Nature Chemistry

# Towards Quantum Chemistry on a Quantum Computer

Lanyon BP, Whitfield JD, Gillett GG, Goggin ME, Almeida MP, Kassal I,
Biamonte JD, Mohseni M, Powell BJ, Barbieri M, Aspuru-Guzik A, White AG.

Presented by: Xuenan Wang

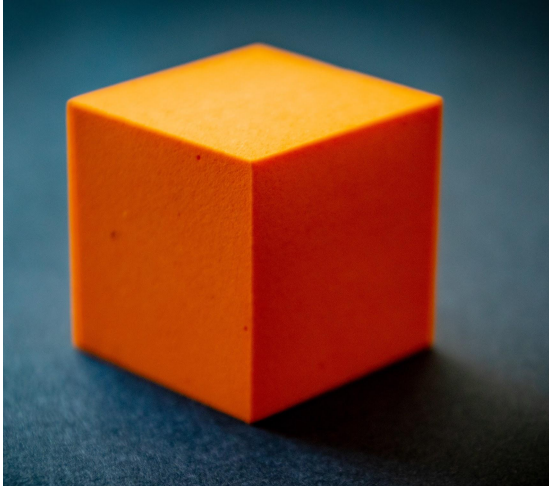# Outline

- Problem to solve

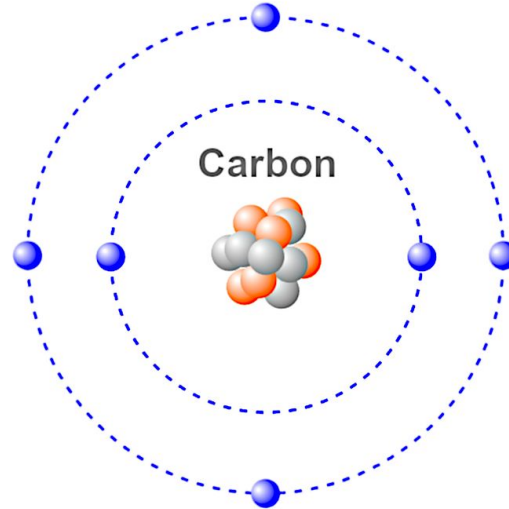- Experiment

- 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."

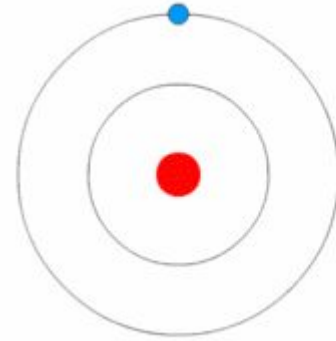# First Principles Calculations



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."
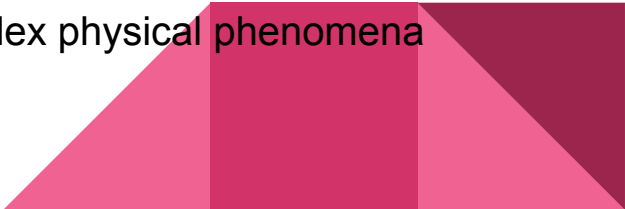


The Niels Bohr model of Hydrogen atom.

# 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.
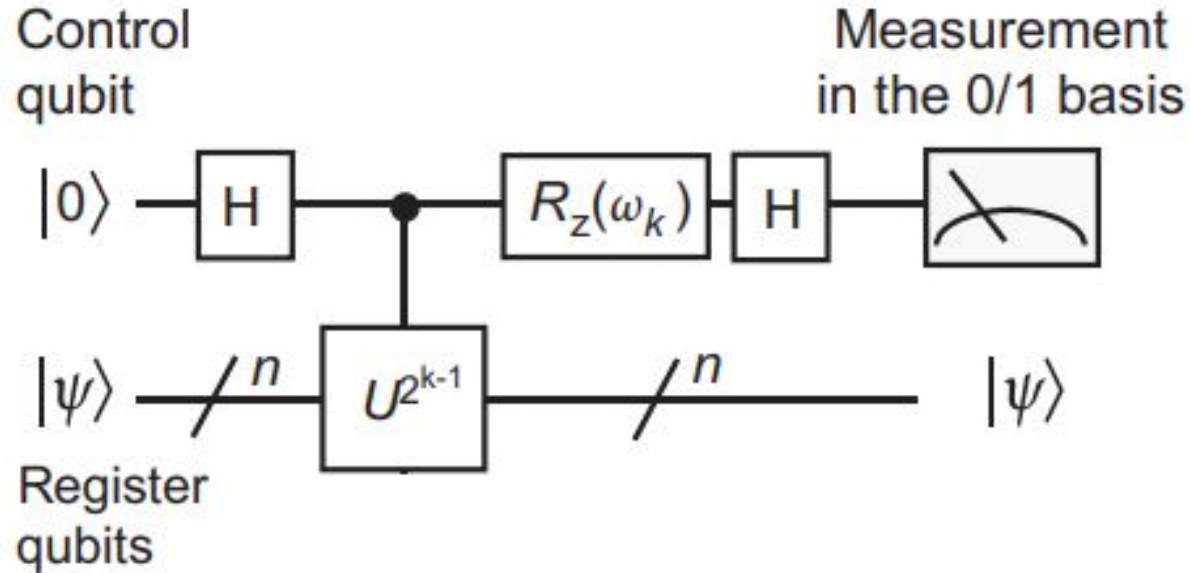
# First Principles Calculations

The Many-Electron Schrödinger Equation

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

**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.
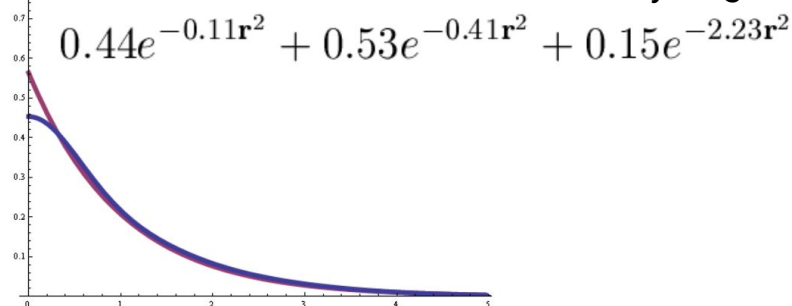
# Encoding Wave Function into Qubits

## 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

$$0.44e^{-0.11\mathbf{r}^2} + 0.53e^{-0.41\mathbf{r}^2} + 0.15e^{-2.23\mathbf{r}^2}$$
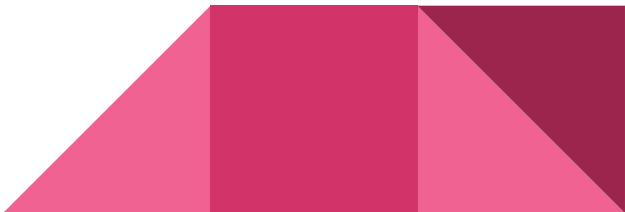
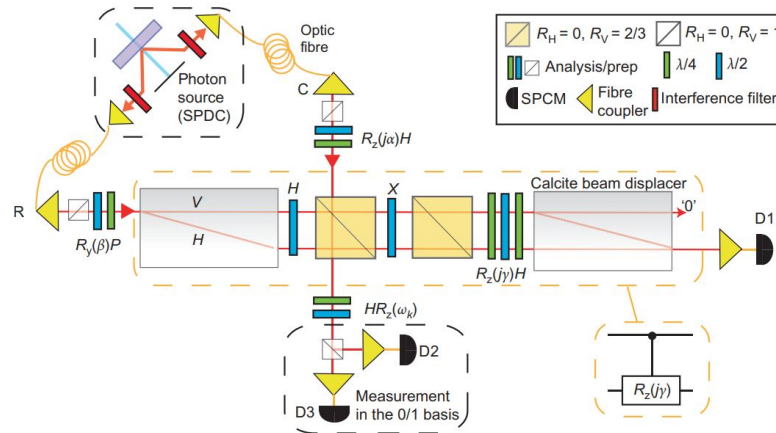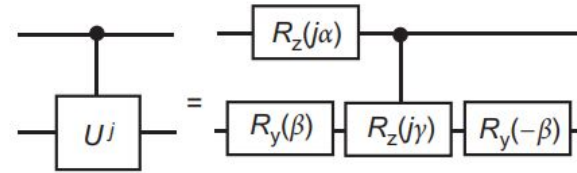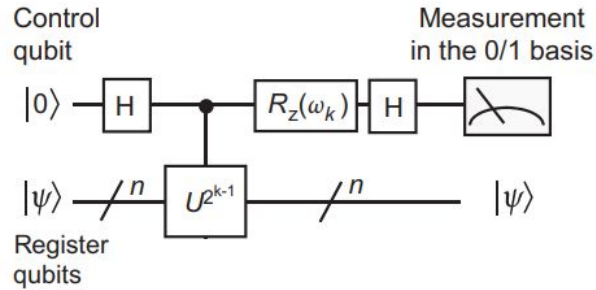# Encoding Wave Function into Qubits

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.

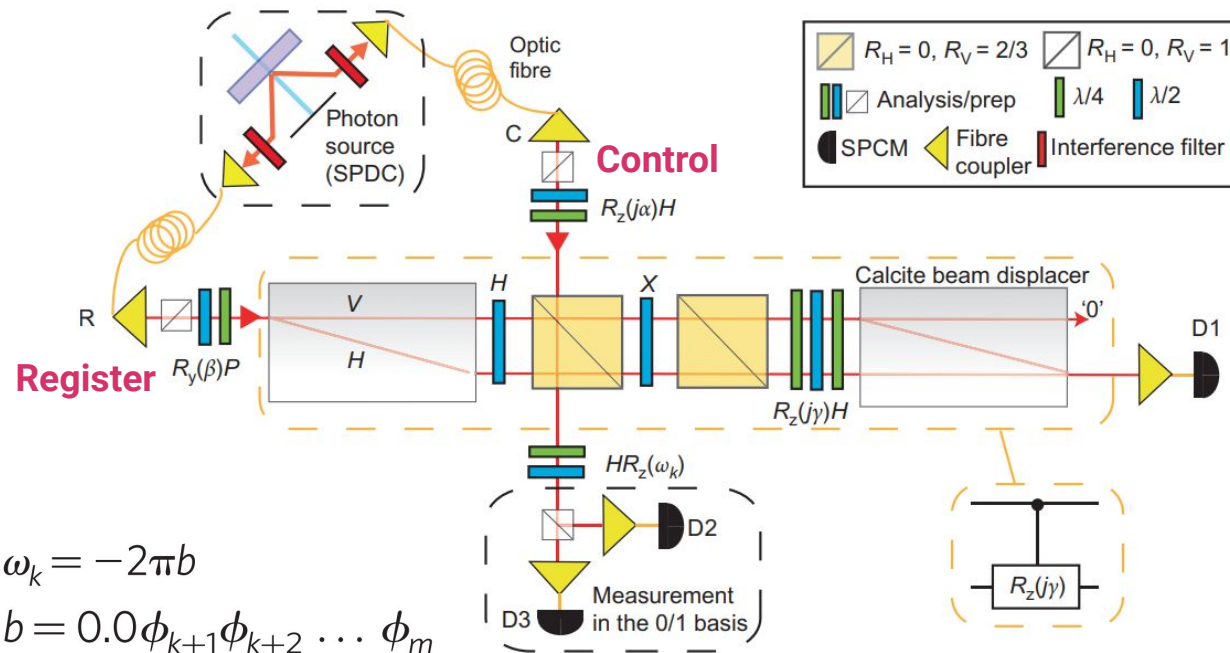Estimating the eigenvalues of 2×2 matrices is the simplest problem for the IPEA.

# 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



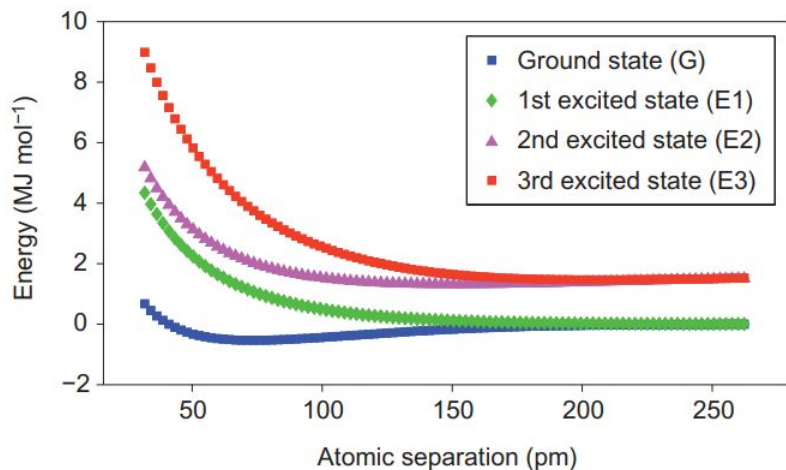To produce an m-bit approximation to the phase of the eigenstate, we need to repeat this algorithm m times.

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

$\omega_k = -2\pi b$

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

starting from the least significant ($\phi_m$)

# 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 $H^{(1,6)}$
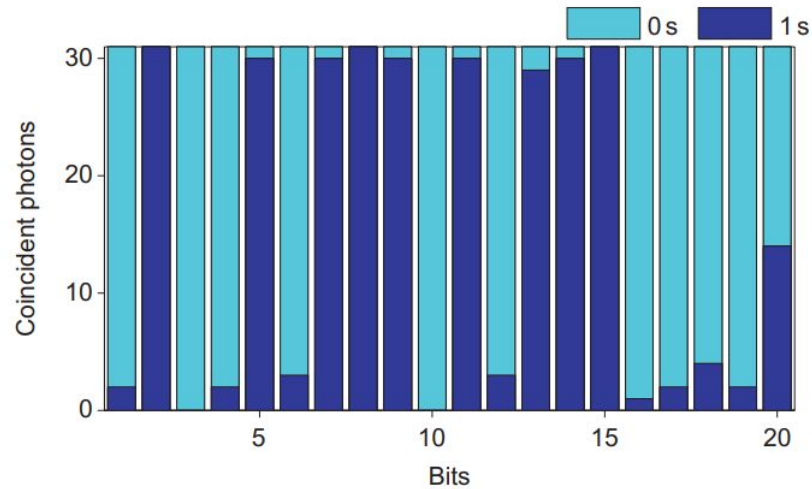
$$E = 2\pi\phi E_{\mathrm{h}} + (e^2/4\pi\varepsilon R) - E_{\infty}$$

Proton-proton
Coulomb energy
at atomic
separation R

Ground state energy of
two hydrogen atoms
at infinite separation

# Result



**73.48pm**

# Result
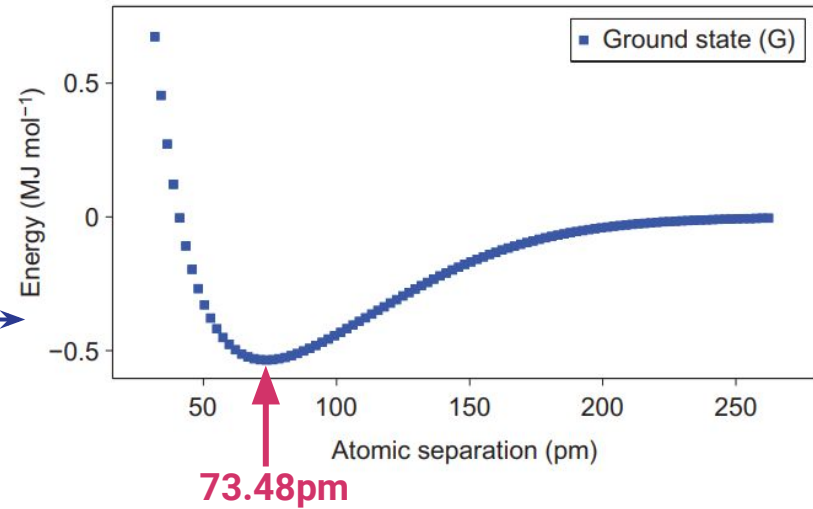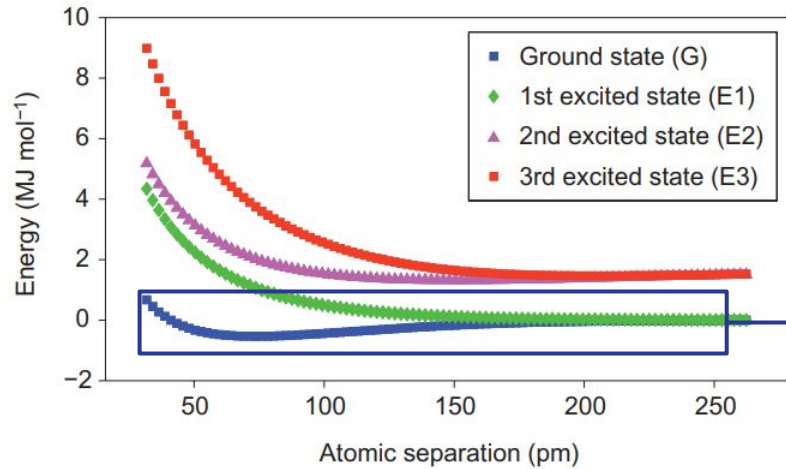


0.01001011101011100000

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?

Thank you