

Towards Quantum Chemistry On a Quantum Computer

A (really short) Group Meeting,
April 27, 2011
Dylan Mahler

Summary

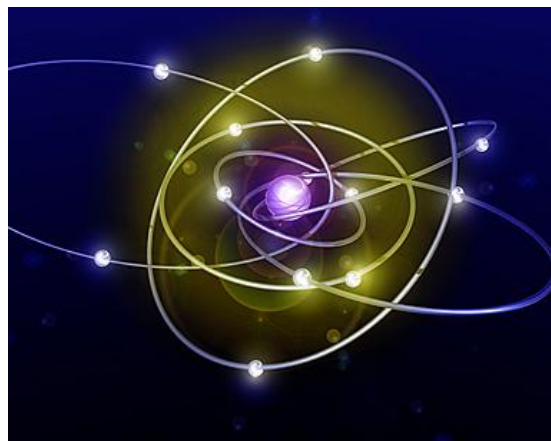
- Quantum Chemistry?!
- Phase Estimation
- Iterative Phase Estimation
- The Experiment

Towards quantum chemistry on a quantum computer

B. P. Lanyon^{1,2*}, J. D. Whitfield⁴, G. G. Gillett^{1,2}, M. E. Goggin^{1,5}, M. P. Almeida^{1,2}, I. Kassal⁴,
J. D. Biamonte^{4†}, M. Mohseni^{4†}, B. J. Powell^{1,3}, M. Barbieri^{1,2†}, A. Aspuru-Guzik^{4*} and A. G. White^{1,2}

Exact first-principles calculations of molecular properties are currently intractable because their computational cost grows exponentially with both the number of atoms and basis set size. A solution is to move to a radically different model of computing by building a quantum computer, which is a device that uses quantum systems themselves to store and process data. Here we report the application of the latest photonic quantum computer technology to calculate properties of the smallest molecular system: the hydrogen molecule in a minimal basis. We calculate the complete energy spectrum to 20 bits of precision and discuss how the technique can be expanded to solve large-scale chemical problems that lie beyond the reach of modern supercomputers. These results represent an early practical step toward a powerful tool with a broad range of quantum-chemical applications.

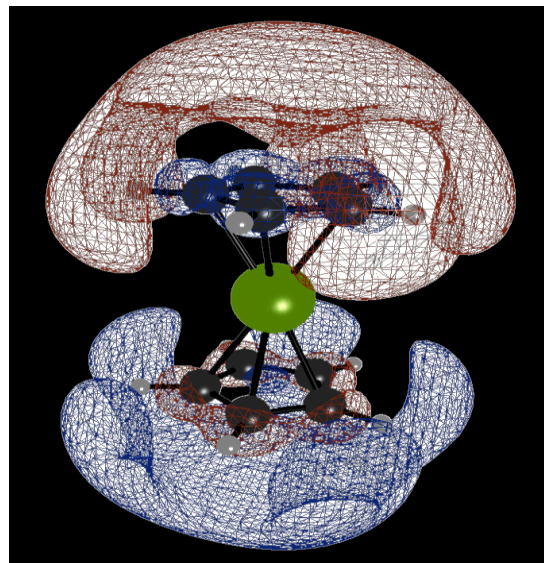
Quantum Chemistry



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Problem!

- Number of orbital configurations grows exponentially!
- For N orbitals and m electrons:

$$\binom{N}{m} \approx \frac{N^m}{m!}$$

Problem

- Simulating this on a classical computer gets really hard really fast.
- But quantum computers grow linearly with an exponential amount of resources!
 - Use them to simulate dynamics, calculate wavefunctions, and calculate eigenenergies:

Feynman, R. P. Simulating physics with computers.
Int. J. Theor. Phys. 21, 467–488 (1982)

(Very) General Idea

- We have a Hamiltonian, H , which we would like to calculate the eigenenergies of.
- Prepare the eigenstate we would like to learn about and allow simulate action of H :

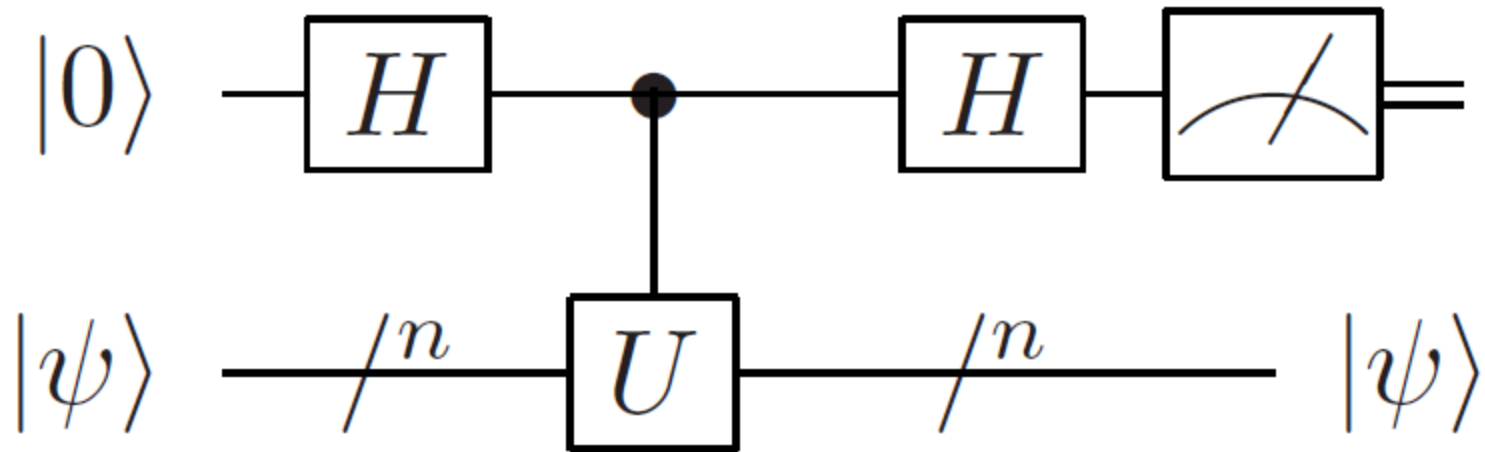
$$e^{-(i\hat{H}t/\hbar)} |\psi\rangle = e^{-(iEt/\hbar)} |\psi\rangle = e^{-i2\pi\phi} |\psi\rangle$$

- If we can estimate ϕ , we can estimate E .

Phase Estimation

- If I give you a unitary, how can you measure its eigenvalues?
- For those more experimentally-minded: how do we measure phase?

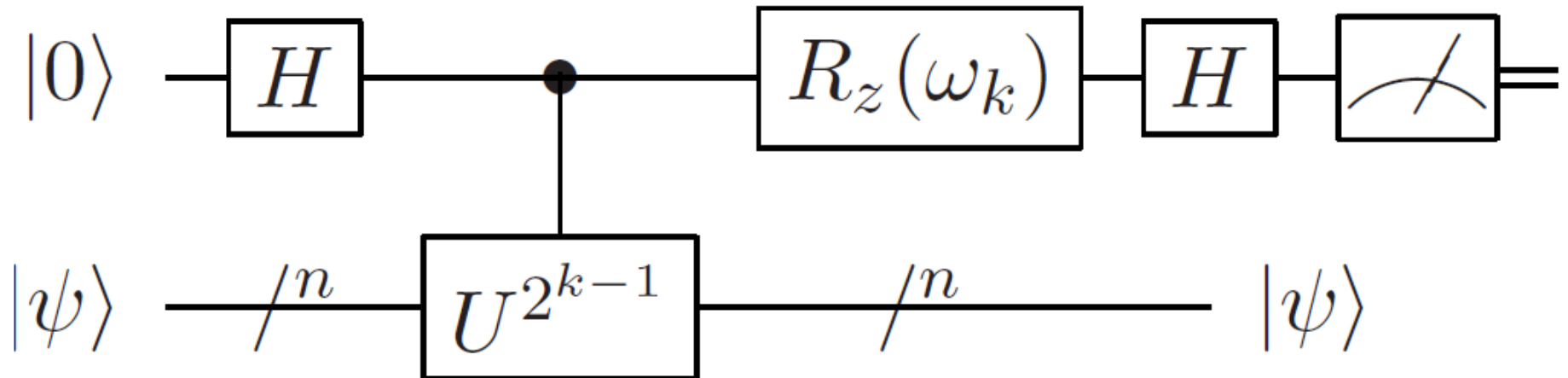
Naïve Method: Homodyne



$$\frac{1}{2}[(1 + e^{i2\pi\phi})|0\rangle + (1 - e^{i2\pi\phi})|1\rangle]|\Psi\rangle$$

$$P_0 = \cos^2(\pi\phi)$$

Iterative Phase Estimation



Math Alert!!

- Assume a binary expansion:

$$\phi = (0.\phi_1\phi_2\dots\phi_m000\dots)$$

- Now apply $U^{2^{m-1}}$:

$$\phi = (\phi_1\phi_2\dots\phi_{m-1}\cdot\phi_m)$$

- Then:

$$P_0 = \cos^2[\pi(0.\phi_m00\dots)]$$

Math Alert!!

- Assume a binary expansion:

$$\phi = (0.\phi_1\phi_2\dots\phi_m000\dots)$$

- Now apply $U^{2^{m-2}}$:

$$\phi = (\phi_1\phi_2\dots\phi_{m-2}\cdot\phi_{m-1}\phi_m)$$

- Now set $\omega_{m-1} = -2\pi(0.0\phi_m)$

$$P_0 = \cos^2[\pi(0.\phi_{m-1}00\dots)]$$

Deep breath...

Summary so far

- We can calculate eigenenergies given:
 - An implementation for U
 - A way to estimate phase efficiently, which in turn requires the ability to implement a controlled- U (many times!)

The H₂ Molecule

- Hamiltonian of the form:

$$\hat{H} = \sum_{p,q} h_{pq} \hat{a}_p^\dagger \hat{a}_q + \frac{1}{2} \sum_{p,q,r,s} h_{pqrs} \hat{a}_p^\dagger \hat{a}_q^\dagger \hat{a}_r \hat{a}_s,$$

- Forget that, its unimportant.

The H₂ Molecule

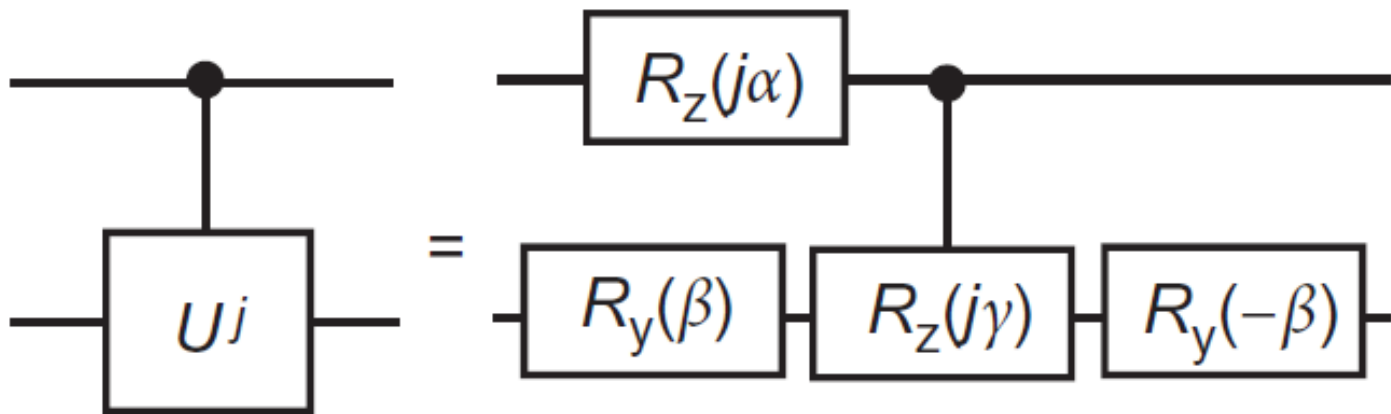
- What IS important: H is of the form

$$H = \begin{pmatrix} A & 0 & 0 & 0 & 0 & 0 \\ 0 & B & 0 & 0 & 0 & 0 \\ 0 & 0 & C & D & 0 & 0 \\ 0 & 0 & E & F & 0 & 0 \\ 0 & 0 & 0 & 0 & G & H \\ 0 & 0 & 0 & 0 & I & J \end{pmatrix}$$

- Block diagonal with single qubit blocks!
- We only need single qubits to simulate this!

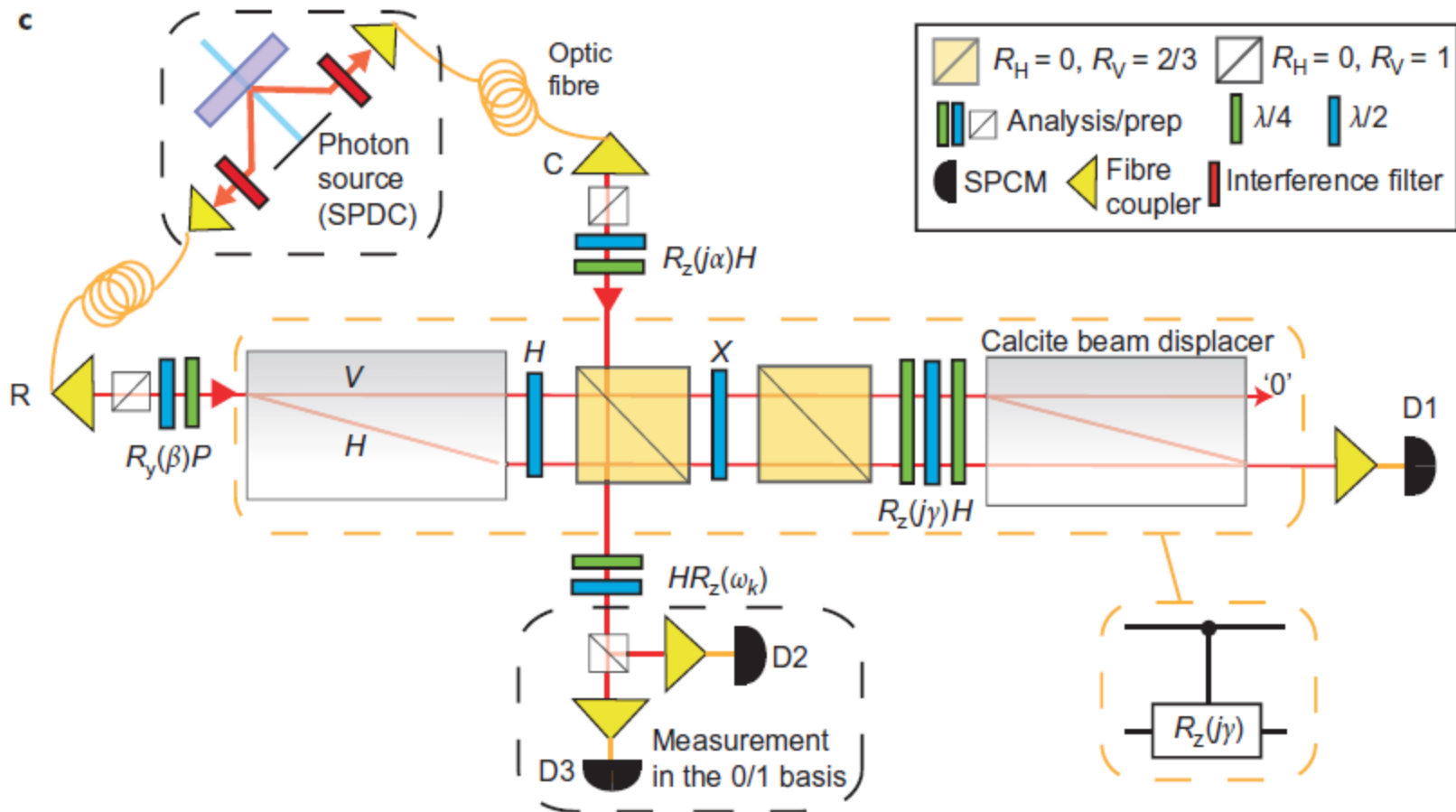
Almost at the experiment...

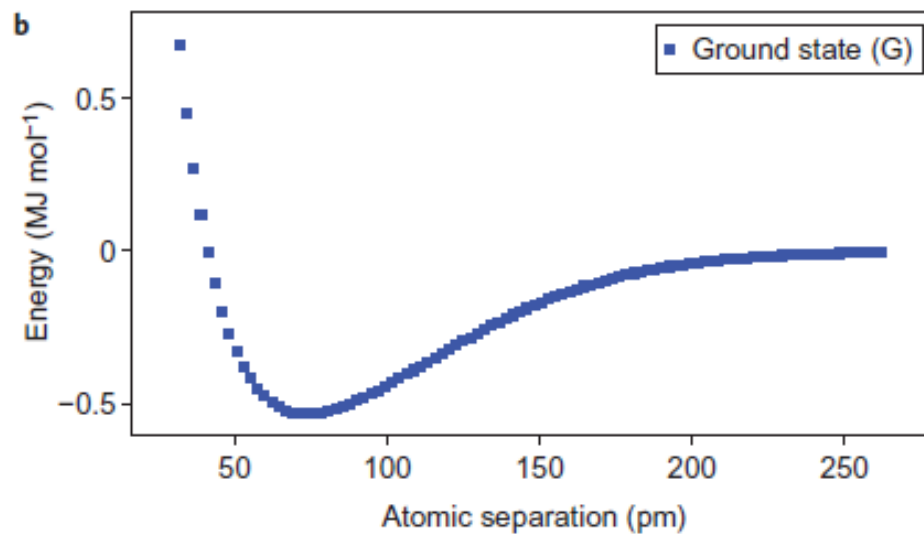
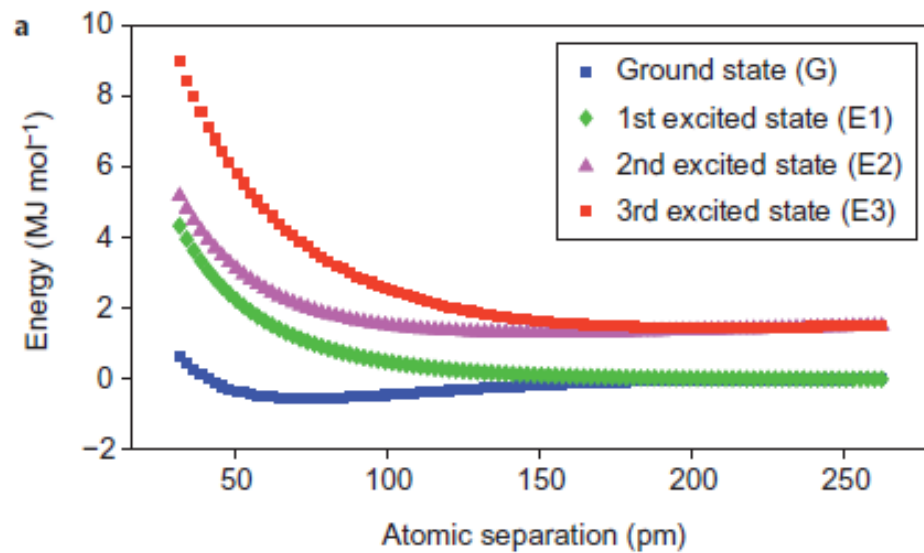
$$\hat{U} = e^{i\alpha} \hat{R}_y(\beta) \hat{R}_z(\gamma) \hat{R}_y(-\beta)$$



Simplifying quantum logic using higher-dimensional Hilbert spaces

Benjamin P. Lanyon^{1*}, Marco Barbieri¹, Marcelo P. Almeida¹, Thomas Jennewein^{1,2}, Timothy C. Ralph¹,
Kevin J. Resch^{1,3}, Geoff J. Pryde^{1,4}, Jeremy L. O'Brien^{1,5}, Alexei Gilchrist^{1,6} and Andrew G. White¹





Conclusions

- Demonstrated a proof of principle simulation of the hydrogen molecule in a linear optics set up.

CAVEATS:

- started from known eigenstates (huge cheat)
- Hamiltonian simple enough to make U^k easy
- a true simulation of this Hamiltonian requires approx. 522 gates!

Thank you,