Quantum Metropolis Sampling

David Poulin

Département de Physique
Université de Sherbrooke

Joint work with: K. Temme, T. Osborne, K. Vollbrecht, and F. Verstraete

Workshop on quantum Algorithms, Computational Models, and Foundations of Quantum Mechanics
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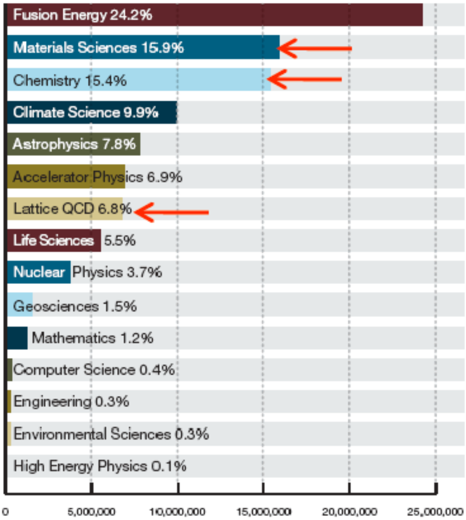
July 2010

Next's year Canadian Quantum Information Summer School
and
Student Conference
June 6th to 17th 2011
Jouvence, Parc National du Mont Orford (near Sherbrooke Qc)


Outline

What are computers used for?



From talk by F. Verstraete, from a talk by S. Aaronson, from a talk by A. Aspuru-Guzik

What are they computing?

Inputs

- A local Hamiltonian $H = \sum_k h_k$:
  - $\|h_k\| = \mathcal{O}(1)$.
  - h_k acts on a few particles, i.e. $h_k = I \otimes I \otimes A \otimes I \otimes I \otimes B \otimes I \otimes I$.
- An efficiently specifiable state ρ, e.g.
  - The Gibbs state $\rho_G(\beta) = \frac{1}{Z} e^{-\beta H}$.
  - The ground state of H, i.e. $\rho_G(\infty)$.
  - Physically relevance: thermal equilibrium at temperature $\frac{1}{\beta}$.

Output

$\langle X(t)Y\rangle = \mathrm{Tr}\{Xe^{-iHt}Ye^{iHt}\rho_G(\beta)\}$ for one-body operators X and Y.

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Why is this complicated?

$$\mathrm{Tr}\{Xe^{-iHt}Ye^{iHt}\rho\}$$

- Matrix multiplication in vector space $\mathcal{H}$ of dimension exponential with the number of particles.

- ρ is not specified in a useful format:
  - E.g., $\rho \propto e^{-\beta H}$.
  - Computing its matrix elements ρ_{ij} is hard.

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Some partial solutions

- Weakly interacting particles: $H = H_0 + \epsilon V$.
  - Perturbation theory
  - Hartree-Fock
  - Density functional theory
  - etc.
- Weakly entangled particles/one dimension
  - Renormalization methods (NRG, DMRG, MPS, PEPES).
  - Other variational methods (Laughlin state, Moore-Read).
- Unfrustrated bosonic systems
  - Quantum Monte Carlo $e^{-\beta H} \sim (I - \epsilon H) \otimes (I - \epsilon H) \otimes \dots$

The interesting physics appears to lie outside the scope covered by these methods.

- Standard model for elementary particle masses
- Hubbard model for superconductivity
- Coulomb force for molecular binding energies

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Outline

Original motivation

International Journal of Theoretical Physics, Vol. 21, Nos. 6/7, 1982

Simulating Physics with Computers

Richard P. Feynman

Department of Physics, California Institute of Technology, Pasadena, California 91107

Received May 7, 1981

1. INTRODUCTION

On the program it says this is a keynote speech—and I don't know what a keynote speech is. I do not intend in any way to suggest what should be in this meeting as a keynote of the subjects or anything like that. I have my own things to say and to talk about and there's no implication that anybody needs to talk about the same thing or anything like it. So what I want to talk about is what Mike Dertouzos suggested that nobody would talk about. I want to talk about the problem of simulating physics with computers and I mean that in a specific way which I am going to explain.

Original motivation

International Journal of Theoretical Physics, Vol. 21, Nos. 6/7, 1982

Simulating Physics with Computers

be understood very well in analyzing the situation. And I'm not happy with all the analyses that go with just the classical theory, because nature isn't classical, dammit, and if you want to make a simulation of nature, you'd better make it quantum mechanical, and by golly it's a wonderful problem, because it doesn't look so easy. Thank you.

I. INTRODUCTION

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with it, with quantum-mechanical rules). For example, the spin waves in a spin lattice imitating Bose-particles in the field theory. I therefore believe it's true that with a suitable class of quantum machines you could imitate any quantum system, including the physical world. But I don't know whether the general theory of this intersimulation of quantum systems has

Solving the dynamics

Lloyd's idea, '96

$$\exp(-it\sum_k h_k) = \left[\prod_k \exp(-ih_k/N)\right]^N + \mathcal{O}(\frac{1}{N^2})$$

So we can integrate Schrödinger's equation, solve $\dot{\rho} = -i[H, \rho]$.

How do we specify the initial conditions $\rho_G(\beta)$?

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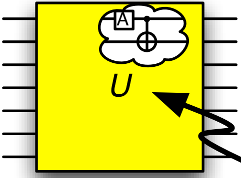

# of gates = poly(n,t,ε^{-1})

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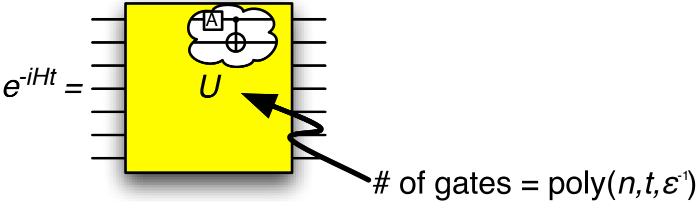

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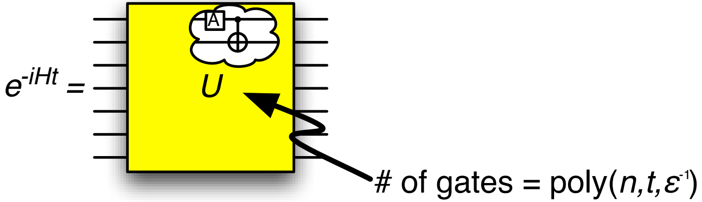

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Approaches to $\rho_G(\beta)$

- Simulate evolution of "system+bath" and Metropolis-like.
  - Conditions for thermalization not reproduced (poorly understood).
- Use adiabatic evolution $H(t) = (1 - t/T)H_0 + t/TH_{hard}$
  - Must avoid quantum phase transition.
  - Limited to ground state.
- Use Grover-like algorithm to search ground state.
  - Slow.

Approaches to $\rho_G(\beta)$

PHYSICAL REVIEW A, VOLUME 61, 022301

Problem of equilibration and the computation of correlation functions on a quantum computer

Barbara M. Terhal[1] and David P. DiVincenzo[2]
[1]*ITF, Universiteit van Amsterdam,Valckenierstraat 65, 1018 XE Amsterdam, The Netherlands and CWI, Kruislaan 413, 1098 SJ Amsterdam, The Netherlands*
[2]*IBM Thomas J. Watson Research Center, Yorktown Heights, New York 10598*
(Received 2 November 1998; revised manuscript received 16 August 1999; published 4 January 2000)

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A Quantum Adiabatic Evolution Algorithm Applied to Random Instances of an NP-Complete Problem

Edward Farhi,[1*] Jeffrey Goldstone,[1] Sam Gutmann,[2]
Joshua Lapan,[3] Andrew Lundgren,[3] Daniel Preda[3]

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A Quantum Adiabatic Evolution Algorithm Applied to Random

PRL **102,** 130503 (2009) PHYSICAL REVIEW LETTERS week ending 3 APRIL 2009

Preparing Ground States of Quantum Many-Body Systems on a Quantum Computer

David Poulin[1,*] and Pawel Wocjan[2]
[1]*Département de Physique, Université de Sherbrooke, Sherbrooke, Québec, Canada*
[2]*School of Electrical Engineering and Computer Science, University of Central Florida, Orlando, Florida, USA*
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PRL **102,** 130503 (2009) PHYSICAL REVIEW LETTERS week ending 3 APRIL 2009

Preparing Ground States of Quantum Many-Body Systems on a Quantum Computer

PRL **103,** 220502 (2009) PHYSICAL REVIEW LETTERS week ending 27 NOVEMBER 2009

Sampling from the Thermal Quantum Gibbs State and Evaluating Partition Functions with a Quantum Computer

David Poulin[1] and Pawel Wocjan[2]
[1]*Département de Physique, Université de Sherbrooke, Québec, Canada, J1K 2R1*
[2]*School of Electrical Engineering and Computer Science, University of Central Florida, Florida 32816-2362, USA*
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How is this problem solved for classical systems?

Use Markov Chain Monte Carlo to sample from $p_G(x) = \frac{1}{Z} e^{-\beta E(x)}$

The Metropolis algorithm

1. Start from a random configuration x of energy $E(x)$.
2. Generate a new configuration y by changing x at a few locations.
3. Accept / reject new configuration with $w_{xy} = min\{1, e^{\beta(E(x)-E(y))}\}$:
   - Accept $x \leftarrow y$ with probability w_{xy}.
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Equation of State Calculations by Fast Computing Machines

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Markov chain

$$x_0 \xrightarrow{P(x_1|x_0)} x_1 \xrightarrow{P(x_2|x_1)} x_2 \ldots x_{n-1} \xrightarrow{P(x_n|x_{n-1})} x_n$$

Detailed balance condition

The distribution $p_G(x) = \frac{1}{Z} e^{-\beta H(x)}$ obeys the condition

$$p_G(x) P(y|x) = p_G(y) P(x|y)$$

so it is the fixed point of the Markov chain $P(x|y)$.

Convergence rate

The convergence rate is given by the inverse spectral gap Δ^{-1} of the stochastic matrix $P(x|y)$: $n \in \mathcal{O}(\Delta^{-1})$.
Δ^{-1} appears to scale polynomially for problems of interest.

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Outline

Can't we do the same with quantum systems?

Objective

CPTP map $\mathcal{E}$ such that $\mathcal{E}^n(\rho_0) \rightarrow \frac{1}{\mathcal{Z}} e^{-\beta H}$ for large enough n.

Straightforward generalization of Metropolis

1. Start from a random energy eigenstate ψ_i of energy E_i.
2. Generate a new "nearby" energy eigenstate ψ_j of energy E_j.
3. Accept / reject new configuration with $w_{ij} = min\{1, e^{\beta(E_i - E_j)}\}$:
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CPTP map $\mathcal{E}$ such that $\mathcal{E}^n(\rho_0) \to \frac{1}{\mathcal{Z}} e^{-\beta H}$ for large enough n.

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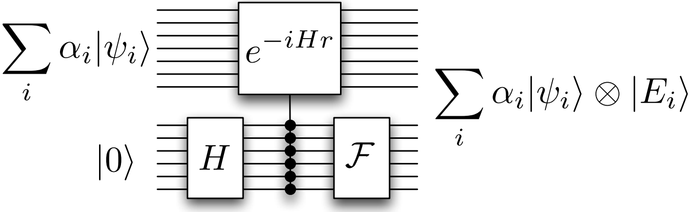

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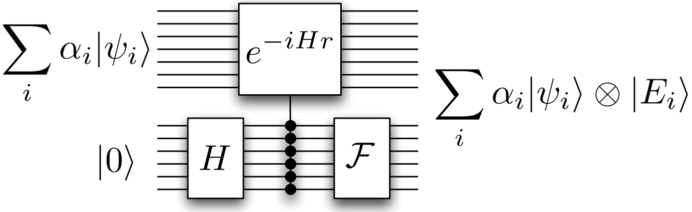

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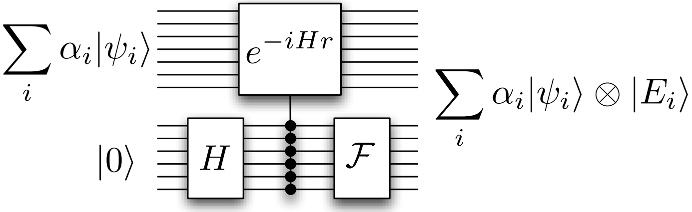

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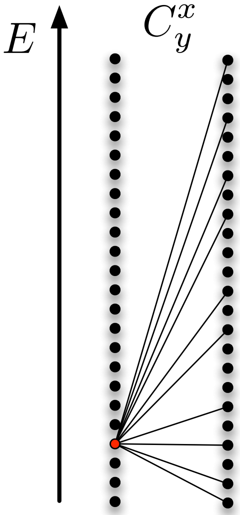

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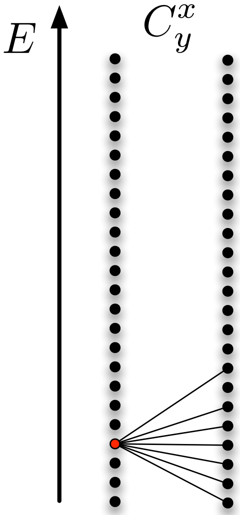

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Measure last qubit:

- If the outcome is 0, measure the "energy register" to learn E_j and return to step 2.
- If the outcome is 1, go back to state ψ_i.

This is already better because only one bit of information was learned–accepr/reject–so less damage was made to the state.

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Undoing binary measurement, Marriott & Watrous '05

Ingredients

- Initial state $|\psi\rangle$.
- Circuit for measurement $\mathcal{P} = \{P, P^\perp\}$ with $P = |\psi\rangle\langle\psi|$.
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Goal

Starting from $Q^\perp|\psi\rangle$, go back to $|\psi\rangle$.

Solution

Iterate $\mathcal{P}$ and $\mathcal{Q}$ measurements until outcome P is obtained.

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Repeat m times, probability of failure is $\sim p^{-m}$.

We can reject the update $\rightarrow$ quantum Metropolis step $\mathcal{E}$.

Quantum detailed balance

$$\sqrt{p_m p_n}\langle\psi_i|\mathcal{E}(|\psi_m\rangle\langle\psi_n|)|\psi_j\rangle = \sqrt{p_i p_j}\langle\psi_m|\mathcal{E}(|\psi_i\rangle\langle\psi_j|)|\psi_n\rangle$$

Hence $\rho_G = \sum_j p_j|\psi_j\rangle\langle\psi_j|$ is the fixed point, $p_j \propto e^{-\beta E_j}$.

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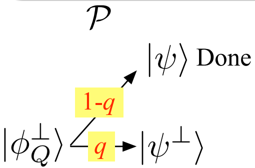

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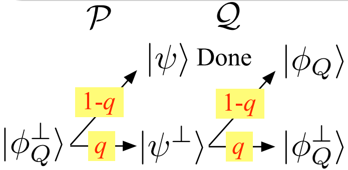

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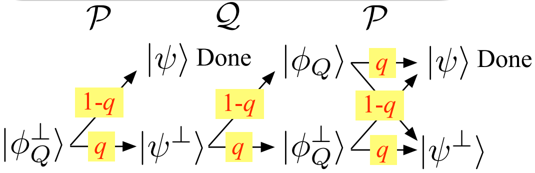

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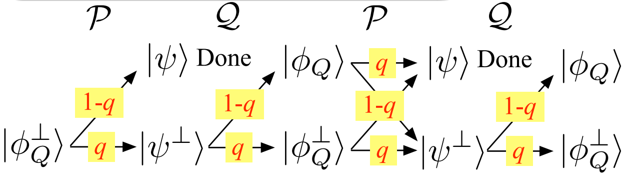

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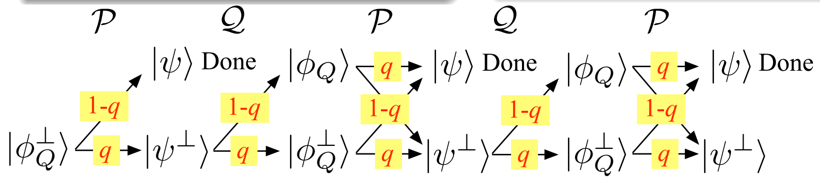

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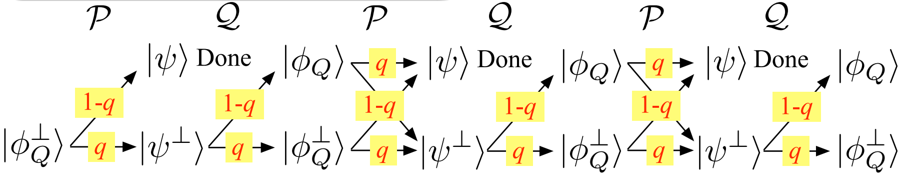

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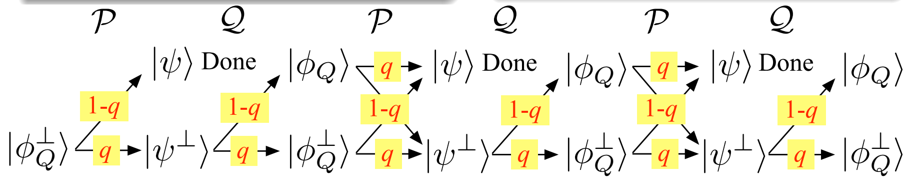

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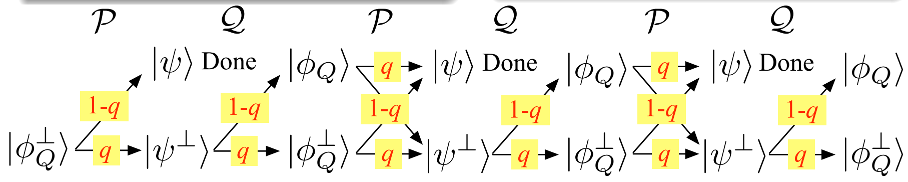

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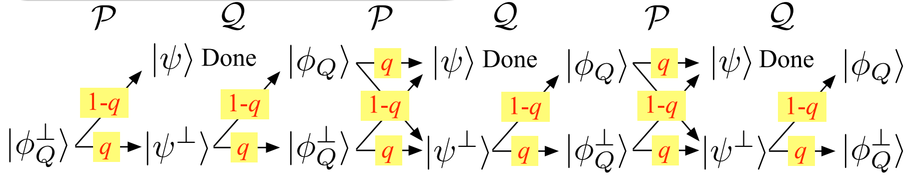

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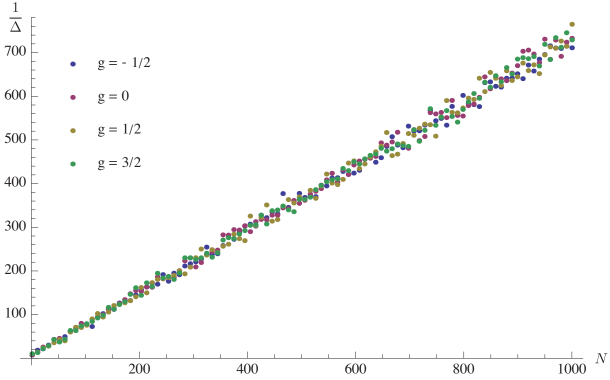
Inverse gap for XY model at $T = 0$

The model

$$H = \sum_k \sigma_k^x \sigma_{k+1}^x + \sigma_k^y \sigma_{k+1}^y + g\sigma_k^z$$

The local moves

$$C_k = \left(\bigotimes_{j=1}^{k-1} \sigma_j^z \right) \sigma_k^x$$



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- They require initializing the quantum computer in physically relevant state.
- The classical problem is solved by the Metropolis algorithm.
  - Rapidly mixing Markov chain to sample from Gibbs distribution.
  - Cleaver unphysical moves can be much faster than "system+bath" simulation.
- We have shown how to leverage the full power of the Metropolis algorithm to the quantum setting.
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