Title: Quantum Metropolis sampling

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Abstract: Quantum computers have emerged as the natural architecture to study the physics of strongly correlated many-body quantum systems, thus providing a major new impetus to the field of many-body quantum physics. While the method of choice for simulating classical many-body systems has long since been the ubiquitous Monte Carlo method, the formulation of a generalization of this method to the quantum regime has been impeded by the fundamental peculiarities of quantum mechanics, including, interference effects and the no-cloning theorem.
We overcome those difficulties by constructing a quantum algorithm to sample from the Gibbs distribution of a quantum Hamiltonian at arbitrary temperatures, both for bosonic and fermionic systems. This is a further step in validating the quantum computer as a full quantum simulator, with a wealth of possible applications to quantum chemistry, condensed matter physics and high energy physics.

universität wien

Quantum Metropolis Sampling

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arXiv: 0911.3635

Perimeter Institute
November 10th

Overview

- Brief motivation
- Description of the algorithm
- Analysis of the algorithm and comments on rapid mixing
- Example circuit for 5 - qubits

Feynman 1982

- "I'm not happy with all the analysis that go with just 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"

Three paths to enlightenment

Solve the many body Schrödinger equation

$$\hat{H}|\psi\rangle = E|\psi\rangle$$

Classical simulation of quantum systems

Weakly interacting systems: perturbation theory, DFT, HF, etc...

Strongly interacting systems: variational methods, RG, Quantum Monte Carlo, etc ...

Build a Quantum Simulator

cf. Cirac, Zoller et al.

Optical lattices,...

Simulation of quantum systems on a universal Quantum Computer

Achievements in Quantum Simulation

- Lloyd '96:

  Dynamics: Any local Hamiltonian Evolution can be simulated with a quantum circuit!

$$\exp\left(-i\delta t \sum_\alpha H_\alpha\right) \approx \prod_\alpha \exp\left(-i\delta t\ H_\alpha\right) + \mathcal{O}(\delta t^2)$$

Central Idea! Trotter decomposition.

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- To some extend this can already give access to static properties!

1) Prepare ground states:

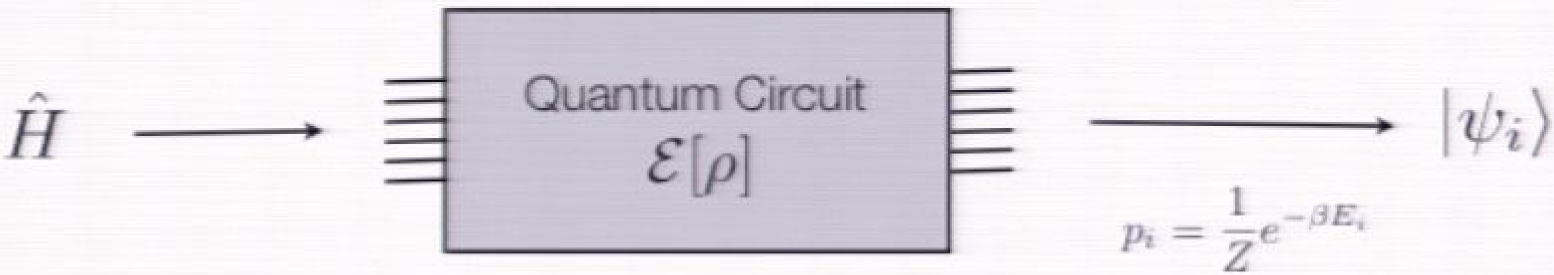
Farhi, Goldstone, Gutmann and Sipser '00:
Adiabatic quantum computation

2) Prepare the Gibbs state:

Terhal and DiVincenzo'00:
Joint evolution "system + bath"

Quantum Metropolis Sampling

- Sample from the eigenstates of some Quantum Hamiltonian



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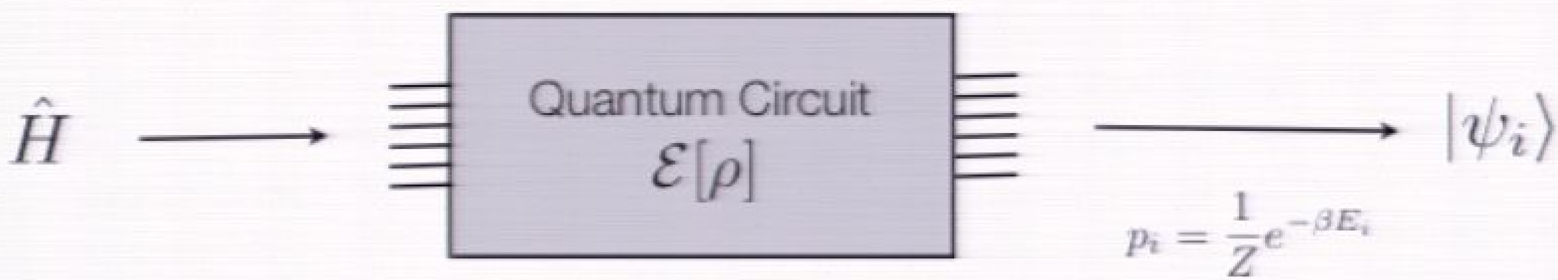

- Empirical average of M samples

$$\frac{1}{Z} e^{-\beta \hat{H}} \approx \frac{1}{M} \sum_{k=1}^{M} |\psi_{i_k}\rangle\langle\psi_{i_k}|$$

with error $\sim \frac{1}{\sqrt{M}}$

The Metropolis Algorithm

- Compute averages:

$$\langle x \rangle = \frac{\sum_i x_i e^{-\beta E_i}}{\sum_i e^{-\beta E_i}}$$

for example, Ising: $$H_i = \sum_{ij} J_{ij} s_i s_j + \sum_i K_i s_i \qquad \uparrow\downarrow\downarrow\uparrow\downarrow \ldots$$

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$$S^n p_0 \xrightarrow[n \to \infty]{} p_G = \frac{1}{Z} e^{-\beta H}$$

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$$S^n p_0 \xrightarrow[n \to \infty]{} p_G = \frac{1}{Z} e^{-\beta H}$$

- Detailed balance ensures the desired F.P.

$$p_i \, S_{i \to j} = p_j \, S_{j \to i}$$

The basic steps of the Metropolis Algorithm

- Basic steps in the algorithm

step 1) move from one state to the other

$$\uparrow\downarrow\downarrow\uparrow\downarrow\ldots \xrightarrow{C_{ij}} \uparrow\downarrow\downarrow\uparrow\uparrow\ldots$$

$$E_i = H(\uparrow\downarrow\downarrow\uparrow\downarrow\ldots)$$

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$$E_i = H(\uparrow\downarrow\downarrow\uparrow\downarrow\ldots)$$

step 2) accept / reject new state

$$w = \min\left(1, e^{-\beta(E_j - E_i)}\right)$$

accept new state with prob w

reject new state with prob $1 - w$ and keep old state

The Basic Problems for a quantized version!

- How do we prepare the eigenstates?

- How do we construct “local” moves between two eigenstates?

- How do we implement the accept/reject step?

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Keep the new sample or go back to the old state with a specific probability!

This is the most subtle step, because one has to perform a measurement!

The Naive Approach! (which does not work !)

- Just repeat the classical Metropolis steps!

step 1) $$|\psi_i\rangle \xrightarrow[C]{} \sum_k c_{ki}|\psi_k\rangle \xrightarrow[\Phi]{|c_{ij}|^2} |\psi_j\rangle$$

step 2) accept / reject

accept ✓ $$f_{ij} = \min\left(1, e^{-\beta(E_j - E_i)}\right)$$ reject ✗

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- Reject step fails! After the energy measurement we can not go back!

We can not undo the measurement!

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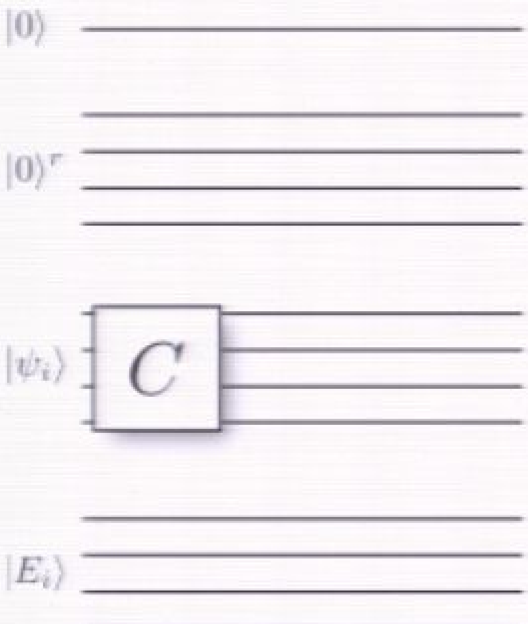
We asked for to much Information! In the end we just want to answer a binary question:

accept or reject?

Tracking the Metropolis steps



choose a random unitary : C

we need to require :

$$d\mu(C) = d\mu(C^\dagger)$$

$$|\psi_i\rangle \rightarrow \quad C|\psi_i\rangle = \sum_k c_i^k \; |\psi_k E_i \; 0^r \; 0\rangle$$

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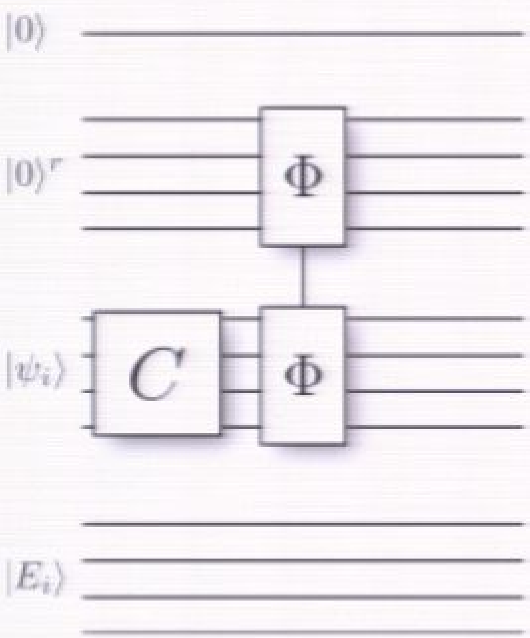

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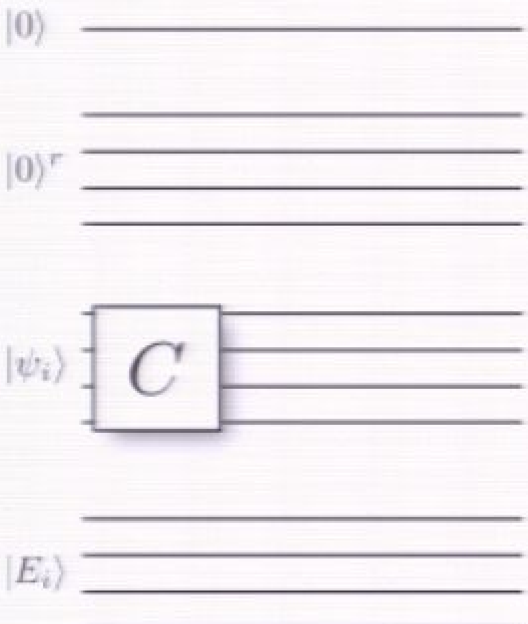

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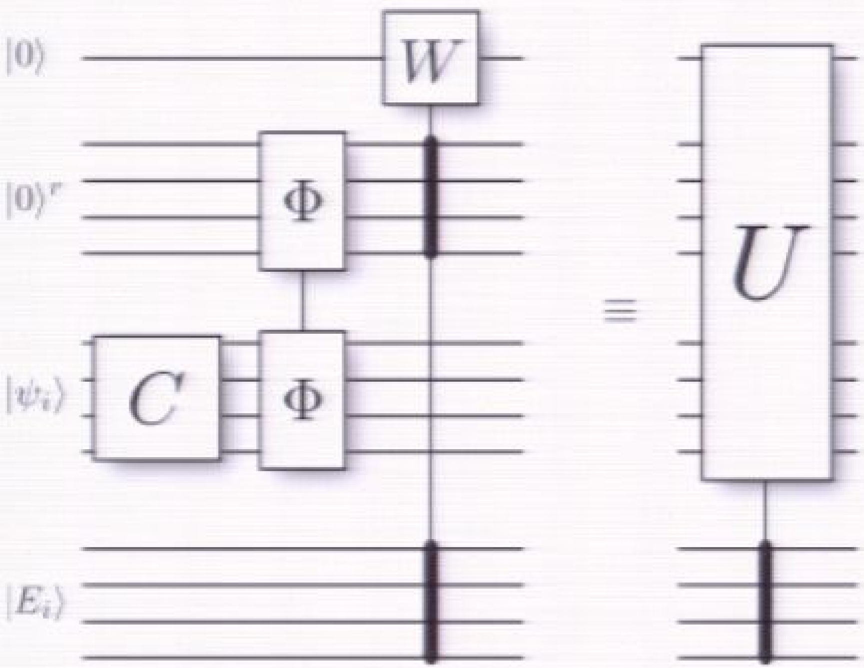

$$W(E_k, E_i) = \begin{pmatrix} \sqrt{1-f_{ik}} & \sqrt{f_{ik}} \\ \sqrt{f_{ik}} & -\sqrt{1-f_{ik}} \end{pmatrix}$$

$$f_{ik} = \min\left(1, \exp\left(-\beta\left(E_k - E_i\right)\right)\right)$$

$$|\psi_i\rangle \to U|\psi_i\rangle = \underbrace{\sum_k c_k^i \sqrt{f_k^i}|E_i\ \psi_k\ E_k\rangle\,|1\rangle}_{|\psi_i^A\rangle} + \underbrace{\sum_k c_k^i \sqrt{1-f_k^i}|E_i\ \psi_k\ E_k\rangle\,|0\rangle}_{|\psi_i^R\rangle}$$

accept   reject

accept / reject

- only measure the last qubit!

1) accept: $|1\rangle$ prepare $|\psi^A\rangle$ then measure both P.E. registers

with $|c_{ik}|^2 f_{ik} \quad \rightarrow \quad |\psi_k\rangle$

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Idea: non-deterministic rejection!

Just ask the binary question:
are we back to the original state or not?

Marriott & Watrous '05 (QMA Games)

- Work in an effective 2D subspace:

define: $Q = U \, \mathbb{I} \otimes |1\rangle\langle 1| \, U^\dagger$

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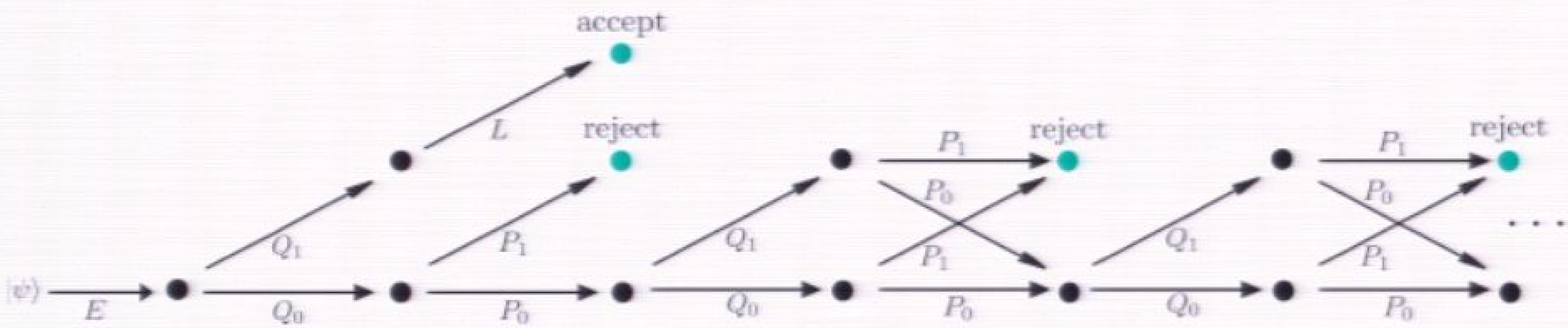
- Perform alternating measurements: $QPQPQ\ldots$



How long does the rejection take?

- A Lemma for two projectors (Jordan 1875)

$$P_1 = \begin{pmatrix} \mathbb{I} & 0 \\ 0 & 0 \end{pmatrix} \qquad Q_1 = \begin{pmatrix} D & \sqrt{D(\mathbb{I}-D)} \\ \sqrt{D(\mathbb{I}-D)} & \mathbb{I}-D \end{pmatrix}$$

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- effective 2D subspace:

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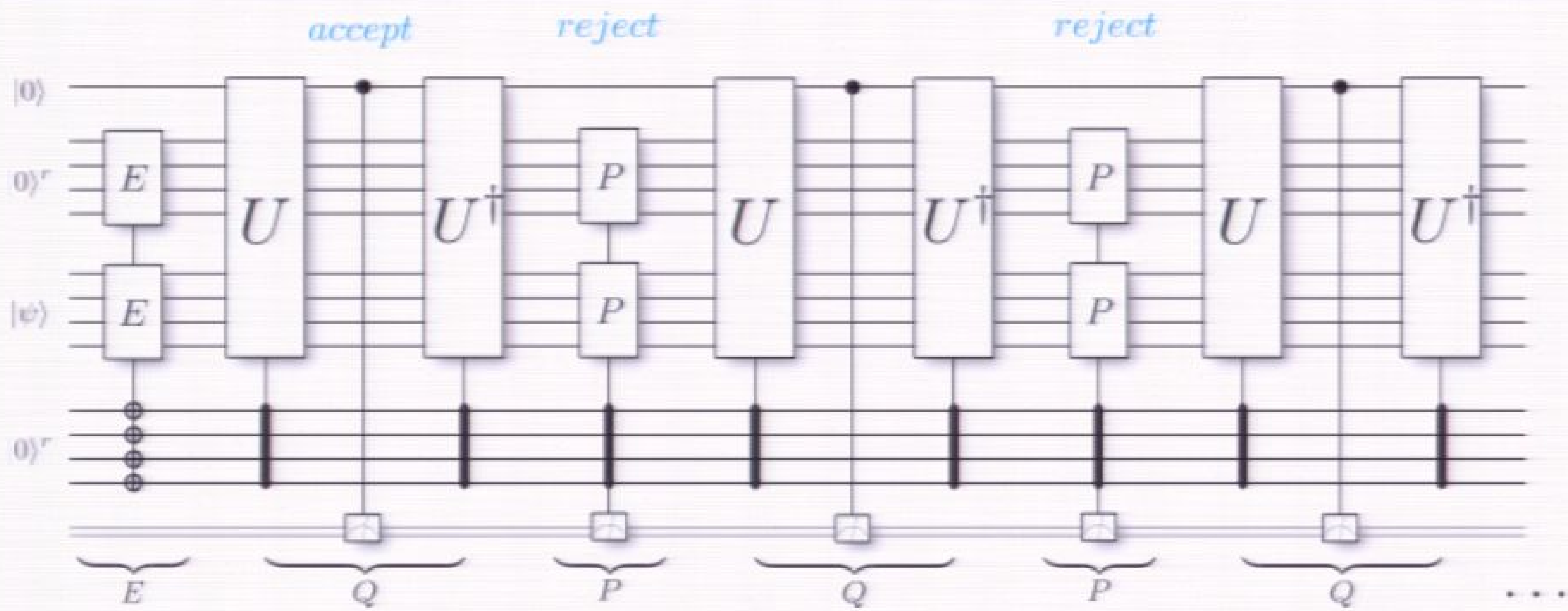
- Bound on the failure probability after m steps.

$$p^{\text{fail}}(m) \leq d^*(1-d^*)(d^{*2} + (1-d^*)^2)^m$$

The full circuit



corresponds to a single application of the cp-map $\mathcal{E}[\rho]$
on the physical level

$$\mathcal{E}[\rho] = A[\rho] + \sum_{k=0}^{\infty} B_k[\rho]$$

Can we ensure the Algorithm does what we want?

- Does the Markov chain converge to the Gibbs state?

  is $\rho = \frac{1}{Z}\exp(-\beta H)$ the FP of the chain?

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$$\left\| \mathcal{E}^n[\rho_0] - \frac{1}{Z} e^{-\beta H} \right\|_{tr} \leq \epsilon \qquad n(\epsilon) \leq \text{poly(system size)}$$

Will depend on the problem and on the updates C

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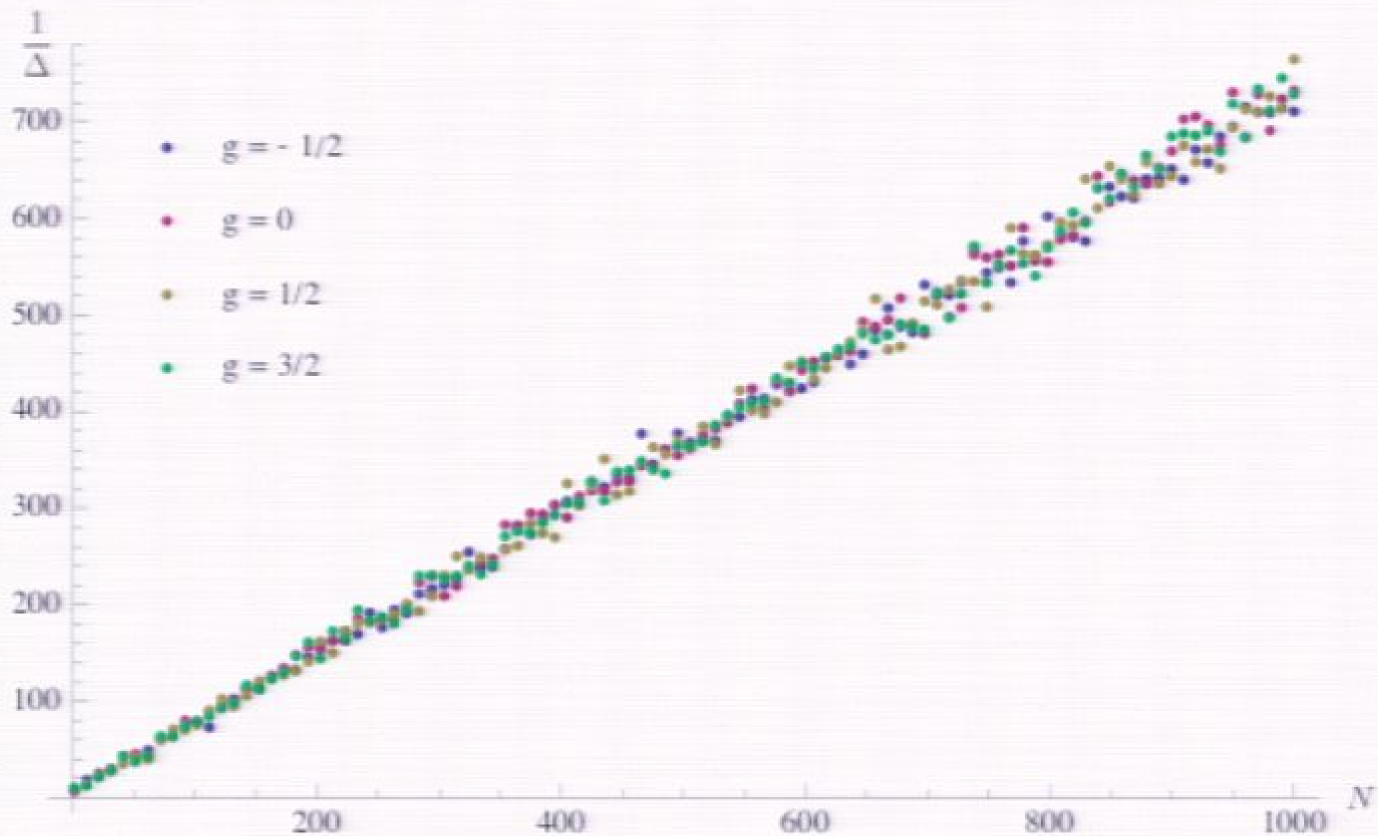
- Imperfections of the Implementation?

  Imperfections due to the simulation (trotter error)

  Imperfections due to the phase estimation algorithm

Rapid Mixing: A simple example system

- inverse Gap of CP-map at T = 0



$$C = X_1$$

$$\hat{H} = \sum X_k X_{k+1} + Y_k Y_{k+1} + g Z_k$$

Small interlude: the quantum χ^2- distance

- classical χ^2- distance

$$\chi^2(p,q) = \sum_i \frac{(p_i - q_i)^2}{q_i}$$

serves as upper bound

$$\|p-q\|_1^2 \leq \chi^2(p,q)$$

gives access to bounding the mixing time (Fill, Diaconis, Strook '91)

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with the inversion $\Omega_\sigma^k[\rho]$ a non-commutative : $\dfrac{``\rho"}{\sigma}$

Quantum detailed balance

- Inversion serves to define quantum detailed balance:

$$\mathcal{E}^* \circ \Omega_\sigma^k = \Omega_\sigma^k \circ \mathcal{E}$$

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Example: $\Omega_\sigma^{1/2}[\rho] = \frac{1}{\sqrt{\sigma}}\rho\frac{1}{\sqrt{\sigma}}$

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

then $\sigma = \sum_i p_i|\psi_i\rangle\langle\psi_i|$ is the fixed point of the CP-map

Fixed point and Degeneracies

- Check detailed balance for the CP-map with degeneracies

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- The fixed point is unique if we ensure ergodicity. Choose:

$C \in$ Universal gate set

What about errors?

- Errors due to simulations: (Childs '04 , Berry '07)

simulation time $T_H = cs^2 t_0 N(\log_*(N))^2 9^{\sqrt{\log(s^2 t_0/\epsilon_H)}}$

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- Errors due to phase estimation

Minimize fluctuations due to median method
(Nagaj, Wocjan, Zhang '09)

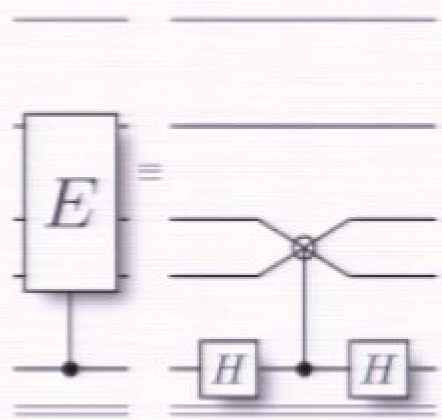
$$\left\| \frac{e^{-\beta H}}{Z} - \sigma \right\|_{tr} \leq \mathcal{O}\left(\frac{1}{1-\eta_{tr}} \frac{m}{2e(1-c)} \frac{4\pi}{t} \beta 2^{-r} \right)$$

An implementation scheme

- Implementation for 2-qubit Heisenberg hamiltonain

$$H = -\frac{1}{2}\vec{S}_1 \circ \vec{S}_2 \qquad t = \frac{\pi}{2}$$

  - Controlled evolution corresponds to Fredkin gate



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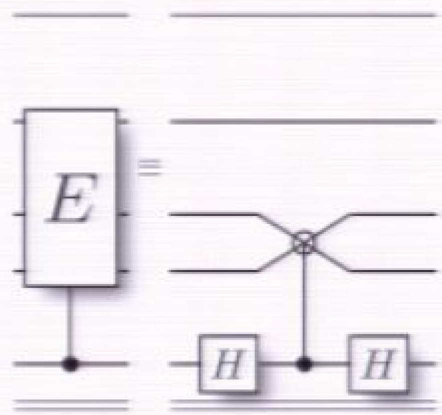

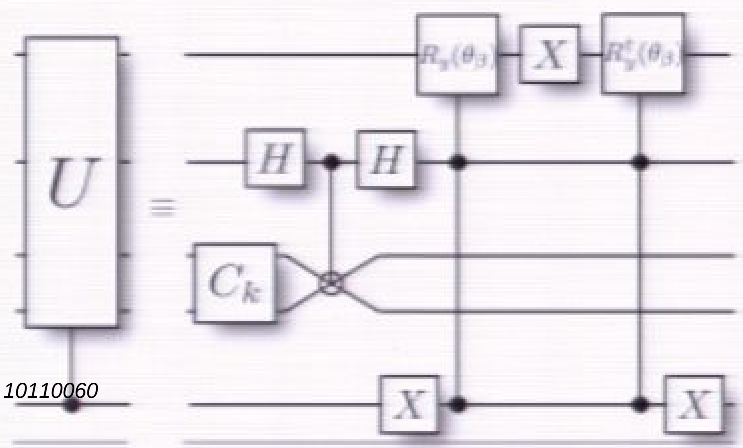

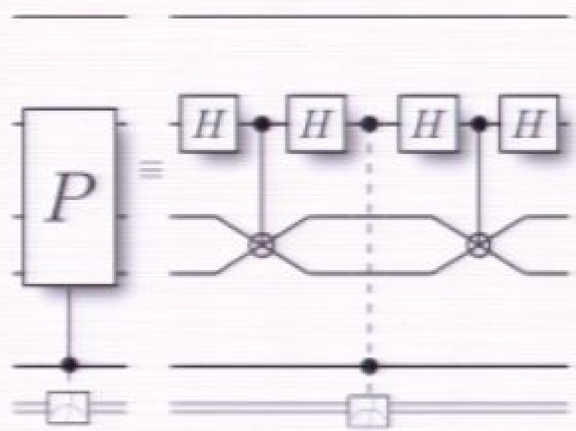

Conclusions

- We took a step in the right direction towards solving the Problem of finding a general purpose algorithm for computing static properties of quantum many body problems!
- Small scale implementations already make sense and should be possible with todays technology
- The problem was again turned into a sampling problem! Universal quantum computation can be seen as the preparation of samples from a time invariant completely positive map! (Verstraete, Wolf and Cirac '09)
- This suggests that one should look for further quantum algorithms in this framework. The classical Metropolis algorithm gave rise to simulated annealing. (Kirkpatrick et al. 1981)

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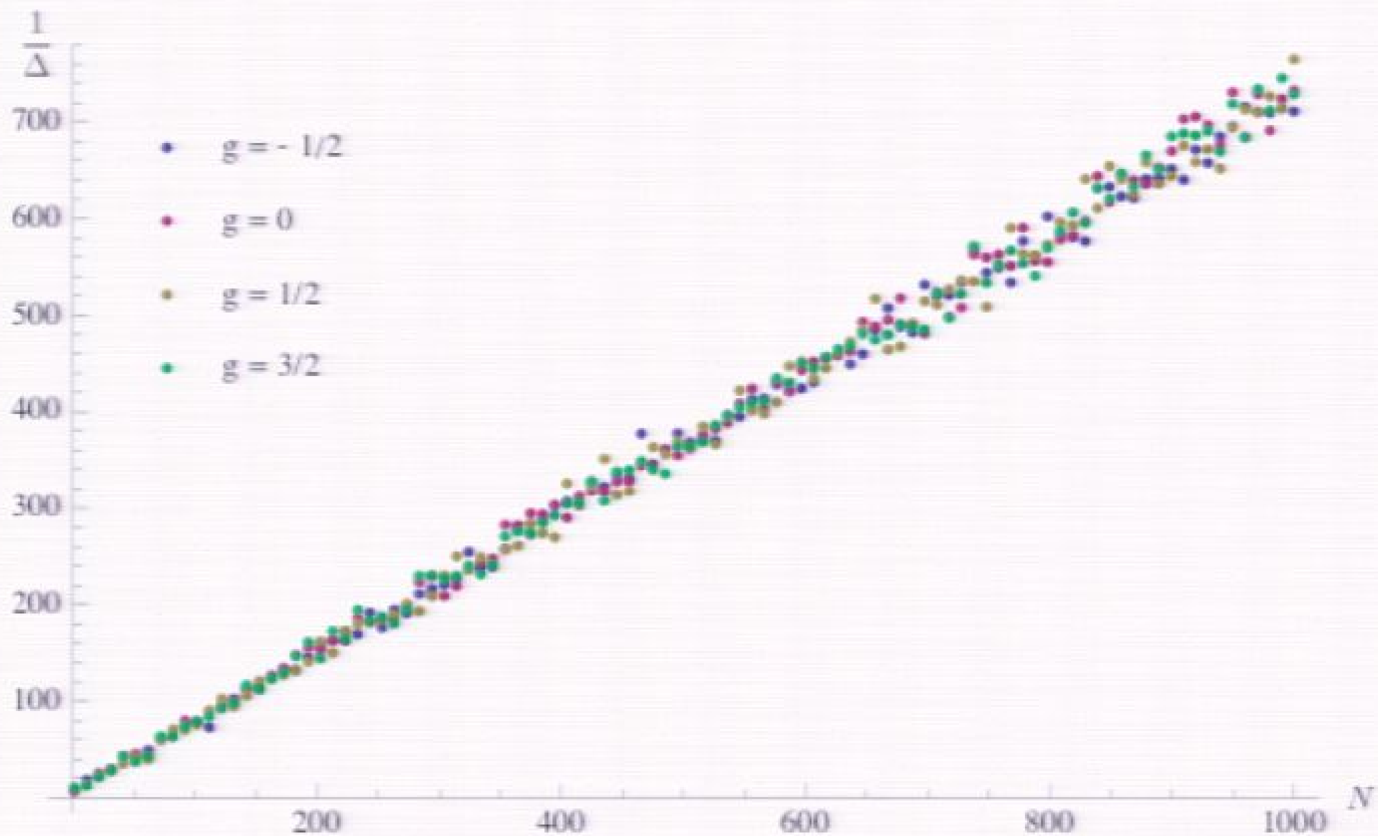

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