap closes exponentially ⇒ Inefficient
If the gap closes polynomially ⇒ Efficient

There are infinite-many possible H_0

Quantum Simulations of Fermionic Systems

$H \to H_{ferm}(c_i^\dagger; c_j)$

Creation; annihilation

$\{c_i^+, c_j\} = \delta_{ij}$

$c_1^\dagger c_3^\dagger |vac\rangle \to$ (1) (2) (3) (4) (5)

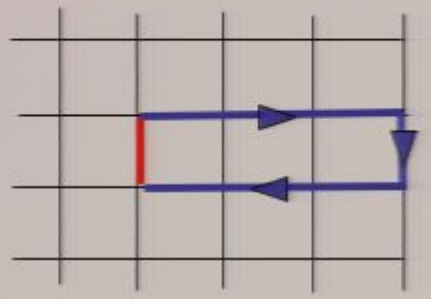
Jordan-Wigner Transf. $\left\{ c_j^\dagger \to \prod_{i=1}^{j-1} \sigma_z^i \sigma_+^j \right.$

$|vac\rangle \to |1_1 1_2 \cdots 1_N\rangle$

$c_1^\dagger c_3^\dagger |vac\rangle \to |0_1 1_2 0_3 1_4 1_5\rangle$

Mapped fermionic model

$G_{ferm}(t) = \langle vac|U^\dagger e^{iH_{ferm}t} U|vac\rangle \to G(t) = \langle 0_1 \cdots 0_N|U'^\dagger e^{iHt} U'|0_1 \cdots 0_N\rangle$



The transformation is efficient: it can be efficiently done + gates can be efficiently implemented

Quantum Simulations of Bosonic Systems

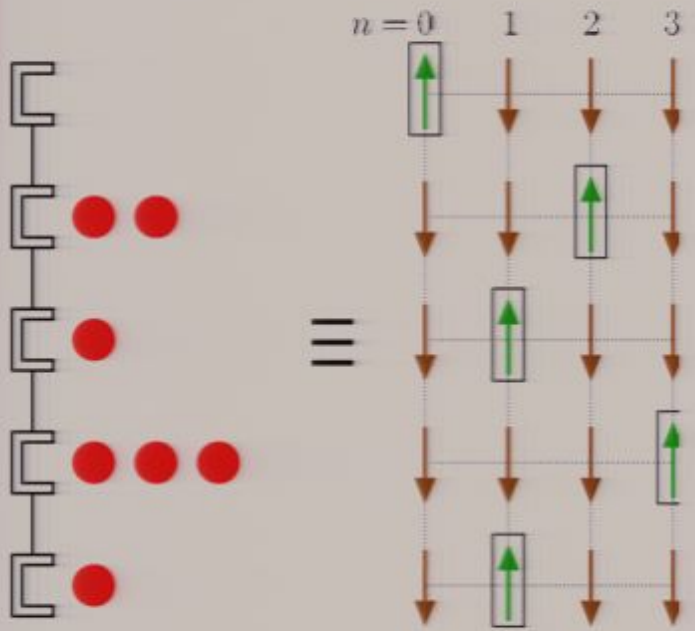
$$H \rightarrow H_{bos}(b_i^\dagger; b_j)$$

Creation; annihilation

$$\left[b_i^+, b_j\right] = \delta_{ij}$$

$$b_1^\dagger b_3^\dagger |n^1 n^2 n^3\rangle \propto$$

If the number of bosons is preserved, a mapping is possible…



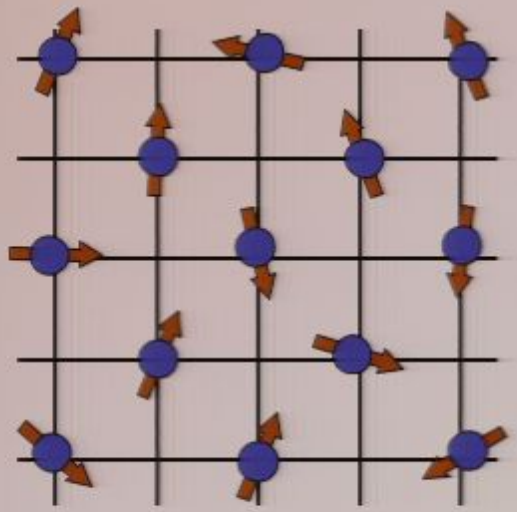
Max. 3 bosons/site

$$b_j^\dagger \rightarrow \sum_{n=0}^{N_P-1} \sqrt{n+1}\sigma_-^{n,j}\sigma_+^{n+1,j}$$

$$|\phi_\alpha\rangle = \frac{1}{2\sqrt{3}} b_1^\dagger (b_2^\dagger)^3 b_3^\dagger (b_1^\dagger)^2 |\text{vac}\rangle$$

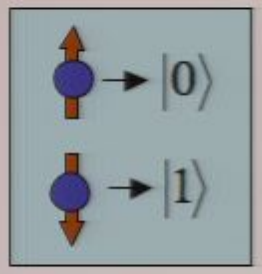
Efficient mapping

Quantum Simulations of Classical Systems



$$T; H = f(\sigma_z^i)$$

$$H_{Ising} = \sum_{<i,j>} J_{ij}\sigma_z^i\sigma_z^j$$



$$\beta = (k_B T)^{-1}; S_\tau = \langle \tau | S | \tau \rangle; |\tau\rangle = |010...0\rangle$$

$$|\psi(T)\rangle = \sum_\tau e^{-\beta E_\tau / 2} |\tau\rangle = e^{-\beta H/2} \sum_\tau |\tau\rangle$$

$$\frac{\sum_\tau A_\tau e^{-\beta E_\tau}}{\sum_\tau e^{-\beta E_\tau}} = \frac{\langle \psi(T) | A | \psi(T) \rangle}{\langle \psi(T) | \psi(T) \rangle}$$

resources required for its preparation determines the complexity of simulating classical systems with QCs

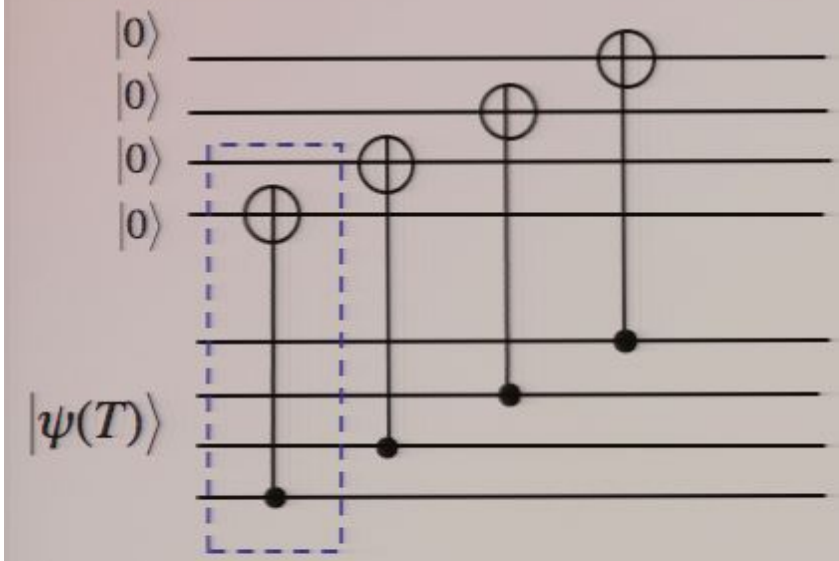
Many Classical (optimization) problems are NP-hard (Barahona'85)

Quantum Simulations of Classical Systems

$$|\psi(T)\rangle = e^{-\beta H/2} \sum_{\tau} |\tau\rangle$$ (Gibbs state)

Thermalization with unitaries

Purification



$$|0\rangle\langle 0| \otimes I + |1\rangle\langle 1| \otimes \sigma_x$$

Actual thermal state

$$|\overline{\psi}(T)\rangle = \sum_{\tau} e^{-\beta E_\tau/2} |\tau\rangle \otimes |\tau\rangle \Rightarrow \rho_S \propto e^{-\beta H}$$

Classical entropy ⇔ (bipartite)Entanglement of formation

Quantum Simulations of Classical Systems

One dimensional Ising model: Efficient Quantum Simulation

$$H_{Ising} = \sum_j J_j \sigma_z^j \sigma_z^{j+1}$$

$$|\psi(T)\rangle = e^{-\beta H_{Ising}/2} \sum_\tau |\tau\rangle = \prod_j (a_j + b_j \sigma_z^j \sigma_z^{j+1}) \sum_\tau |\tau\rangle$$

$$\left(a_3 + b_3 \sigma_z^3 \sigma_z^4\right)\left(a_2 + b_2 \sigma_z^2 \sigma_z^3\right)\left(a_1 + b_1 \sigma_z^1 \sigma_z^2\right) \sum_\tau |\tau\rangle$$

$$\sigma_x^4 \equiv 1$$

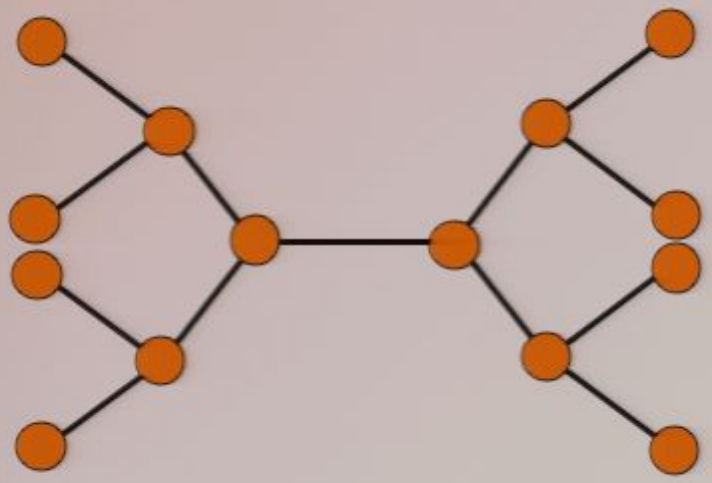
$$\left(a_3 + b_3 \sigma_z^3 \sigma_z^4 \sigma_x^4\right) = a_3 + i b_3 \sigma_z^3 \sigma_y^4 \propto e^{i\theta_4 \sigma_z^3 \sigma_y^4}$$

$$\Rightarrow \quad |\psi(T)\rangle = e^{i\theta_N \sigma_z^N \sigma_y^{N-1}} \ldots e^{i\theta_2 \sigma_z^3 \sigma_y^2} e^{i\theta_1 \sigma_z^2 \sigma_y^1} \sum_\tau |\tau\rangle$$

(This approach can't be used for the two-dimensional model)

Quantum Simulations of Classical Systems

Trees and Matrix Product States: Efficient Classical Simulation



$$H = \sum_{\langle i,j \rangle} J_{ij} \sigma_z^i \sigma_z^j + \sum_i B_i \sigma_z^i$$

$|\psi(T)\rangle$ can be represented with a tree tensor network

(F. Verstraete, et. al.)

⇨ Any classical lattice model in a tree can be efficiently classically simulated

(G. Vidal, et. al. ; H. Briegel, et. al.)

Quantum Simulations of Classical Systems

Quantum Adiabatic Evolution I: Simulated Annealing

$$|\psi(T)\rangle = e^{-\beta H/2}\sum_{\tau}|\tau\rangle \Rightarrow \sigma_x^j|\psi(T)\rangle = e^{-\beta H_j}|\psi(T)\rangle$$

$$\sigma_x^j H \sigma_x^j = H - 2H_j; H_j = \sigma_z^j \otimes \eta_j$$

fluctuations

$$H_q(T) = \sum_j e^{\beta H_j} - \sigma_x^j \Rightarrow H_q(T)|\psi(T)\rangle = 0$$ (unique ground state)

- $T >> 1 \Rightarrow |\psi(T)\rangle \approx \sum_{\tau}|\tau\rangle = |+\rangle_1 \otimes ... \otimes |+\rangle_N; |+\rangle = |0\rangle + |1\rangle$

$$H_q = AMA^{-1}$$

Trans. matrix

- Adiabatic evolution by slow decrease of parameter T (quantum v. simulated annealing)

$$T(t) \approx N/\log(t) \rightarrow \forall H$$ (remain in equilibrium Worst-case: inefficient)

Quantum Simulations of Classical Systems

Classical Adiabatic Evolution: Equivalence of rates

$\overrightarrow{P}_a \propto (p_a^1, \cdots, p_a^{2^N})$ (distribution at time step a)

$\overrightarrow{P}_{eq} \propto (e^{-\beta E_1}, \cdots, e^{-\beta E_{2^N}})$ (equilibrium)

$$\overrightarrow{P}_a = [M(T)]^a \overrightarrow{P}_0 \; ; \; \overrightarrow{P}_{eq} = \overrightarrow{P}_{a \to \infty}$$

⇨ Rate of convergence is determined by the gap of *M*

$$T(t) \approx N / \log(t) \to \forall H$$

(similar scaling obtained by S. Geman and D. Geman '84)

The classical system is always close to equilibrium

Quantum Simulations of Classical Systems

Quantum Adiabatic Evolution I: Simulated Annealing

$$|\psi(T)\rangle = e^{-\beta H/2}\sum_{\tau}|\tau\rangle \Rightarrow \sigma_x^j|\psi(T)\rangle = e^{-\beta H_j}|\psi(T)\rangle$$

$$\sigma_x^j H \sigma_x^j = H - 2H_j; H_j = \sigma_z^j \otimes \eta_j$$

fluctuations

$$H_q(T) = \sum_j e^{\beta H_j} - \sigma_x^j \Rightarrow H_q(T)|\psi(T)\rangle = 0$$ (unique ground state)

- $T >> 1 \Rightarrow |\psi(T)\rangle \approx \sum_{\tau}|\tau\rangle = |+\rangle_1 \otimes ... \otimes |+\rangle_N; |+\rangle = |0\rangle + |1\rangle$

$$H_q = AMA^{-1}$$

Trans. matrix

- Adiabatic evolution by slow decrease of parameter T (quantum v. simulated annealing)

$$T(t) \approx N/\log(t) \rightarrow \forall H$$ (remain in equilibrium Worst-case: inefficient)

Quantum Simulations of Classical Systems

Classical Adiabatic Evolution: Equivalence of rates

$\overrightarrow{P}_a \propto (p_a^1, \cdots, p_a^{2^N})$ (distribution at time step a)

$\overrightarrow{P}_{eq} \propto (e^{-\beta E_1}, \cdots, e^{-\beta E_{2^N}})$ (equilibrium)

$$\overrightarrow{P}_a = [M(T)]^a \overrightarrow{P}_0 \; ; \; \overrightarrow{P}_{eq} = \overrightarrow{P}_{a \to \infty}$$

⇨ Rate of convergence is determined by the gap of *M*

$$T(t) \approx N / \log(t) \to \forall H$$

(similar scaling obtained by S. Geman and D. Geman '84)

The classical system is always close to equilibrium

Quantum Simulations of Classical Systems

Quantum Adiabatic Evolution II: Quantum Annealing $T>0$

$$\tilde{H}_q(\gamma) = H(\sigma_z^j) - \gamma \sum_j \sigma_x^j \; ; \; \gamma(0) \gg 1 \; , \; \gamma(t \gg 1) \to 0 \; \; ; \; (T=0)$$

(Farhi, et. al.)

$$H_q(\gamma) = \sum_j e^{\beta H_j} - \gamma \sigma_x^j \Rightarrow H_q(\gamma = 1)\left|\psi(T)\right\rangle = 0 \qquad (T > 0)$$

- $\gamma >> 1 \Rightarrow \left|\psi(T)\right\rangle \approx \sum_\tau \left|\tau\right\rangle = \left|+\right\rangle_1 \otimes ... \otimes \left|+\right\rangle_N$

- Adiabatic evolution by slow decrease of parameter γ (quantum annealing for $T>0$)

$$\boxed{\gamma(t) \approx (Nt)^{-1/N} \to \forall H}$$

(remain in equilibrium
Worst-case: inefficient)

For particular problems: see how the gap closes…

A similar rate was obtained for the classical simulation of QA with Monte-Carlo Techniques (H. Nishimori'06)

Quantum Simulations of Classical Systems

Adiabatic evolution

Classical phase transition

Quantum phase transition

$$|\psi(\gamma)\rangle = e^{-\tilde{H}(\gamma)/2}\sum_{\tau}|\tau\rangle; \tilde{H}(\gamma=1)=\beta H$$

(quantum annealing)

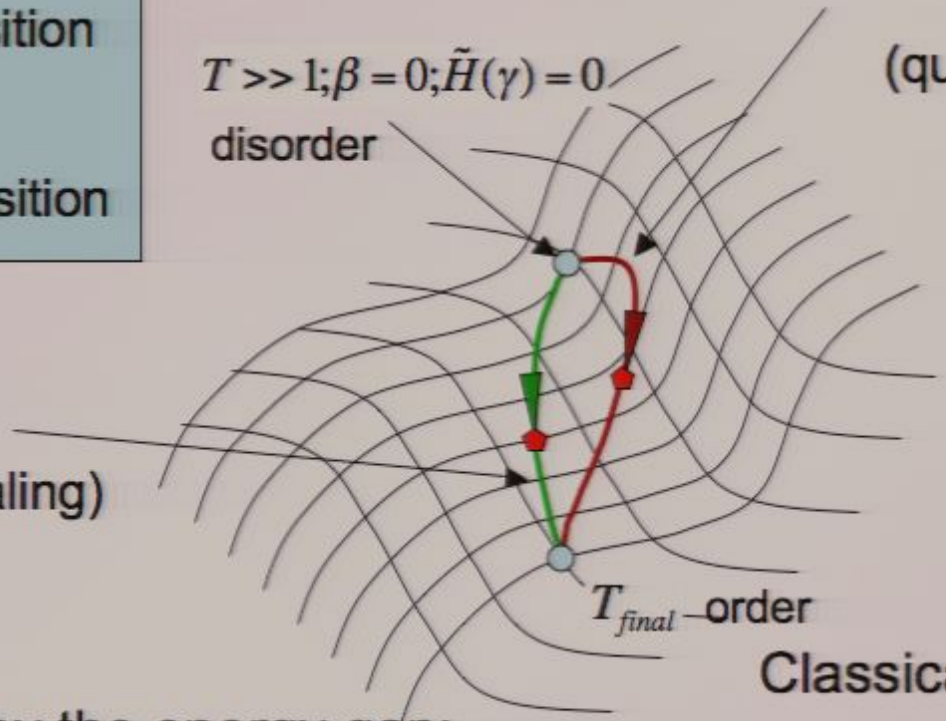
Can we find its classical path?

$T >> 1; \beta = 0; \tilde{H}(\gamma) = 0$

disorder

$$|\psi(T)\rangle = e^{-\beta H/2}\sum_{\tau}|\tau\rangle$$

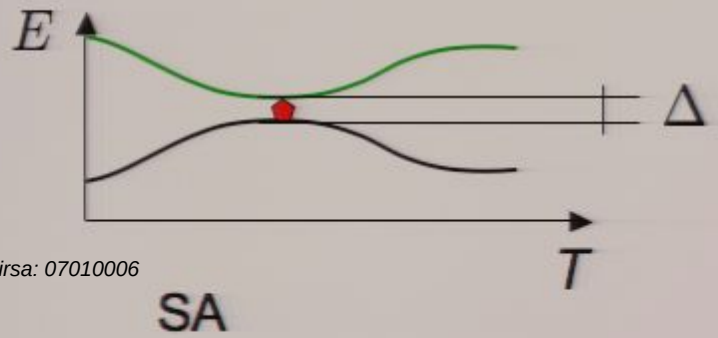
(Qv simulated annealing)

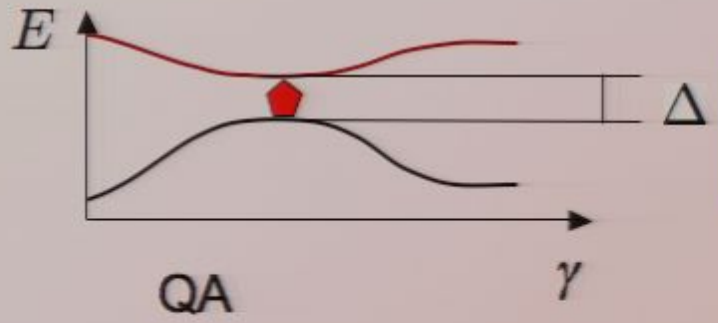


T_{final} – order

Classical *H's*

Time is determined by the energy gap:





Is QA (T>0) more efficient?

Conclusions + Future Work:

-A QC seems to be a powerful tool for quantum simulations (Exponential Speed-Up in some cases)

$$G(t) = \langle \phi | e^{iHt} \phi \rangle$$

-However, a CC can efficiently compute *G(t)* in some particular cases (Clifford algebra, Gen. Coh. States, etc…)

-Ground state properties…. Adiabatic QC?

-Efficient quantum simulations of fermionic and bosonic systems through algebra and Hilbert space mappings

Conclusions + Future Work:

-Simulation of Classical Systems: Quantum annealing for finite *T*
Convergence rates, etc.

Open questions:

Is there any (quadratic) speed-up by simulating classical systems on QCs?

Is there a classical interpretation of quantum annealing (without going to d+1)?