Nature Chemistry

Towards Quantum Chemistry on a Quantum Computer

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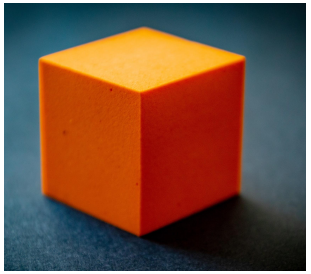
Outline

- Problem to solve
- Experiment
- Influence

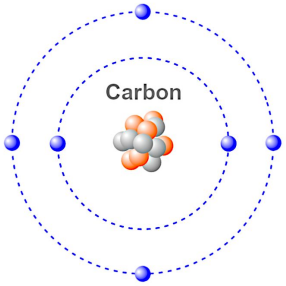
The problem

"**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."

First Principles Calculations



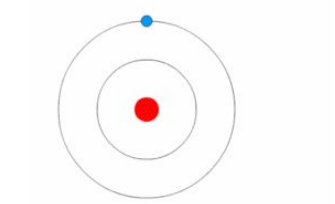
Condensed Matter



Atoms and Molecules

First Principles Calculations

"For the most part, the way this is done is to pick a particular macroscopic phenomenon, which has been well studied experimentally, and to build empirical, or semi-empirical, models to describe the experimentally observed results."



The Niels Bohr model of Hydrogen atom.

First Principles Calculations

The first principles approach to condensed matter theory is entirely different from this. It starts from what we know about all condensed matter systems - that they are made of **atoms**, which in turn are made of **a positively charged nucleus**, and **a number of negatively charged electrons**. The interactions between atoms, such as chemical and molecular bonding, are determined by the **interactions of their constituent electrons and nuclei**.

All of the physics of condensed matter systems arises ultimately from these basic interactions.

If we can model these interactions accurately, then all of the complex physical phenomena that arise from them should emerge naturally in our calculations.

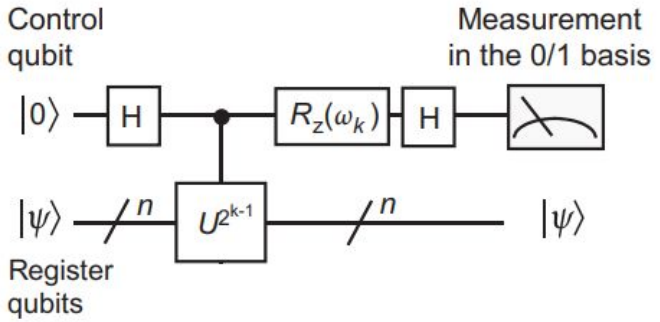
First Principles Calculations

The Many-Electron Schrödinger Equation

$$\hat{T}\Psi_{\mathrm{MB}} + \hat{V}\Psi_{\mathrm{MB}} = -i\frac{d\Psi_{\mathrm{MB}}}{dt},$$

Intractable Computational Problem even for Supercomputers

Linear Optic Quantum Computer(2 qubits)



Methodology

1. Encoding a molecular wave function into qubits;
2. Simulating its time evolution using quantum logic gates;
3. Extracting the approximate energy using the phase estimation algorithm.

Encoding Wave Function into Qubits

Basis Set

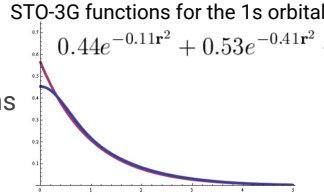
A set of functions (called basis functions) that is used to represent the electronic wave function in the Hartree–Fock method or density-functional theory in order to turn the partial differential equations of the model into algebraic equations suitable for efficient implementation on a computer.

Minimal Basis Sets

STO-3G, 3 Gaussian primitive functions comprising a single basis function.

STO-3G functions for the 1s orbital of a hydrogen atom

$$0.44e^{-0.11\mathbf{r}^2} + 0.53e^{-0.41\mathbf{r}^2} + 0.15e^{-2.23\mathbf{r}^2}$$



Encoding Wave Function into Qubits

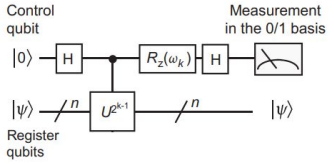
Six two-electron configurations

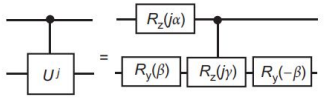
$$\{\Phi_i\}_{i=1}^{6} \rightarrow \{\Phi_1, \Phi_6\} \quad \{\Phi_2\} \quad \{\Phi_3, \Phi_4\} \quad \{\Phi_5\}$$

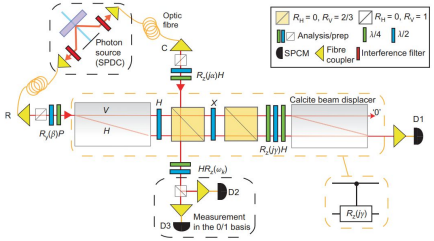
Finding the eigenvalues of the two 2×2 submatrices in the Hamiltonian, $H^{(1,6)}$ and $H^{(3,4)}$, is what we need.

Estimating the eigenvalues of 2×2 matrices is the simplest problem for the IPEA.

Experiment Design



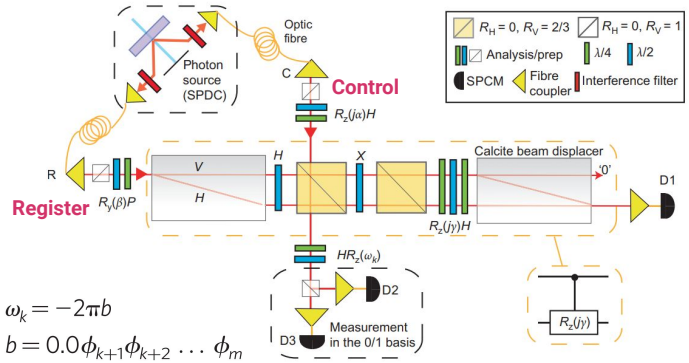




$$\hat{U} = e^{i\alpha}\hat{R}_y(\beta)\hat{R}_z(\gamma)\hat{R}_y(-\beta)$$

A series of rotations of the one-qubit Hilbert space.

Experiment Design



$\omega_k = -2\pi b$

$b = 0.0\phi_{k+1}\phi_{k+2}\dots\phi_m$

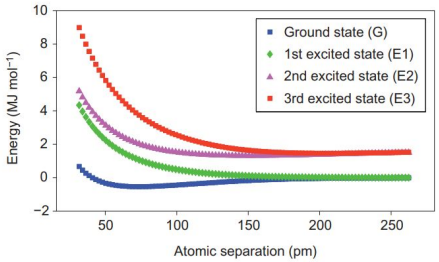
starting from the least significant (ϕ_m)

To produce an m-bit approximation to the phase of the eigenstate, we need to repeat this algorithm m times.

IF control horizontally polarized:
Nothing is changed
IF control vertically polarized:
$\hat{U}^{2^{k-1}}$ is implemented on the register

Problem to solve | Experiment | Influence

Result



Each point was calculated with a 20-bin iterative phase estimation algorithm, using n=31 samples per bit.

- Ground state (G) – Low Eigenvalue of $H^{(1,6)}$
- 1st excited state (E1) – Low Eigenvalue of $H^{(3,4)}$
- 2nd excited state (E2) – High Eigenvalue of $H^{(3,4)}$
- 3rd excited state (E3) – High Eigenvalue of $H^{(1,6)}$

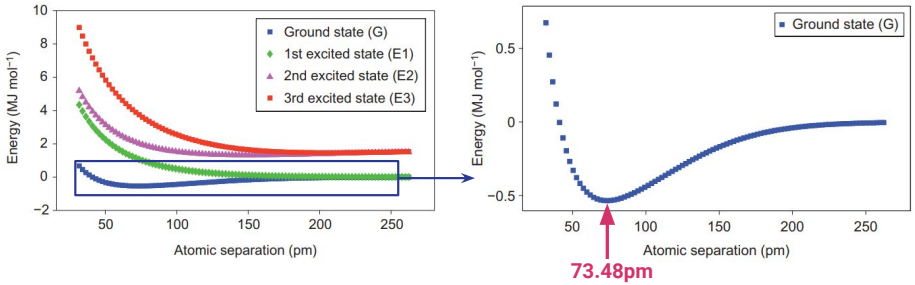
$$E = 2\pi\phi E_h + (e^2/4\pi\varepsilon R) - E_\infty$$

Proton-proton Coulomb energy at atomic separation R

Ground state energy of two hydrogen atoms at infinite separation

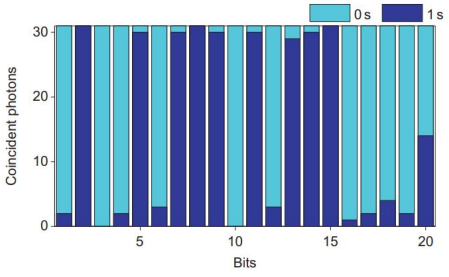
Problem to solve | Experiment | Influence

Result



Problem to solve | Experiment | Influence

Result



0.01001011101011100000

Equal to the exact value of minimal basis, to a precision of $\pm 2^{-20} E_h$

Impact

Previous Idea:

[1] Feynman, R.P. Simulating physics with computers. Int J Theor Phys 21, 467–488 (1982). https://doi.org/10.1007/BF02650179
[2] Lloyd, Seth. "Universal quantum simulators." Science (1996): 1073-1078.
[3] Abrams, Daniel S., and Seth Lloyd. "Simulation of many-body Fermi systems on a universal quantum computer." Physical Review Letters 79.13 (1997): 2586.

Previous Algorithm:

[1] Brown, Kenneth R., Robert J. Clark, and Isaac L. Chuang. "Limitations of quantum simulation examined by simulating a pairing Hamiltonian using nuclear magnetic resonance." Physical review letters 97.5 (2006): 050504.
[2] Somaroo, S., et al. "Quantum simulations on a quantum computer." Physical review letters 82.26 (1999): 5381.
[3] Yang, Xiaodong, et al. "Experimental simulation of a pairing Hamiltonian on an NMR quantum computer." Chemical physics letters 422.1-3 (2006): 20-24.
[4] Friedenauer, Axel, et al. "Simulating a quantum magnet with trapped ions." Nature Physics 4.10 (2008): 757-761.
[5] Gerritsma, Rene, et al. "Quantum simulation of the Dirac equation." Nature 463.7277 (2010): 68-71.

Experimentally proved the feasibility of quantum computer simulating particles.

Is it believable?

Yes.

Nature Chemistry

582 citations in 10 years.

Limitations

- 2-qubits quantum computer
- STO-3G H_2 model
- Non-scalable implementation of IPEA

Questions?