Quantum Metropolis Sampling

Kristan Temme, K. Vollbrecht, T. Osborne,
D. Poulin, F. Verstraete
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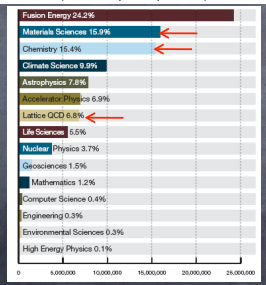
Quantum Simulation

- Principal use of quantum computers: quantum simulation

Use of DoE supercomputers by area
(from a talk by Alán Aspuru-Guzik)



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

Quantum Chemistry

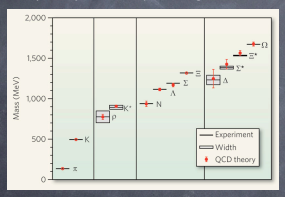
- Determination of the binding energy of molecules
  - electronic structure calculations (determination of electronic ground state energy for a given location of the nuclei)

$$\mathcal{H} = \sum_{ijkl} f_{ijkl} \hat{a}_i^\dagger \hat{a}_j^\dagger \hat{a}_k \hat{a}_l$$

- Simulation of molecular dynamics:
  - Born-Oppenheimer / Car-Parrinello
  - grand challenge: describe protein surrounded by water molecules over the period of 1 sec.

Quantum Chromodynamics

- Determination of masses of hadrons (e.g. proton) from first principles (i.e. quarks, gluons in QCD); in practice: lattice QCD



Finally, let me add a note of critical perspective. The accurate, controlled calculation of hadron masses is a notable milestone. But the fact that it has taken decades to reach this milestone, and that even today it marks the frontier of ingenuity and computer power, emphasizes the limitations of existing methodology and challenges us to develop more powerful techniques. QCD is far from being the only area in which the challenge of solving known quantum equations accurately is crucial. Large parts of chemistry and materials science pose similar mathematical challenges. There have been some remarkable recent developments in the simulation of quantum many-body systems, using essentially new techniques[9]. Can the new methods be brought to bear on QCD? In any case, it seems likely that future progress on these various fronts will benefit from cross-fertilization. The consequences could be enormous. To quote Richard Feynman[6]: "Today we cannot see whether Schrödinger's equation contains frogs, musical composers, or morality — or whether it does not. We cannot say whether something beyond it like God is needed, or not. And so we can all hold strong opinions either way."

Durr et al., Science '08; Wilczek, Nature '08

Condensed Matter Physics

- Material Science: determine band structure, spectral function, etc; note that this only makes sense in systems for which there is a description possible in terms of an effective free theory
- Quantum Impurity problems: extract spectral information
- Bottleneck: Simulation of effective Hamiltonians like the Hubbard model (cfr. present experiments with cold atoms or concept of topological quantum order)

$$\mathcal{H} = t \sum_{ij} a^\dagger_{i\uparrow} a_{j\uparrow} + a^\dagger_{i\downarrow} a_{j\downarrow} + U \sum_i n_{i\uparrow} n_{i\downarrow}$$

  - determine phase diagram as a function of the temperature, filling factor and t/U

Quantum Simulation:

- In principle, we just have to simulate the many-body Schrodinger equation

$$\{-\frac{\hbar^2}{2m}\sum_j \nabla_j^2 - \sum_{j,\ell}\frac{Ze^2}{|r_j - R_\ell|} + \frac{1}{2}\sum_{j\neq j'}\frac{e^2}{|r_j - r'_j|} - E\}\Psi = 0$$

  - Dirac: "The underlying physical laws necessary for the mathematical theory of a large part of physics and the whole of chemistry are thus completely known, and the difficulty is only that the exact application of these laws leads to equations much too complicated to be soluble. It therefore becomes desirable that approximate practical methods of applying quantum mechanics should be developed, which can lead to an explanation of the main features of complex atomic systems without too much computation."
- In practice: work with effective or discretized Hamiltonians (e.g. Hubbard model, lattice QCD, Gaussian or plane wave basis sets, ...)
  - PS: does anybody know how to derive the many-body Schrodinger equation as the nonrelativistic limit of a quantum field theory; what about many-body versions of the Dirac equation?
- Fundamental problem: "exponential wall"

3 paths to enlightenment

- Classical Simulation of quantum systems
- Building a Quantum Simulator (cfr. Cirac, Lukin, Zoller et al.)
- Simulating quantum systems on a quantum computer

Classical Simulation of Quantum Many-Body Systems

- Weakly interacting systems: Hartree-Fock, Density Functional Theory, perturbation theory, coupled cluster, ...
- Strongly interacting systems: renormalization group, variational methods, ...
  - NRG, DMRG, Matrix Product States, MERA, ...
  - Laughlin states, Resonating Valence Bond States, ...
  - Quantum Monte Carlo: for static properties of non-frustrated bosonic systems!
  - Full CI, ... (exponential scaling)
- In all those methods: fundamental limitations for extracting spectral information (e.g. too much entanglement in case of variational wavefunctions, phases in case of Monte Carlo, limited to ground state energies, ...)

- Feynman '82:
  - "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"

- Lloyd '96:

  Any unitary evolution generated by a local quantum Hamiltonian can be simulated efficiently by a quantum circuit

$$\mathcal{T}\exp\left(i\int_0^{\delta t} dt \sum_\alpha H_\alpha(t)\right) \simeq \prod_\alpha \mathcal{T}\exp\left(i\int_0^{\delta t} dt H_\alpha(t)\right) + O(\delta t^2)$$

  - Can be used to prepare ground states under some restricted conditions (gap): adiabatic time evolution (Farhi et al.)

How to simulate ground and/or thermal states of generic Hamiltonians?

- Actually, this is already a difficult problem for classical systems: classically, the configuration space also explodes exponentially as a function of the particles/spins/...
- It was only with the advent of "fast computing machines" that a generic solution was found by Metropolis, Rosenbluth and Teller in 1952:
  - "We devised a general method to calculate the properties of any substance comprising individual molecules with classical statistics."

The Metropolis algorithm

- Let's for simplicity consider a classical Ising spin system with Hamiltonian

$$\mathcal{H} = \sum_{ij} J_{ij} s_i s_j + \sum_i K_i s_i$$

- Instead of simulating the action of a heat bath (which would require much more resources and would be very slow), Metropolis et al. set up a stochastic map that flips spins from one configuration i to another one j in a controlled random way:

$$|\uparrow\uparrow\downarrow\uparrow\downarrow \ldots\rangle \to |\uparrow\downarrow\downarrow\uparrow\downarrow \ldots\rangle$$

$$p_{i\to j} = \min\left(1, \exp\left(-\beta(E_j - E_i)\right)\right)$$

  - The stationary state of this stochastic map is the Gibbs state with

$$p_i = \frac{\exp(-\beta E_i)}{Z}$$

Detailed Balance

$$\text{if } S_{i\to j} p_i = S_{j\to i} p_j \text{ then } \textstyle\sum_i S_{i\to j} p_i = \sum_i S_{j\to i} p_j = p_j$$

- Alternative to Metropolis: If one does a careful analysis of the case of system adiabatically coupled to a system of thermal harmonic oscillators, one gets a different stochastic map that also obeys detailed balance:

$$p_{i\to j} \simeq \left| \frac{(E_i - E_j)^\alpha}{1 - \exp\left(-\beta(E_i - E_j)\right)} \right|$$

- Convergence rate: relaxation time is inversely proportional to the spectral gap of the stochastic matrix
  - Magic of Metropolis / Monte Carlo: gap scales typically as an inverse polynomial in the system size, i.e. the method is efficient!

Quantum Metropolis

- Challenge: how to set up a similar algorithm for a quantum computer?
  - would allow to sample from the Gibbs state from an arbitrary Hamiltonian (spins, bosons, fermions)
  - Replace stochastic map with completely positive map
    - how to guarantee that Gibbs state is the fixed point of this CP-map?
- Problem has been around since the early days of quantum computing: most elementary algorithm for quantum simulation

B. Terhal and D. DiVincenzo, '00

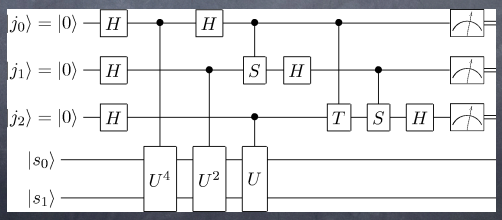
- **Basic task:**

Sample from the eigenstates $|\psi_\alpha\rangle$
of a Hamiltonian $H = \sum_\alpha E_\alpha |\psi_\alpha\rangle\langle\psi_\alpha|$
with probability $p(E_\alpha) \simeq \exp(-\beta E_\alpha)$

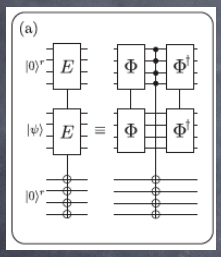
- Three basic problems that have to be solved to construct the quantum analogue of Metropolis:
  - 1. How to prepare eigenstates of a Hamiltonian?
  - 2. How to construct "local moves" that map eigenstates to eigenstates and guarantee mixing (i.e. ergodicity and detailed balance)
  - 3. How to reject a move (no-cloning!)

Preparing eigenstates

- Easy: just measure the energy!
- The ubiquitous quantum phase estimation algorithm does precisely that as a non-demolition measurement (von Neumann measurement)
  - append ancilla's that will encode the energy in binary format; efficient for sparse (e.g. local) Hamiltonians. Note that the cost is exponential in the number of digits of precision needed, so only poly precision can be obtained!



$$\sum_i x_i|\psi_i\rangle|0\rangle \rightarrow \sum_i x_i|\psi_i\rangle|E_i\rangle$$



$$\sum_i x_i|\psi_i\rangle|0\rangle|0\rangle \rightarrow \sum_i x_i|\psi_i\rangle|E_i\rangle|0\rangle$$

Local moves

- For generic systems, we clearly do not know how to construct unitaries that map one eigenstate to another one (unlike classical case!)
- We therefore implement a random local unitary, and work in superposition:

$$|\psi_i\rangle \rightarrow \hat{C}|\psi_i\rangle = \sum_k x_k^i |\psi_k\rangle$$

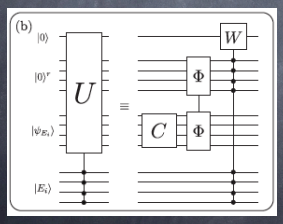
  - If this unitary is chosen from a family that forms a universal gate set for quantum computation, then the ergodicity problem is settled
  - As we will see, the notion of quantum detailed balance requires C to be Hermitean

Metropolis step

$$\sum_k x_k^i |\psi_k\rangle|E_i\rangle \rightarrow \underbrace{\sum_k x_k^i \sqrt{f_k^i}|\psi_k\rangle|E_i\rangle|E_k\rangle}_{|\psi_i^+\rangle}|1\rangle + \underbrace{\sum_k x_k^i \sqrt{1-f_k^i}|\psi_k\rangle|E_i\rangle|E_k\rangle}_{|\psi_i^-\rangle}|0\rangle$$

$$f_k^i = \min\left(1, \exp\left(-\beta(E_k - E_i)\right)\right)$$

Such a transformation can be implemented by the following quantum circuit:



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

The State |1> corresponds to accepting the move, |0> to a rejection of the move

$$\sum_k x_k^i |\psi_k\rangle |E_i\rangle \quad \rightarrow \quad \underbrace{\sum_k x_k^i \sqrt{f_k^i} |\psi_k\rangle |E_i\rangle |E_k\rangle}_{|\psi_i^+\rangle} |1\rangle + \underbrace{\sum_k x_k^i \sqrt{1-f_k^i} |\psi_k\rangle |E_i\rangle |E_k\rangle}_{|\psi_i^-\rangle} |0\rangle$$

$$f_k^i \quad = \quad \min\left(1, \exp\left(-\beta(E_k - E_i)\right)\right)$$

- We proceed by measuring this 1-qubit register in the computational basis; note that this only reveals 1 bit of information (accept or reject)
  - in case of a an accept move |1>: we trace out all ancilla's and start all over (i.e. we succeeded doing one Metropolis step)
  - in case of a reject move |0>: we have to undo what we did!
    - How to undo a quantum measurement? Seems to be in violation with no-cloning...
    - can be done in a recursive way (similar trick was used by Watrous in his work on zero-knowledge proofs)

Undoing a 1-bit measurement

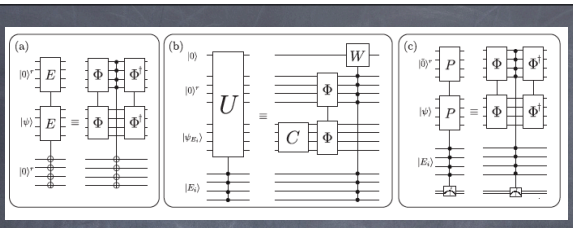
- Basic theorem in linear algebra: given two projectors P and Q, then there is a basis in which they have the following form:

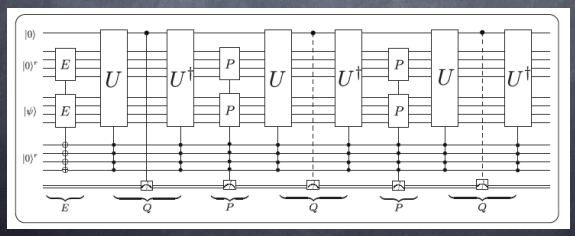
$$P_1 = \begin{pmatrix} \mathbb{I}_p & 0_{n-p,p} \\ 0_{p,n-p} & 0_{n-p,n-p} \end{pmatrix}$$

$$Q_1 = \begin{pmatrix} D_p & \sqrt{D_p(\mathbb{I}_p - D_p)} & 0 & 0 \\ \sqrt{D_p(\mathbb{I}_p - D_p)} & \mathbb{I}_p - D_p & 0 & 0 \\ 0 & 0 & \mathbb{I}_{q-p} & 0 \\ 0 & 0 & 0 & 0_{n-(q+p),n-(q+p)} \end{pmatrix}$$

- How does this help us?
  - Define P to be the projector given by the Metropolis step
  - Define Q to be the projector on the energy subspace corresponding to the original state
  - A recursive application of P,Q,P,Q,... leads to a probability increasing exponentially fast to 1 of ending up in the same subspace as the original one, hence allowing to implement a reject move !

$$D_{fail}(n) = \begin{pmatrix} D(\mathbb{I}-D)(D^2+(\mathbb{I}-D)^2)^n & -\sqrt{D(\mathbb{I}-D)}(D^2+(\mathbb{I}-D)^2)^n & 0 & 0 \\ -\sqrt{D(\mathbb{I}-D)}(D^2+(\mathbb{I}-D)^2)^n & D^2(D^2+(\mathbb{I}-D)^2)^n & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$





Technical details

- In quantum system, we typically have exponential degeneracy and hence this procedure will not undo the measurement but just prepare another state with the same energy
  - this is actually fine: this means that the reject moves are not useless but also lead to mixing!
- Why is the fixed point of this completely positive map the Gibbs state?
  - quantum version of detailed balance:

Lemma: Detailed balance criterium Let $\{|\psi_i\rangle\}$ be a complete basis of the physical Hilbert space and let $\{p_i\}$ be a probability distribution on this basis. Furthermore, assume that a completely positive map $\mathcal{E}(\rho) = \sum_\mu A_\mu \rho A_\mu^\dagger$ obeys

$$\sqrt{p_n p_m}\langle\psi_i|\mathcal{E}(|\psi_n\rangle\langle\psi_m|)|\psi_j\rangle = \sqrt{p_i p_j}\langle\psi_m|\mathcal{E}(|\psi_j\rangle\langle\psi_i|)|\psi_n\rangle, \tag{56}$$

then $\sigma = \sum_i p_i |\psi_i\rangle\langle\psi_i|$ and $\mathcal{E}$ obey the detailed balance condition. Therefore σ is the fixed point of $\mathcal{E}$.

- Quantum Phase estimation algorithm does not work with infinite precision, and hence QPE corresponds to POVM and not to Projective measurement. How to deal with this?

Conclusion

- Quantum Simulation is and will be the central task in quantum information processing
- Quantum Metropolis algorithm is an efficient way of simulating thermal/ground states of many-body quantum systems
  - "We develop a general method, suitable for quantum computing machines, to calculate the properties of any substance comprising interacting quantum molecules"
  - might lead to novel dissipation-based quantum algorithms: dissipation based quantum algorithms (cfr. FV, M. Wolf, I. Cirac, Nat. Phys. '09); graph isomorphism???
  - Proving efficiency is extremely hard, even for classical Metropolis
- Quantum mechanics is subtle and allows to overcome seemingly impossible tasks (i.e. undoing a quantum measurement, as long as it gave not too much information)
- Small scale implementations on a few qubits already make sense