Quantum Computation for Chemistry

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Quantum Information Science Workshop, Vienna, VA 2009

D. Bacon, Science 317 (2007), p. 1876, September 28

PHYSICS

Does Our Universe Allow for Robust Quantum Computation?

Dave Bacon

Computers operating purely according to the laws of quantum theory might break modern cryptographic codes (*1*), revolutionize quantum chemical calculations (*2*), and overturn the most basic limits to computing (*3*). Standing in the way of creating these dream machines is the fact that quantum computers do not like to maintain their quantum nature, but instead have a propensity to decay into machines obeying the classical tum system. Left out, however, is the question of whether the theorem actually holds in an experimental setting: Does our universe allow for robust quantum computation?

This is a hard question because the cost (the number of experiments needed) of characterizing the properties of quantum systems useful for fault-tolerant computation rises exponentially with the number of quantum systems (*9*, *10*). Emerson *et al.* have found a

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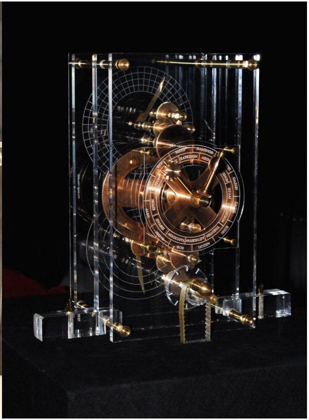
Antikythera device

Built around 150-100 B.C. (Ancient mechanical quantum simulator)



Computer simulation

From “Image and Logic: A material culture of microphysics”, 1997

Without the computer-based simulation, the material culture of late-twentieth-century microphysics is not mereley inconvenienced – it does not exist. Nor this is only true for particle detectors – machines including the huge plasma-heating Tokamaks, the complex fission-fusion nuclear weapons, the guidance systems of rockets are inseparable from their virtual counterparts – all are bound to simulations.

–Peter Galison

S. F. Boys, EDSAC and Gaussian orbitals

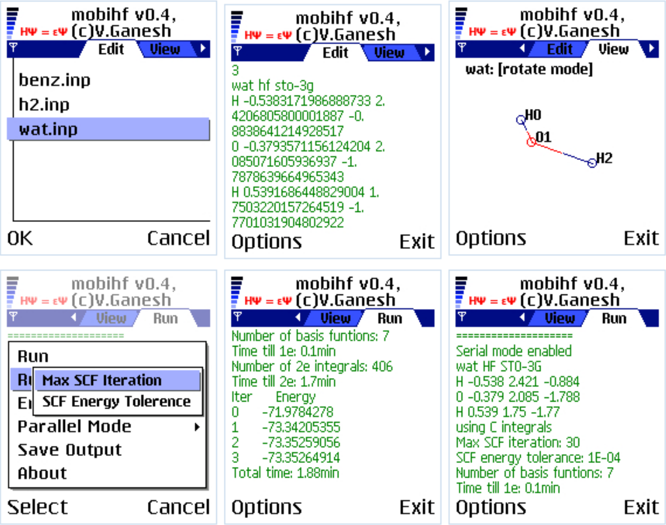
Boys, Cook, Reeves and Shavitt, **Nature**, 178, 1207 (1956)

AUTOMATIC FUNDAMENTAL CALCULATIONS OF MOLECULAR STRUCTURE

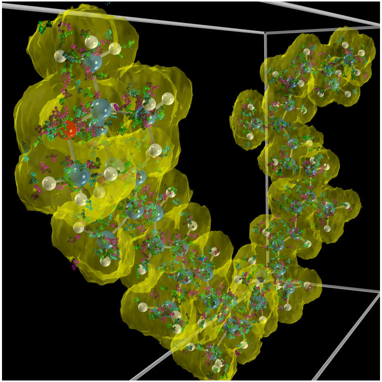
By Dr. S. F. BOYS, Dr. G. B. COOK, C. M. REEVES and I. SHAVITT

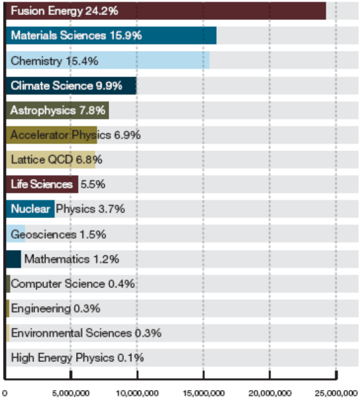
Theoretical Chemistry Department, University of Cambridge

Cell phone quantum chemistry: **mobimol**



High-performance quantum chemistry calculations

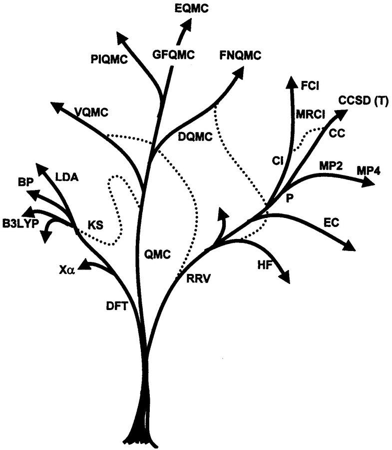




Spheroidene molecule QMC calculation (250,000 hours of CPU time),
Usage allocation per area, NERSC Supercomputers (DOE), (2007)

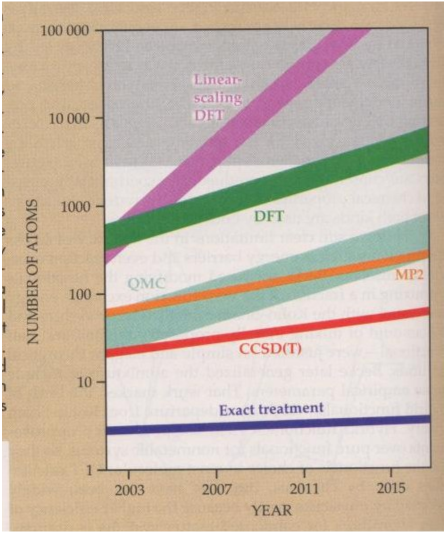
Traditional Mexican ceramics and quantum chemistry methods

The tree of life



Traditional Computational Chemistry Roadmap

Martin Head-Gordon, *Physics Today* April, 2008

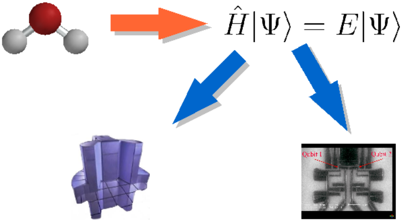


R. P. Feynman, *Simulating physics with computers*
Int. J. Theo. Phys., 21, (1982)

Computational Chemistry vs. Quantum Simulation

Feynman's Proposal

$$
\begin{aligned}
|\Psi^{mol}\rangle &\rightarrow |\Psi^{QC}\rangle \\
\hat{U}^{mol}(t) = e^{-i\hat{H}^{mol}t} &\rightarrow \hat{U}^{QC}(t) = e^{-i\hat{H}^{QC}t}
\end{aligned}
$$



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

quantum emulation

Quantum algorithms for simulation:
Zalka, Lloyd, Lidar, Cleve, Aharonov, Chuang, Brown, Love, Ortiz, Somma, Gubernatis, Kais, Nori, Aspuru-Guzik, ...

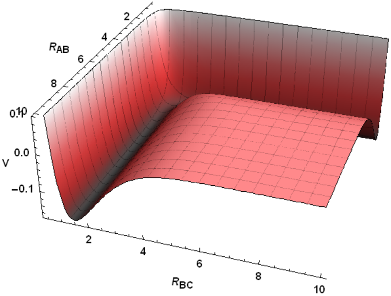
The quantum advantage

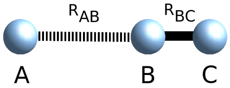
Computational task	Classical cost	Quantum cost
Factoring	$e^{O(n^{1/3} \log^{2/3} n)}$	$O(n^2 \log n \log \log n)$
Search	$O(n)$	$O(\sqrt{n})$
Full CI	$e^{O(n)}$	$O(n^5)$
Chemical dynamics	$e^{O(n)}$	$O(n^2)$
Protein folding	$e^{O(n)}$	?

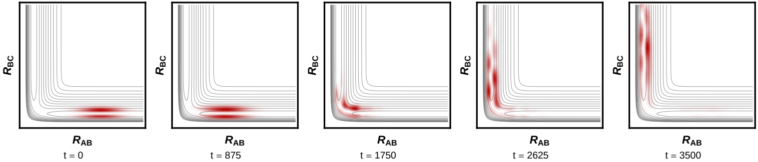
- Full CI: Aspuru-Guzik et. al, **Science** (2005). Huang, Kais, Aspuru-Guzik, Hoffman, **Phys. Chem. Chem. Phys.** 10, 5388 (2008); Gradients: Kassal, Aspuru-Guzik, *to be submitted*.
- Chemical dynamics: Kassal, Jordan, Mohseni, Love, Aspuru-Guzik, **Proc. Nat. Acad. Sci.** 105, 1868 (2008), Ward, Kassal, Aspuru-Guzik, **J. Chem. Phys.** (2009) In Press. arxiv:0812.2681
- Protein folding (random heteropolymer minima): Perdomo, Truncik, Tubert-Brohman, Rose, Aspuru-Guzik. **Phys. Rev. A.** 78, 1, 021320 (2008)

Chemical reaction dynamics

Kassal, . . . , Aspuru-Guzik **PNAS (2008)**







Reaction dynamics algorithm

Kassal, . . . , Aspuru-Guzik **PNAS (2008)**, Ward, Kassal, Aspuru-Guzik **J. Chem. Phys. In press (2009)**

Input

- The Hamiltonian of the system, $\hat{H} = \hat{T} + \hat{V} = \frac{\hat{p}^2}{2m} + \hat{V}(\mathbf{x})$
- An initial condition for the wave packet

Steps

- Initialize wavefunction using a proper mapping to qubits
- Propagate in time
- Measure observables

Output

- Reaction probability
- Thermal rate constant
- State-to-state distributions

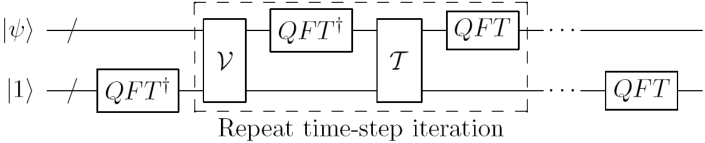
Split-operator (Trotter) method

For a short timestep, δt,

$$U(\delta t) \approx e^{-iT\delta t} e^{-iV\delta t}.$$

Note that the potential operator V is diagonal in position **R** and T is diagonal in momentum **P**. Use diagonal representation of operators.

$$|\psi(\delta t)\rangle = \mathrm{FT}\, e^{-iT\delta t}\, \mathrm{FT}^{-1}\, e^{-iV\delta t}\, |\psi(0)\rangle\,.$$



$$|\psi\rangle \rightarrow e^{-iV\delta t}\,|\psi\rangle = \sum_{x=0}^{2^n-1} a_x e^{-iV(x)\delta x}\,|x\rangle$$

A quantum architecture for an error correcting quantum computer

A. Steane. How to build a 300-bit, 1-gigaop quantum computer, Quantum Information and Computation, 7, 171 (2007)

- 300 logical qubits
- Encoded in $\approx$ 10,000 physical qubits
- Ion-trap implementation
- Within error-correcting threshold and able to carry out 10^9 quantum gates.

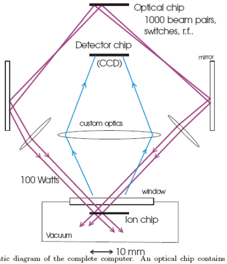
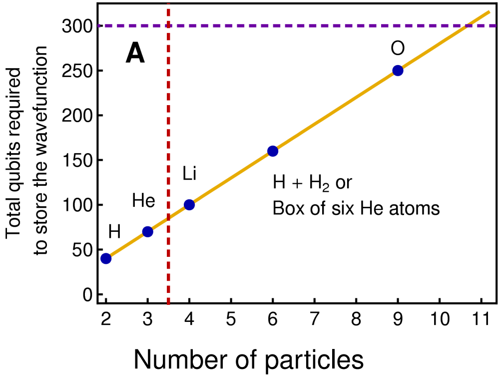


Fig. 1. Schematic diagram of the complete computer. An optical chip contains laser sources, optical switches and r.f. control circuitry for the laser pulses; the multiple laser beams (2 of 1000 pairs are shown) are imaged onto an 'ion chip' (IC) in vacuum, containing the array of ion traps and the control circuitry for moving ions around. The detector registers optical fluorescence; its elements could alternatively be incorporated onto the IC. The optical chip could alternatively be placed inside the vacuum chamber, close to the IC, or else replaced by conventional methods

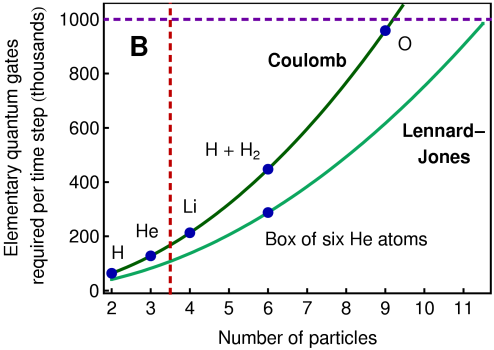
Qubit requirements



$n = 10$, i.e., a grid of 1024 points per dimension

$(3N - 2)n$ qubits are required

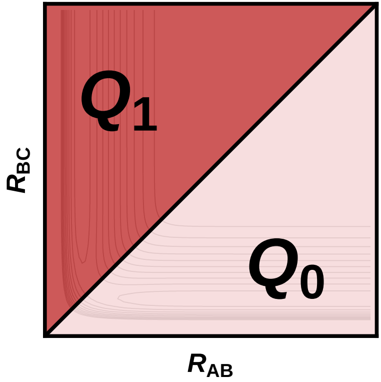
Quantum gate requirements

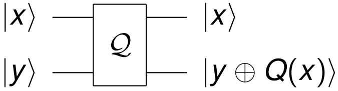


$n = 10$, i.e. a grid of 2^{30} points
Coloumb: $\frac{75}{4}n^3 + \frac{51}{2}n^2$ elementary gates per step per pair of particles.
Lennard-Jones: $\frac{25}{2}n^3 + 12n^2$ gates per step per pair of particles.

Determination of observables

Has the wave packet crossed the barrier?

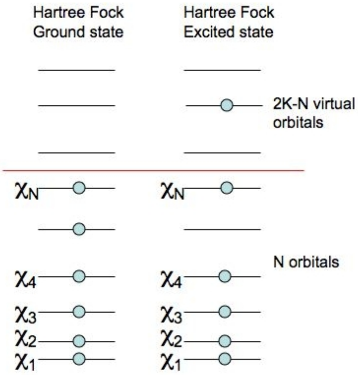




$$\mathcal{Q}\,|x, y, 0\rangle = \begin{cases} |x, y, 0\rangle & \text{if } \; y < x \\ |x, y, 1\rangle & \text{if } \; y \geq x \end{cases}$$

Measuring the ancilla gives the transition probability.

HF Determinants



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

Full Configuration Interaction (FCI)

Aspuru-Guzik *et al*, **Science (2005)**, Wang *et al.*, **PCCP (2008)**

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 exact results within the given basis.

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

$$e^{-i\hat{H}t} \approx \left[\prod_X e^{-i\hat{h}_X t/M} \right]^M \qquad \hat{a}_p^\dagger \hat{a}_q \rightarrow \hat{X}^p \hat{X}^q \left[\prod_{i=p+1}^{q-1} \hat{\sigma}_z^i \right] \hat{P}_0^p \hat{P}_1^q$$

- Number of Terms in $\hat{H}$ grows as N_{basis}^4
- Each term involves a controlled action on at most 4 qubits
- Few gates required by term

Time Evolution

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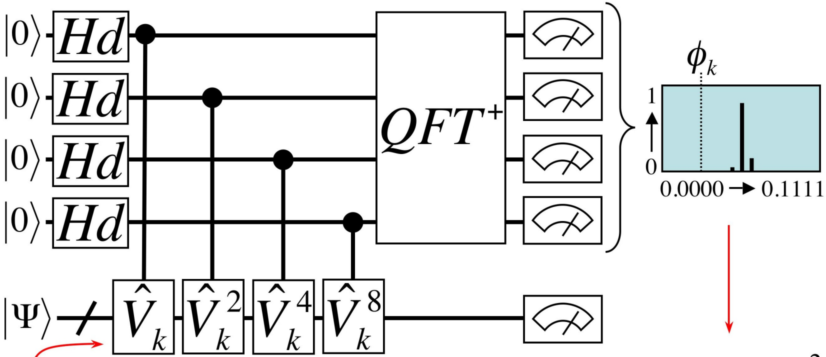
Phase Estimation: A Recursive Algorithm

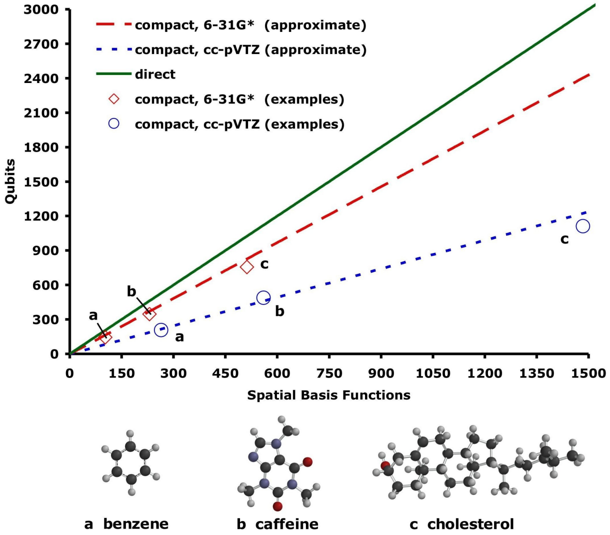
Get a lower bound and measure the difference . . . repeatedly . . . as much as you want.



$$\hat{V}_0 = \hat{U}$$

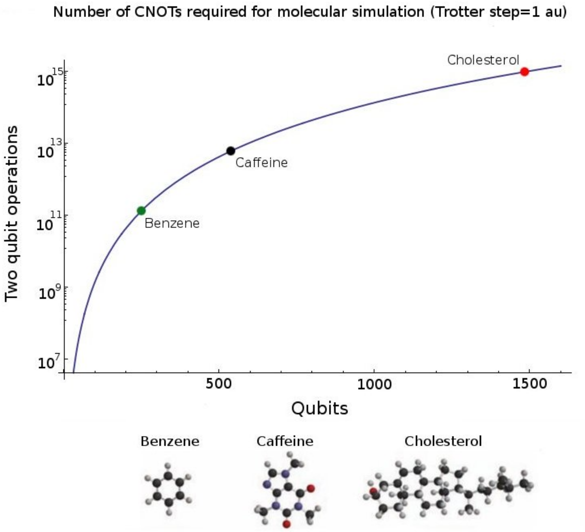
$$\hat{V}_k = \left[\exp\left(-i2\pi\phi_{k-1}\right)\hat{V}_{k-1}\right]^2$$

Qubit Requirements



Two-qubit gates required for simulating molecules

Whitfield, Biamonte, AAG, In Preparation



Ken Brown (GA Tech): Error Correction analysis

Quantum simulation of Ising Model in a Transverse magnetic field

Challenges

- Hardware is unreliable
  - Passive Error Prevention
  - Active Error Correction

- Simulating systems with protected subspaces.

  Energy protection arguments fail in the interaction picture

  KRB, Phys. Rev. A, 022327 (2007) arXiv:0705.2370

- Quantum simulation on a fault-tolerant quantum computer.

  Resource requirements for fault-tolerant quantum simulation:
  the transverse Ising model ground state arXiv:0810.5626
  C.R. Clark and KRB, Georgia Tech
  T.S. Metodi and S.D. Gasster, Aerospace Corporation

Ken Brown (GA Tech)

Quantum Logic Array Model

T. S. Metodi, D. D. Thaker, A. W. Cross, F. T. Chong, and I. L. Chuang (2005), MICRO 38.

- Tile Based Architecture
- Communication by qubit movement
- Specifically designed based on ion traps.
- Extendable to other models
  - Quantum Dots

J. M. Taylor, et al.,
Nature Physics **1**, 177 (2005).

Logical Qubit 1
+ ancilla for error correction
+ ancilla for operations

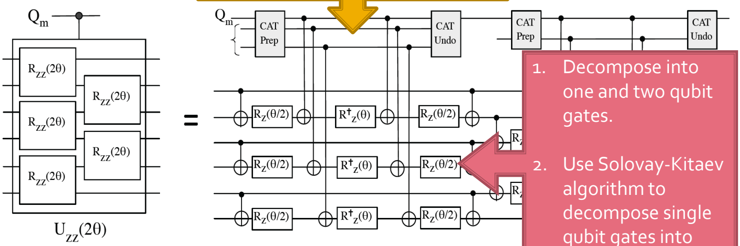
Logical Qubit 2
+ ancilla for error correction
+ ancilla for operations

Ken Brown (GA Tech): Error correction

Quantum simulation of Ising Model in a Transverse magnetic field

Parallelize and Decompose

Cat States for Parallelization (|0000…>+|1111…>)

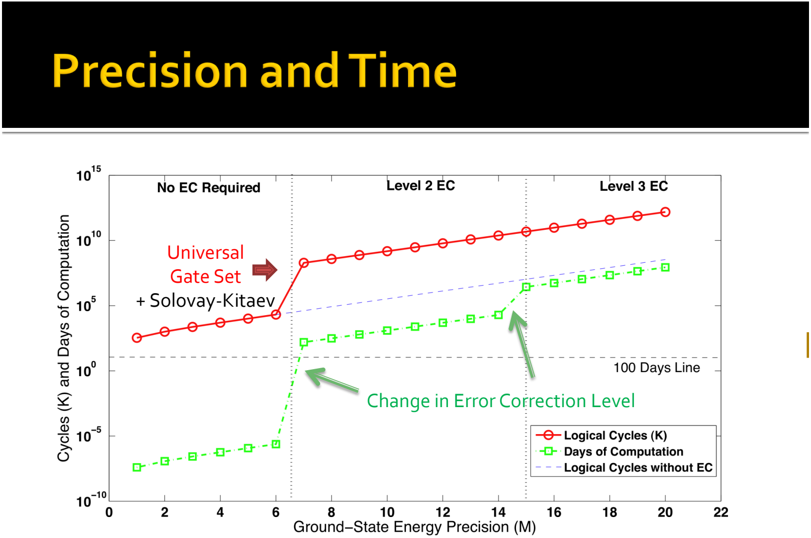


1. Decompose into one and two qubit gates.
2. Use Solovay-Kitaev algorithm to decompose single qubit gates into H,T, X,Z,Y

Phase Bit Precision > Trotter Error > Solovay-Kitaev Error

Ken Brown (GA Tech): Quantum Resources

Quantum simulation of Ising Model in a Transverse magnetic field



N=100 TIM

Quantum optics for quantum chemistry

First quantum chemistry quantum computing experiment, 2008

Lanyon *et al.*. In review.

Quantum Technology Lab - Brisbane, Australia


Ben Lanyon


Andrew White


M. DeAlmeida


Geoff Gillet

Aspuru-Guzik research group - Harvard, USA

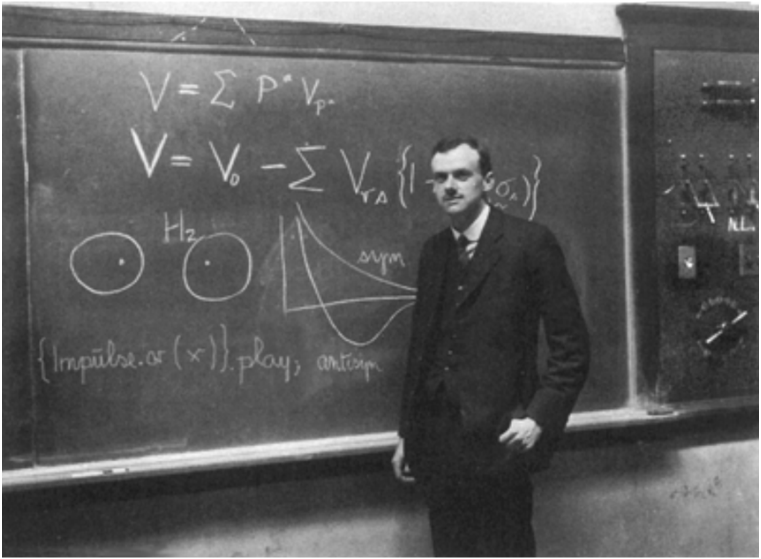

James Whitfield


Ivan Kassal

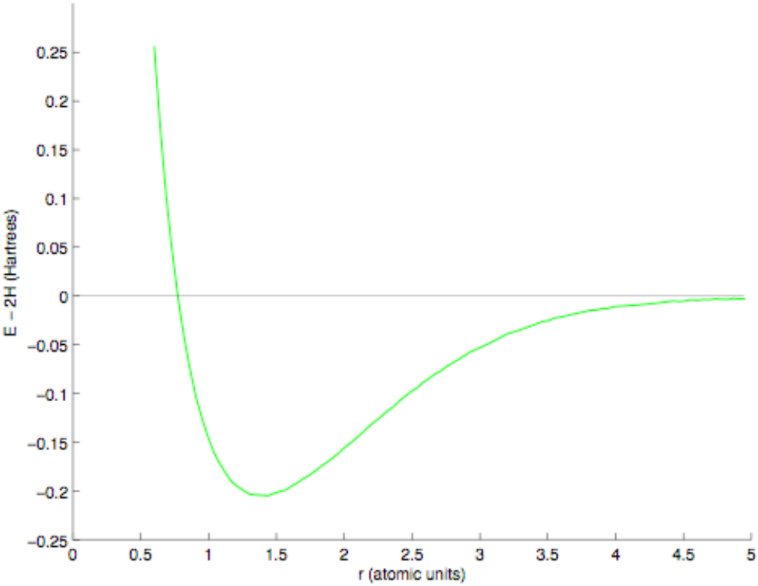

Alejandro Perdomo


Masoud Mohseni

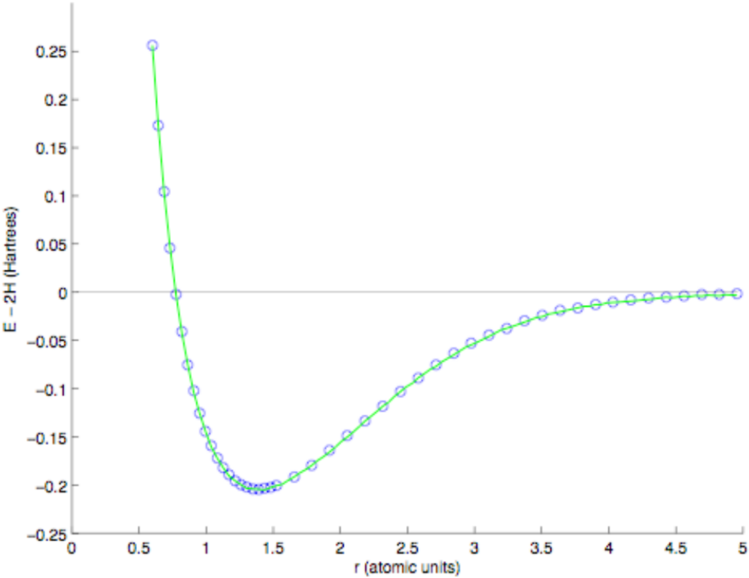
The hydrogen molecule



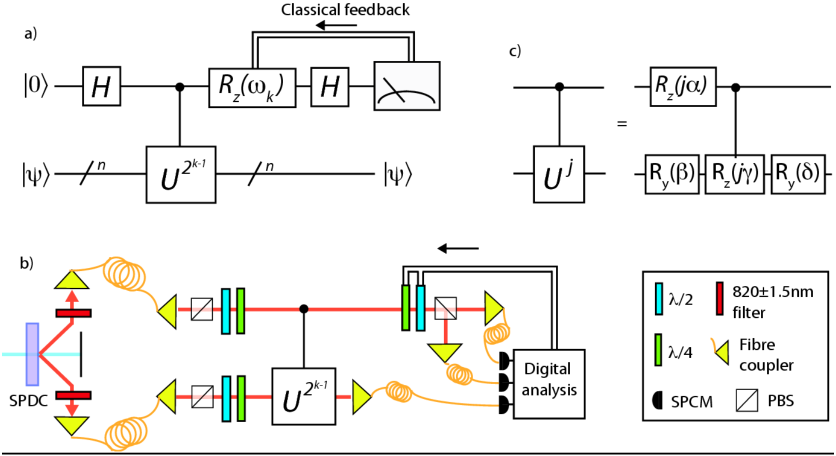
H_2 STO-3G Basis set Full CI

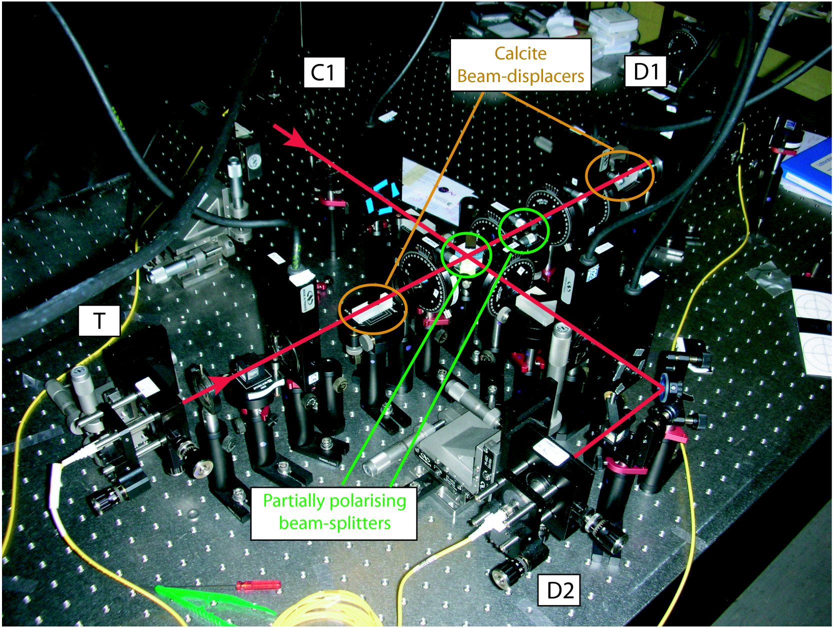


H_2 FCI Quantum computer experiment

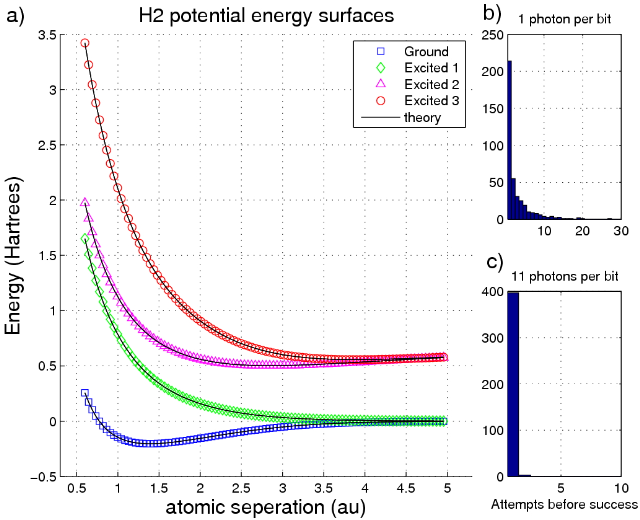


Experimental setup



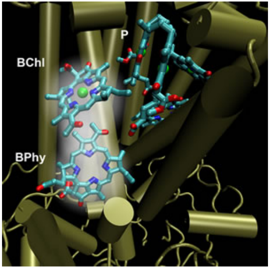

C1
Calcite
Beam-displacers
D1
T
Partially polarising
beam-splitters
D2

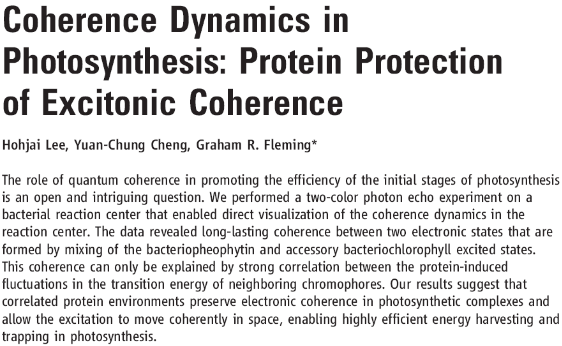
Experimental curves and number of photons per point



Quantum coherence in photosynthesis

Revealed by ultrafast four-wave mixing experiments




Coherence Dynamics in Photosynthesis: Protein Protection of Excitonic Coherence

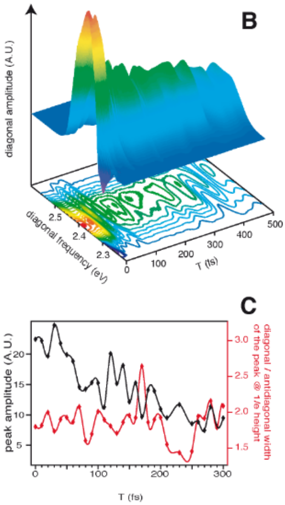
Hohjai Lee, Yuan-Chung Cheng, Graham R. Fleming*

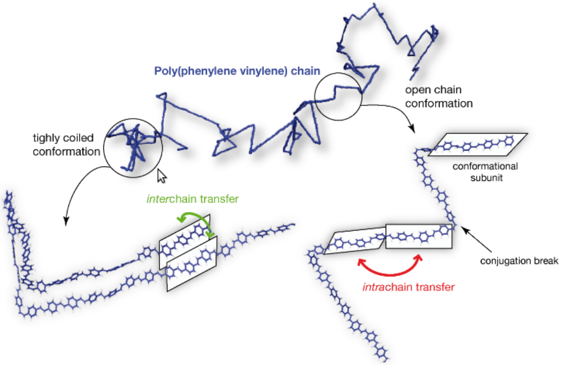
The role of quantum coherence in promoting the efficiency of the initial stages of photosynthesis is an open and intriguing question. We performed a two-color photon echo experiment on a bacterial reaction center that enabled direct visualization of the coherence dynamics in the reaction center. The data revealed long-lasting coherence between two electronic states that are formed by mixing of the bacteriopheophytin and accessory bacteriochlorophyll excited states. This coherence can only be explained by strong correlation between the protein-induced fluctuations in the transition energy of neighboring chromophores. Our results suggest that correlated protein environments preserve electronic coherence in photosynthetic complexes and allow the excitation to move coherently in space, enabling highly efficient energy harvesting and trapping in photosynthesis.

Lee, Cheng and Fleming, Science **316** 5830 (2007)

Evidence for wavelike energy transfer through quantum coherence in photosynthetic complexes, Engel, . . . , Fleming, Nature **446** 782 (2007)

Room temperature coherence observed in a conjugated polymer at **room temperature** for hundreds of femtoseconds.





E. Collini, G. Scholes, Science, **323**, 369 (2009)

Dendrimers

Quantum walks on “perfect” trees have exponential speedup. What about “imperfect” light-harvesting molecules?

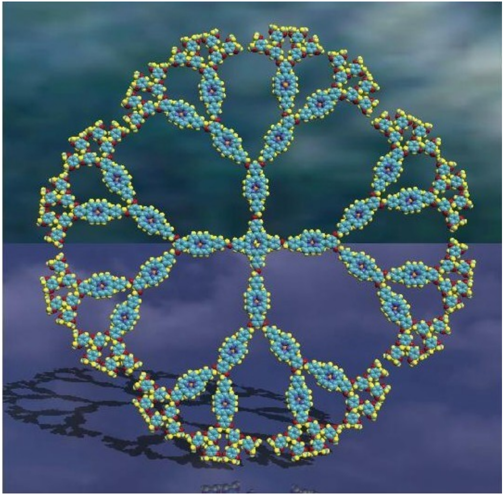
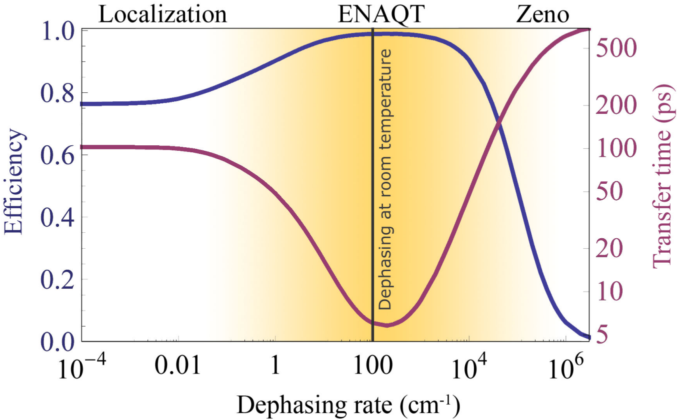


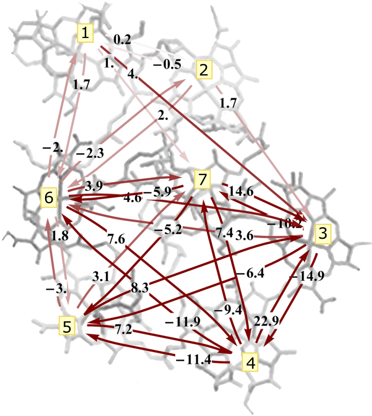
Image: Takuzo Aida, University of Tokyo

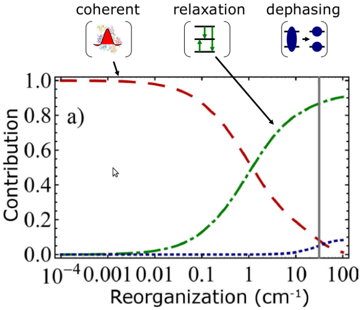
Environment Assisted Quantum Transport (ENAQT)



P. Rebentrost, M. Mohseni, S. Lloyd, A. Aspuru-Guzik
arxiv:0807.0929, *New Journal of Physics* **11 (2009) 033003**
M. Plenio and Huelga, **arxiv:0807.4902**

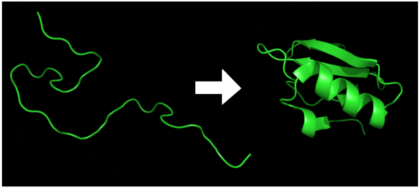
Emergence of “quantum biology” ?

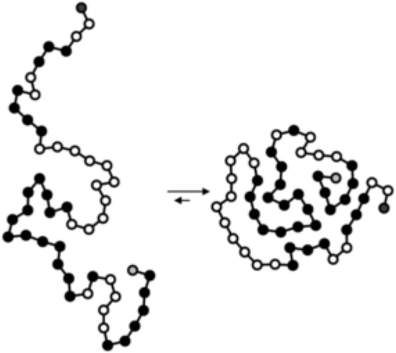




- *J. Chem. Phys. 129, 174106 (2008), New J. Phys., 11, 033003 (2009), arxiv:0806.4725*
- *Other quantum information scientists involved or interested (not exhaustive):* M. Plenio (Imperial College), B. Whaley (UC Berkeley), Gerald Milburn (Queensland), Hans Briegel (Innsbruck), Vlatko Vedral (Leeds/Singapore), A. Olaya-Castro (UC London), Keye Martin (NRL), M. Lanzagorta (ITT), . . .
- *Conferences.* DARPA (2008), Singapore (2008), Lisbon (this Summer, 2009)

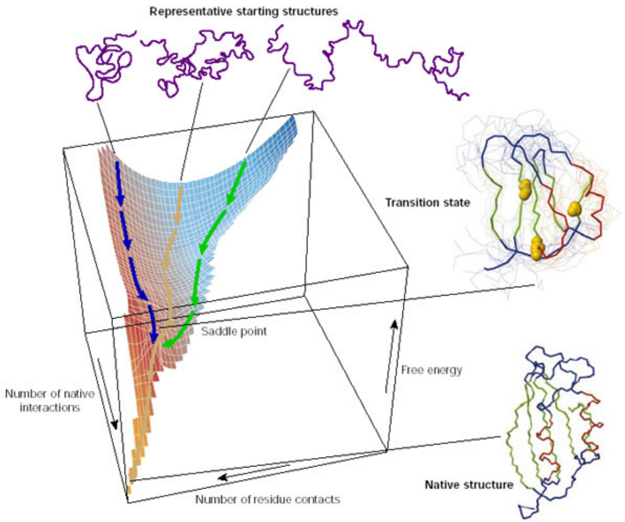
Protein Folding





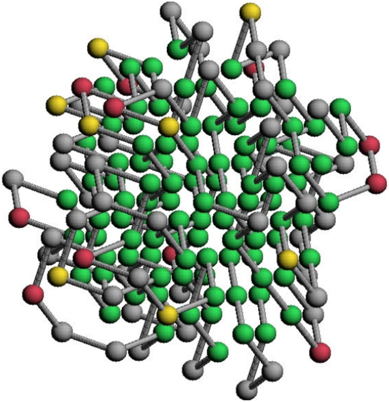
Protein Energy Landscapes

Funnel idea (P. Wolynes)



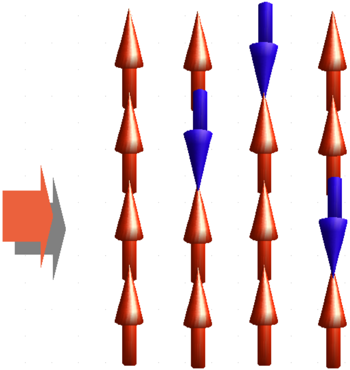
Lattice Protein Models

Mapping to 2D Ising Model in a Magnetic Field



Protein Lattice Model

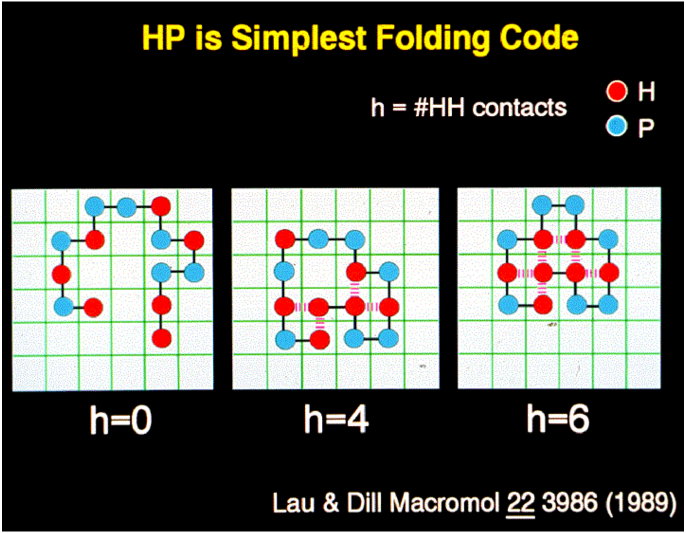
Image: Prof. Backofen, Uni. Freiburg



Classical Ising Model

The hydrophobic-polar (HP) model

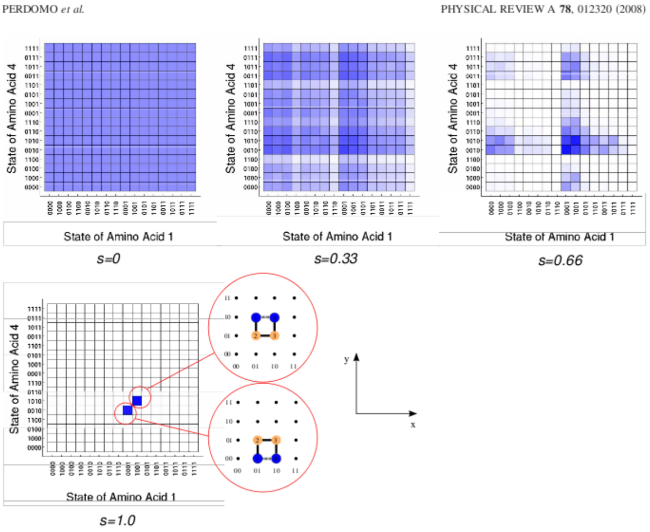
Mapping to 2D Ising Model in a Magnetic Field



Slide Credit: Ken Dill

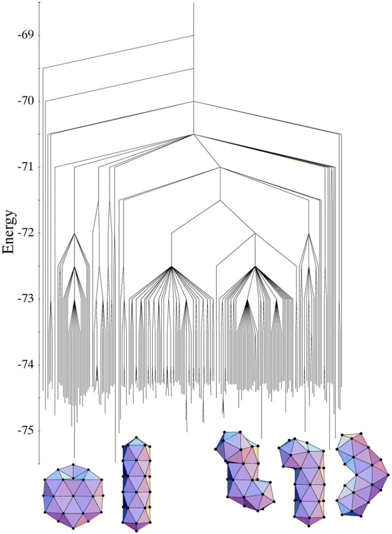
Adiabatic evolution to simplest HP model ground state

Perdomo, . . . , Aspuru-Guzik, Phys. Rev. A (2008)



Energy Landscape: Lennard-Jones Cluster example

David Wales, Cambridge, UK



Grover's Algorithm for optimized Lennard-Jones Cluster

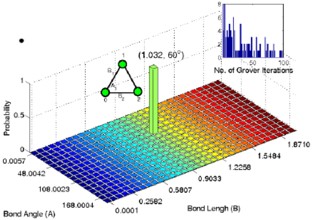


Figure 6.8. Final probability distribution of the wave function for LJ (N=3) cluster. The global minimum located at $B_1 = 1.032, B_2 = 1.032$ and $A_1 = 60^o$. The left inner panel is the distribution of total iteration number before reach the global minimum for 100 search experiments. The right inner panel is the total measure step before reach the global minimum.

- 9 qubits total. 5 for the bond length, 4 for the bond angle
- The final optimized structure are shown in the picture, it is the same as the classical simulation result
- Our next project is try to extend the simulations to N=4, 5,6,…

Conclusions and Outlook

- Quantum computing provides exponential speedups for electronic structure and quantum dynamics
- Interesting quantum algorithms for structure optimization that might exhibit polynomial (quadratic) speedup.
- Quantum information providing insight into photosynthesis and solar energy harvesting
- Other physical chemistry / quantum information connections awaiting to be explored.