Quantum Computation for Quantum Chemistry and Statistical Mechanics

Quantum Computation for Chemistry Applications

Alán Aspuru-Guzik

^a Department of Chemistry and Chemical Biology, Harvard University

> Towler Insitute Vallico Soto, Italy



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Q. Computation for Chemistry

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- What is quantum computation? Classical vs quantum computing.
- Quantum algorithms for finding protein low energy conformations
- Quantum algorithm for molecular energies

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Quantum Simulation vs. Quantum Emulation



quantum simulation (HF, DFT, QMC, CC, FCI,...)

quantum emulation

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Quantum Simulation vs. Quantum Emulation

Why use quantum computers?

Quantum Simulation

- Represent the system using a classical computer
- Exact algorithm (FCI) scales exponentially with the basis set size
- Approximate algorithms (HF, DFT, QMC, CI, CC) scale polynomially

Quantum Emulation

- Map the wave function and Hamiltonian onto another quantum system (quantum computer)
- Exploit the quantum nature of the emulator to achieve polynomial-scaling *exact* algorithms

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Classical Computer





Quantum Computer

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Stages of quantum computation



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Classical bits

- Always has a value of 0 or 1
- A bit can be copied
- Doesn't change if read
- Reading a bit doesn't affect other unread bits.

Quantum bits (qubits)

- All items on the left can fail.
- Superposition states $(a_0|0\rangle + a_1|1\rangle)$

where
$$\sum_i a_i^2 = 1$$

N-qubit state

 $a_1|0...01\rangle + a_2|0...10\rangle \ a_3|0...11\rangle + ...+ a_n|1...11\rangle$

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N-qubit state

$$\begin{array}{lll} a_1|0\dots01\rangle & + & a_2|0\dots10\rangle \\ a_3|0\dots11\rangle & +\dots+ & a_n|1\dots11\rangle \end{array}$$

Measuring qubits

Bloch sphere representation



Properties

• Project system onto $|0\rangle$ or $|1\rangle$: Pr(0) = $|a_0|^2$, Pr(1) = $|a_1|^2$

A (1) > A (2) > A

 Probabilistic result: may require multiple measurements.

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Classical gates

Example circuit: adder



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Quantum gates



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Quantum circuits

Example circuit: quantum Fourier transform



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Quantum Emulation



Feynman's Proposal

$$egin{array}{rcl} |\Psi^{mol}
angle &
ightarrow &|\Psi^{QC}
angle \ \hat{U}^{mol}(t)=m{e}^{-i\hat{H}^{mol}t} &
ightarrow &\hat{U}^{QC}(t)=m{e}^{-i\hat{H}^{QC}t} \end{array}$$

Jordan-Wigner Transformation

Mapping of fermionic systems to spin systems and vice versa R. Somma *et al*, *Phys. Rev. A* **65** 042323 (2002)

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Quantum Emulation III

SOMMA, ORTIZ, GUBERNATIS, KNILL, AND LAFLAMME

Jordan-Wigner transformations

3. 6 **HC Bosons** Spin 1/2 Helium 4 ? Models Physical of Computation Systems (Operator Algebra) Spin 3/2 Electrons ? Fermions S=3 2 atoms -->>

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Josephson-Junction superconducting qubits Quantronics group, Saclay France



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D-Wave Systems's device



Oxidized Silicon wafer using a Niobium trilayer process The Economist, February 15th, 2007 (Others: Nature, Wired, etc.)

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D-Wave Qubit Coupler



$$\mathcal{H} = \sum_{q=a,c} (\epsilon^q \sigma_z^{(q)} + \Delta^q \sigma_x^{(q)}) + J(f_x^b) \sigma_z^{(a)} \sigma_z^{(c)}$$

arXiv:cond-mat/0608253

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The physics

The Hamiltonian

Two-dimensional Ising model in a magnetic field (2DIMM):

$$E(\sigma_1,\ldots,\sigma_N)=\sum_{j=1}^N h_j\sigma_z^j+\sum_{i< j}^N J_{ij}\sigma_z^i\sigma_z^j+\sum_{j=1}^N a_j\sigma_x^j$$

where
$$\sigma_z^i = +1, -1$$

Procedure

- Initialize in a highly quantum state (a_i large)
- Turn on couplings
- As you turn off a_i slowly
- Read-out the answer

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Adiabatic quantum computing

Adiabatic evolution

$$irac{d}{dt}|\Psi(t)
angle = H(t)|\Psi(t)
angle$$

 $H(t) = (1 - rac{t}{T})H(0) + rac{t}{T}H_{problem}$

Hilbert space

 $|z_1\rangle\otimes|z_2\rangle\otimes\cdots\otimes|z_n\rangle$

The ground state of a given spin for the field in **x** is:

$$\frac{1}{\sqrt(2)}(|0\rangle_1+|1\rangle_1)$$

$$|\Psi(0)
angle = rac{1}{2^{n/2}} |z_1 z_2 z_3 z_4
angle >$$

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Adiabatic evolution pictorially



Transverse field on Z-field off

Transverse field off Z-field on

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What can it do?

Maximum independent set



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Maximum Independent Set What is it?



MIS of a graph

A MIS is the largest subset of vertices of a graph for which there is no edge connecting the two.

Computational complexity class

This problem is **NP-Hard** (Nondeterministic Polynomial-time hard)

wikipedia.org/ Independent_set

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Exact Cover

- The problem Hamiltonian H_p is a the sum of a series of constraints, $H_p = \sum_j h_c$.
- Each constraint involves **three** bits: One must have the value 1, and the other two must have 0 value.



Farhi et al. Science 292 (2001) 472 and arxiv.org/000770

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Is there an advantage?

What could a device like this really do?

Careful!

- A quantum device like this one might do better than a classical one in certain random instances of the problem. It might not necessarily do better in other instances.
- Farhi has evidence of quadratic scaling up to 20 qubits for the SAT problem.
- We need to gather evidence for larger systems!

Simulation of classical systems

Somma et al. arxiv:quant-ph/0609216



- Adiabatic QC is very similar to Quantum Annealing (QA) (T=0). Introduce an external transverse magnetic field (e.g. in x) that is lowered with simulation time.
- Simulated Annealing (SA).
- Introduce a simulation temperature T that is lowered with simulation time.

Kirkpatrick *et al.* Science 22 (1983) 671, wikipedia.org/Quantum_annealing

Lattice Protein Models

Mapping to 2D Ising Model in a Magnetic Field



Protein Lattice Model Image: Prof. Backofen, Uni. Freiburg **Classical Ising Model**

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The hydrophobic-polar (HP) model Mapping to 2D Ising Model in a Magnetic Field



Side Credit. Ren Dill

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HP model Hamiltonian (structural constraints)



Onsite repulsion



Hydrophobic interaction



- 2(N-2) log₂ N
 N-local variables are needed!
- But our Ising model is 2-local:
- We need to convert N-local hamiltonian to 2-local

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2-local hamiltonian scaling

Hamiltonian reduction recipe

Replace terms of the form $\sigma_1 \sigma_2 \sigma_3$ with new **ancilla variables** τ_i , α_i :

 $\sigma_1 \sigma_2 \sigma_3 \rightarrow \tau_1 \sigma_3$

Additional complexity

This procedure adds extra terms to the Hamiltonian, such as:

$$\sigma_1 \sigma_2 - (\sigma_1 + \sigma_2) \tau_1 - 2 \alpha_1 (\sigma_1 + \sigma_2 - \tau_1 + 1) + \sigma_1 + \sigma_2 - \tau_1$$

Scaling: $2(N-2)\log_2 N \to 2(N-2)(N^2 - \log_2 N - 1)$

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2-local Hamiltonian scaling plot



About 50,000 "cheap" qubits would be needed to do what a classical computer can do right now.

Carrying out the experiment!

The simplest HP-model case system



Mapping the HP loop

- 2-local network obtained.
- We need a 52-bit device: 8
 - *core* bits and 46

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ancilla bits.

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Partitioning the problem

The simplest HP-model case system



Spin coupling network Locally-optimized domains

Divide and "conquer"

Partitioning schemes (local search) do not guarantee finding the global minimum but have been used with success in numerical (quantum annealing) protocols.

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Low energy conformations on a quantum computer Present and future

Currently

- Numerical simulation of 8192 8-qubit experiments was carried out.
- Colin Truncik at D-Wave is carrying out the experiments on their quantum device.



Near future

- Extend to continuum force fields on a lattice.
- Carry out Experiment for H₂O

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Part II: Quantum Chemistry by Quantum Computation

A. Aspuru-Guzik, A. D. Dutoi, P. J. Love, M. Head-Gordon, *Science* **309** (2005) 3741

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(I) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1)) < ((1))

The quantum chemistry problem



Molecular Hamiltonian

$$\hat{H}^{mol} = \hat{T}_{e} + \hat{T}_{Z} + \hat{V}_{ZZ}(L_{pq}) + \hat{V}_{ee}(r_{ij}) + \hat{V}_{eZ}(R_{pi})$$

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Full Configuration Interaction (FCI)

Wavefunction representation

Expand wavefunction in all HF determinants:

$$|\psi\rangle = \alpha_{0}|\psi^{HF}\rangle + \sum \alpha_{a}^{b}|\psi_{a}^{b}\rangle + \sum \alpha_{ab}^{cd}|\psi_{ab}^{cd}\rangle + \dots$$

Hamiltonian: CI Matrix

Hamiltonian is given by all matrix elements between determinants Solving the matrix eigenvalue problem for this $\binom{2K}{N} \times \binom{2K}{N}$ matrix gives <u>exact</u> results within the given basis.

Basis Functions

Options

o . . .

- Hydrogenic or Atomic (Slater Type Orbitals)
- Plane waves
- Wavelets
- Localized basis (e.g. Gaussians)

Gaussian Basis Sets

- Give compact wavefunction representations
- The exact solution within a good basis set is usually *chemically accurate*.

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Gaussian Basis Sets



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Q. Computation for Chemistry

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• Mapping between $|\Psi^{mol}\rangle$ and $|\Psi^{QC}\rangle$

2 Preparation of $|\Psi_0^{QC}\rangle$

- **Output** Construct $\hat{U}^{QC}(t)$
- Energy Readout (recursive phase estimation algorithm)



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The Phase Estimation Algorithm

R. Cleve *et al*, *Proc. R. Soc. Lond. A* **454** 313 (1998) D. Abrams and S. Lloyd *Phys. Rev. Lett.* **83** 5162 (1999)

Goal

Assume an unitary operator \hat{U} , with eigenvector $|\Psi\rangle$ such that

$$\hat{U}|\Psi
angle=e^{i2\pi\phi}|\Psi
angle,$$

estimate $0 < \phi < 1$.

Conditions

Must be able to prepare a state with large overlap with the eigenstate

• Must be able to gate sequence U^{2^a}

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Phase Estimation: The Fourier State



Choose *t*; $Et = -2\pi\phi$

$$\hat{U}(t)|\Psi
angle=e^{-i\widehat{H}t}|\Psi
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Phase Estimation: The Inverse Fourier Transform



The Quantum Fourier Transform

If $\phi = m/2^b$

$$\frac{1}{\sqrt{2^b}}\sum_n e^{i(2\pi\phi)n}|n\rangle = \frac{1}{\sqrt{2^b}}\sum_n e^{i(2\pi m/2^b)n}|n\rangle = QFT|m\rangle$$

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Phase Estimation: The Inverse Fourier Transform



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$$rac{1}{\sqrt{2^b}}\sum_n e^{i(2\pi\phi)n}|n
angle = rac{1}{\sqrt{2^b}}\sum_n e^{i(2\pi m/2^b)n}|n
angle = QFT|m
angle$$

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Wavefunction Mapping, H₂

Compact Map





Direct Map

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The Non-eigenvector Case

Algorithm Success Probability

- We must prepare the quantum computer in the analog of the molecular ground state.
- We may not be able to construct the ground state exactly.
- Given the trial function $|\Psi_T\rangle$, the algorithm succeeds with probability $|\langle \Psi_0 | \Psi_T \rangle|^2$.

Options

- Use the Hartree-Fock state (for some cases, $|\langle \Psi_0 | \Psi_0^{HF} \rangle|^2 \approx 0.9$)
- Adiabatic state preparation
- Other chemically motivated Ansatzes

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Adiabatic State Preparation

If HF is a bad guess, construct the FCI solution adiabatically.



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A Short Digression: The Adiabatic Theorem

M. Born et al, Zeit. f. Phys. 51 65 (1928) E. Farhi et al, guant-ph/0001106 W. van Dam et al. Proc. 42nd IEEE Symp. (2002)

 $\hat{H}(t) = \hat{H}^{HF} + \frac{t}{\tau} \left(\hat{H}^{FCI} - \hat{H}^{HF} \right)$ $\hat{H}(0)|\Psi(0)\rangle = E_0^{HF}|\Psi(0)\rangle$ $T >> \max_{t} \left(\frac{\left| \langle \Psi_{X}(t) | \hat{H}^{FCI} - \hat{H}^{HF} | \Psi_{0}(t) \rangle \right|}{\left(E_{X}(t) - E_{0}(t) \right)^{2}} \right)$ then $\hat{H}(T)|\Psi(T)\rangle = E_0^{FCI}|\Psi(T)\rangle$

For

if

and

Adiabatic State Preparation for Molecules?

Arguments

- Molecules are insulators
- For a given system, we know a lot of properties of the eigenvalue spectrum from approximate classical methods.
- The gap is larger than the correlation energy
- At each stage in the CI adiabatic state preparation the gap is large
- We <u>conjecture</u> that levels do not cross in between turning on *n*-tuple excitations and *n* + 1 tuple excitations

State Preparation Results

H₂, STO-3G singlet manifold



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Time Evolution

Molecular Hamiltonian

$$\hat{H} = \sum_{X} \hat{h}_{X} = \sum_{p,q} \langle p | \hat{T} + \hat{V}_{N} | q \rangle \hat{a}_{p}^{\dagger} \hat{a}_{q} - \frac{1}{2} \sum_{p,q,r,s} \langle p | \langle q | \hat{V}_{e} | r \rangle | s \rangle \hat{a}_{p}^{\dagger} \hat{a}_{q}^{\dagger} \hat{a}_{r} \hat{a}_{s}$$

Trotter Expansion and Jordan-Wigner Transformation

$$e^{-i\hat{H}t} \approx \left[\prod_{X} e^{-i\hat{h}_{X}t/M}
ight]^{M} \qquad \hat{a}_{p}^{\dagger}\hat{a}_{q} \rightarrow \hat{X}^{p}\hat{X}^{q} \left[\prod_{i=p+1}^{q-1}\hat{\sigma}_{z}^{i}
ight]\hat{P}_{0}^{p}\hat{P}_{1}^{q}$$

• Number of terms in \hat{H} grows as the fourth power of the basis size

- Each term involves a controlled action on at most four qubits at a time
- Absolute bound of less than 400 gates required per term

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Time Evolution

Molecular Hamiltonian

$$\hat{H} = \sum_{X} \hat{h}_{X} = \sum_{p,q} \langle p | \hat{T} + \hat{V}_{N} | q \rangle \hat{a}_{p}^{\dagger} \hat{a}_{q} - \frac{1}{2} \sum_{p,q,r,s} \langle p | \langle q | \hat{V}_{e} | r \rangle | s \rangle \hat{a}_{p}^{\dagger} \hat{a}_{q}^{\dagger} \hat{a}_{r} \hat{a}_{s}$$

Trotter Expansion and Jordan-Wigner Transformation

$$e^{-i\hat{H}t} \approx \left[\prod_{X} e^{-i\hat{h}_{X}t/M}\right]^{M} \qquad \qquad \hat{a}_{p}^{\dagger}\hat{a}_{q} \rightarrow \hat{X}^{p}\hat{X}^{q} \left[\prod_{i=p+1}^{q-1} \hat{\sigma}_{z}^{i}\right] \hat{P}_{0}^{p}\hat{P}_{1}^{q}$$

- Number of terms in \hat{H} grows as the fourth power of the basis size
- Each term involves a controlled action on at most four qubits at a time
- Absolute bound of less than 400 gates required per term

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Q. Computation for Chemistry

Precision Considerations

Qubit Requirements

Need at least *b* bits in readout register for *b* bits of precision

Chemical Accuracy Requirements

For 6 decimal digits of precision at least 20 logical control qubits are needed.

Improvement: Recursive Implementation

- Allows readout register size to be independent of precision
- Fewer consecutive coherent gates

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Phase Estimation: A Recursive Algorithm

Get a lower bound and measure the difference ... repeatedly ... as much as you want.



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Qubit Requirements



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Q. Computation for Chemistry

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Qubit Requirements

Water molecule

water 🛹	Basis set (number of functions)		
Mapping	STO-3G (7)	6-31G* (19)	cc-pVTZ (58)
compact (singlets)	8	25	42
compact	10	29	47
direct	14	38	116

One of the best classical results:

Exact solution of the electronic Schrödinger equation for water, within a double-polarization (TZ) basis set G. Chan *et al, J. Chem. Phys.* **118** *8551 (2003)*

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Recursive Algorithm Results

 H_2O , 196 determinants / LiH, \approx 1200 determinants



Electronic Energy

H₂O, STO-3G -84.29366<mark>3</mark> vs. -84.29366<mark>5</mark>

LiH, 6-31G -9.1228936 vs. -9.1228934

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Can we do an experiment?

Proposed experimental H₂ emulation

Circuit for an actual calculation (1929 vintage)



The gate sequence for simulation of the H_2 molecule in a minimal basis requires 5 quantum bits and under 40 elementary gates. Within reach of NMR quantum computers!

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Thank you!

Group

Sule Atahan Ivan Tubert-Brohman Ali Najmaie Masoud Mohseni

Ivan Kassal Alejandro Perdomo Leslie Vogt **James Whitfield**

Carlos Amador-Bedolla Laura Dominguez

Michael Wan



Collaborators

Colin Truncik (D-Wave) Anthony Dutoi (Northwestern) Martin Head-Gordon (Berkeley) Peter Love (Haveford) Sabre Kais (Purdue) Hefeng Wang (Purdue)

Alán Aspuru-Guzik (Harvard University)

The Basics

Electronic Structure Problem

Neglect T_Z , treat V_{ZZ} classically

$$\hat{H}^{elec} = -rac{1}{2}\sum_{i=1}^{N}ec{
abla}_{i}^{2} - \sum_{i,L}rac{Z_{L}}{r_{iL}} + \sum_{i>j}^{N}rac{1}{r_{ij}}$$

Find the energy as a function of the Nuclear Coordinates

Solve:

$$E|\Psi
angle=\hat{H}^{elec}|\Psi
angle$$

Ab Initio: only inputs are $\{Z_i\}$, *N* Output is *E*

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The Basics



So what?

Nuclei move on the electronic potential energy surfaces surface (PES) Knowledge of PES enables:

- Minima (equilibrum structures)
- Saddle points (Transition states)
- Reaction rates and mechanisms

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 PES characterize most of physical chemistry

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Traditional Mexican ceramics

The tree of life



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The tree of life

Methods for the solution of Schrödinger's equation



Figure by Jim Anderson

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The tree of life



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- Expand wavefunction in a finite basis of functions
- For Hydrogen, we know a complete basis of eigenfunctions
- Truncation of this basis gives an (incomplete) finite basis
- How do we construct a basis for multi-electron wavefunctions?

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- Approximate multi-electron w.f. using Hydrogenic orbitals
- 2 Consider Hartree-Product w.f.: $|\chi_O^1(1)\rangle \otimes |\chi_O^3(2)\rangle \otimes |\chi_O^4(3)\rangle$
- Neglects interactions also ignores indistinguishability
- Use a Slater Determinant: complete antisymmetrization of Hartree Products

$$|\chi_O^1 \chi_O^3 \chi_O^4 \rangle = \frac{1}{\sqrt{3!}} \sum_{P \in S_3} (-1)^{\operatorname{sign}(P)} P \left[|\chi_O^1(1)\rangle \otimes |\chi_O^3(2)\rangle \otimes |\chi_O^4(3)\rangle \right]$$

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Hartree-Fock



Molecular orbitals

First approximation - neglect e-e interactions Hartree- Fock - treat e-e electrons at mean field level

- Given a set of orbitals compute average potential felt by each electron
- Re-solve the non-interacting problem with this effective potential
- Iterate until convergence
- Result is a set of molecular orbitals

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- HF GS: fill first N orbitals and form Slater Determinant
- 2 There are $\binom{2K}{N}$ occupancy states (configurations)
- These are organized into singles, doubles, triples, etc
- The determinants formed from these configurations form an N-electron basis

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Somma's mapping

And how can we use it for quantum simulation?

Definition: Spin configurations: $[z] \equiv |z_1 z_2 z_3 z_4\rangle$

Thermodynamic variables A at T

$$\langle A \rangle_T = rac{1}{\mathcal{Z}(T)} \sum_{[z]} e^{-eta E[z]} A_{[z]}$$

Example: Ising model $E[z] = J_{ij}z^iz^j$

Classical \rightarrow quantum mapping

$$[Z] \rightarrow |[Z]\rangle$$
$$Z^{i} \rightarrow \sigma_{Z}^{i}$$
$$A \rightarrow \hat{A}$$

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Some goodies

Quantum "Thermodynamic" averages

$$\langle \hat{A} \rangle = Tr[\rho \hat{A}] = \frac{\langle \psi(T) | \hat{A} | \psi(T) \rangle}{\langle \psi(T) | \psi(T) \rangle} \equiv \langle A \rangle_T$$

But, does the Hamiltonian [A, H] = 0 that gives the thermodynamic states **exist**?

It exists! See Henley J. of Phys. Cond. Mat 16 (2004) S891

For any classical statistical-mechanics model with a discrete state space, and endowed with a dynamics satisfying detailed balance (...) a quantum Hamiltonian can be constructed (on the same state space) such that the ground state wavefunction coincides with the classical equilibrium distribution. Furthermore the excited eigenstates correspond to classical relaxation modes (...) Quantum and classical correlation functions are related by analytic continuation to the imaginary time axis.

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How to get the magic $C \rightarrow Q$ Hamiltonian?

Classical master equation

$$rac{d p_i}{d au} = \sum_{j
eq i} (W_{ij} p_j(au) - W_{ji} p_i(au))$$

with $W_{ii} = -\sum_{j \neq i} W_{ji}$

Similarity-transformed transition matrix

$$\hat{W}(T) = e^{-\beta H/2} W(T) e^{\beta H/2}$$

• Shares eigenvalues with W(T)

Here it is!

$$H_q(T) = I - \hat{W}(T)$$

With this Hamiltonian one can show that for T > 0 ($\Psi(T)$) is the 2^{-2} (A (an Aspuru-Guzik (Harvard University) Q. Computation for Chemistry 7-25-07 68/85

Important results of these papers

- **Thermodynamics** of *classical* spin 1/2 can be obtained from the **ground state** of a quantum system with **classical** interactions (determined by T and H) and an external homogeneous transverse field.

•
$$\Psi(T o \infty)
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1D Ising model

$$H_q^j(T) = \sigma_x^j - \cosh(\beta J) - \cosh(\beta J) \sinh(\beta J) (\sigma_z^{j-1} \sigma_z^j + \sigma_z^j \sigma_z^{j+1}) - \sinh(\beta J)^2 \sigma_z^{(j-1)} \sigma_z^{(j+1)} + \sigma_z^j \sigma_z^{j+1} - \sigma_z^j \sigma_z^j \sigma_z^{j+1} - \sigma_z^j \sigma_z^j \sigma_z^{j+1} - \sigma_z^j \sigma_z^j \sigma_z^j - \sigma_z^j \sigma_z^j \sigma_z^j - \sigma_z^j \sigma_z^j \sigma_z^j - \sigma_z^j \sigma_z^j \sigma_z^j \sigma_z^j - \sigma_z^j \sigma_z^j \sigma_z^j \sigma_z^j - \sigma_z^j \sigma_z^j \sigma_z^j \sigma_z^j \sigma_z^j - \sigma_z^j \sigma_z^j \sigma_z^j \sigma_z^j \sigma_z^j \sigma_z^j - \sigma_z^j \sigma$$

Frustrated Hamiltonian, except for T = 0.

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Important results of these papers

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$$\Psi(T \to \infty) \rangle \approx rac{1}{2^{n/2}} |[Z] \rangle > 0$$

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Frustrated Hamiltonian, except for T = 0.

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Why do chemists care?

Plan of attack

- An adiabatic QC like the one described above could yield quantum states that are analogous to thermodynamic states.
- One can obtain statistics for lattice models of interest to chemists at finite temperature

Specific example of interest to us: Protein lattice models

- We have found a mapping of the Hydrophobic-Polar model to a 2DIMM
- Working with D-Wave for experimental realization
- We plan to use Somma's method to study T > 0 states of this model experimentally using their quantum device.

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Why do chemists care?

Plan of attack

- An adiabatic QC like the one described above could yield quantum states that are analogous to thermodynamic states.
- One can obtain statistics for lattice models of interest to chemists at finite temperature

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HP model

Ivan Tubert-Brohman and Colin Truncik (D-Wave) and AAG



Alán Aspuru-Guzik (Harvard University)

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HP model mapping to 52 quantum bits

Ivan Tubert-Brohman and Colin Truncik (D-Wave) and AAG



Alán Aspuru-Guzik (Harvard University)

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David Deutsch

I think the field doesn't need acceptability. The idea will either be valid, or not. The claim will either be true, or not. I think that the normal processes of scientific criticism, peer review and just general discussion in the scientific community is going to test this idea – provided enough information is given of what this idea is. That will be quite independent of what kind of access they provide to the public. However, I think the idea of providing an interface such as you describe is a very good one. I think it's a wonderful idea....

TeQuiLA: A High-Performance QC Simulator



Features

- FREE! Under LGPL
- Reads Isaac Chuang's QAsm (LATEX)
- Fast linear algebra core (parallelizable)
- Pure or mixed states
- Perfect for circuit simulation, experiment design, undergraduate courses, parties,.....

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Excited states: Multiconfigurational Self-Consistent Field (MCSCF)

Work in progress: In collaboration with Sabre Kais, Purdue University

MCSCF in a nutshell

- Choose a subspace $\mathcal{H}_{MCSCF} \subset \mathcal{H}$
- Find the optimal coefficients $C_{\mu i}$ and orbitals ϕ_i self-consistently
- Note: The orbitals will be different to the CI orbitals (natural orbitals)

MCSCF Equations

$$\psi_{MCSCF} = \sum_{K} A_{K} \Phi_{K}, \qquad \Phi_{K} = A_{\prod_{i \in K}} \phi_{i}, \qquad \phi_{i} = \sum_{\mu} \chi_{\mu} C_{\mu i}$$

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MCSCF advantages

$\bullet \ |\langle \Psi_{\textit{MCSCF}} | \Psi_0 \rangle|^2 > |\langle \Psi_{\textit{HF}} | \Psi_0 \rangle|^2$

- Can be prepared classically in polynomial time
- Reproduces better potential energy surfaces and excited states.
- We conjecture that it has a significative overlap with a **polynomial** number of states.

State Preparation

- Use Natural orbital occupation coefficients as a guess, or
- Prepare the MCSCF state efficiently

Valence active space

Capturing the important correlations



- Use near-optimal orbitals (e.g. coming out from imperfect pairing method)
- Only consider excitations of the valence electrons
- Able to treat more exciting chemical problems

Other things we will work on next semster

When the students join the group!

Phase estimation

- Effect of Trotter discretization
- Finish work on effects of noise
- Excited states
- Molecular properties (polarizability, dipole moments)
- Precise gate counts and sequences for series of molecules

Other quantum algorithms

- Finding protein low-energy conformations (Ivan Tubert-Brohman)
- Chemical reaction dynamics (Masoud Mohseni)
- Density Functional theory and correlation (Ali Najmaie)

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Conclusions and Outlook

"We want to use this machine in the same sense ... as a cyclotron is used in a physics laboratory" - John Von Neumann

- Quantum chemistry includes a well-defined set of problems which are optimal candidates for small quantum computers.
- Much chemical intuition available: should enable proof of conjectures about, e.g. adiabatic state preparation
- Experimental realizations yes, please
- Use Tequila to design further small realizable examples
- Further algorithmic improvements, other eigenfunction Ansatzes, active space methods, lattice gas methods, ...

Thank you!



Anthony Dutoi, Peter Love, Martin Head-Gordon



Kinga Partyka, James Whitfield

Also thanks to:

- Mikko Möttönen (Factorization)
- The David Cory group (Jonathan Hodges, Troy Borneman)
- The Martin Head-Gordon group
- D-Wave Systems (funding)

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Reference:

Aspuru-Guzik, Dutoi, Love and Head-Gordon Science 309 5741 (2005)

But where are we?

Active control of qubits



Steffen et al. Science 313 (2006) 1423

Alán Aspuru-Guzik (Harvard University)

Q. Computation for Chemistry

7-25-07 81/85

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Adiabatic State Preparation

If HF is a bad guess, construct the FCI solution adiabatically.

Open question

Discretization effects?



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Adiabatic State Preparation

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Open question

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Adiabatic State Preparation for Molecules?

Arguments

- Molecules are insulators and they often have color (even most polymers).
- For a given system, we know a lot of properties of the eigenvalue spectrum from approximate classical methods.
- Kohn's argument against wave function theories does not lead to an exponential increase in preparation time.

Kohn's Idea

For an group of *K* non-interacting subsystems call $S_1 = |\langle \Psi_0^1 | \Psi_T^1 \rangle|$, then the overall overlap *S* will decrease as S_1^K , but ...

$$\lim_{K\to\infty} \left[1-S_1\right] = \frac{\ln S}{K}$$

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The Aspuru-Guzik Group

Department of Chemistry, Harvard University

Renewable Energy Materials

- Polymer Fuel Cell Membranes
- Nanoparticle/Organic photovoltaic materials

Density Functional Theory development

- Non-local density functional theory
- Connections with quantum information theory

Quantum simulation

- Quantum devices (computers and simulators) and their application to chemistry.
- Connections between quantum algorithms and physical systems.

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