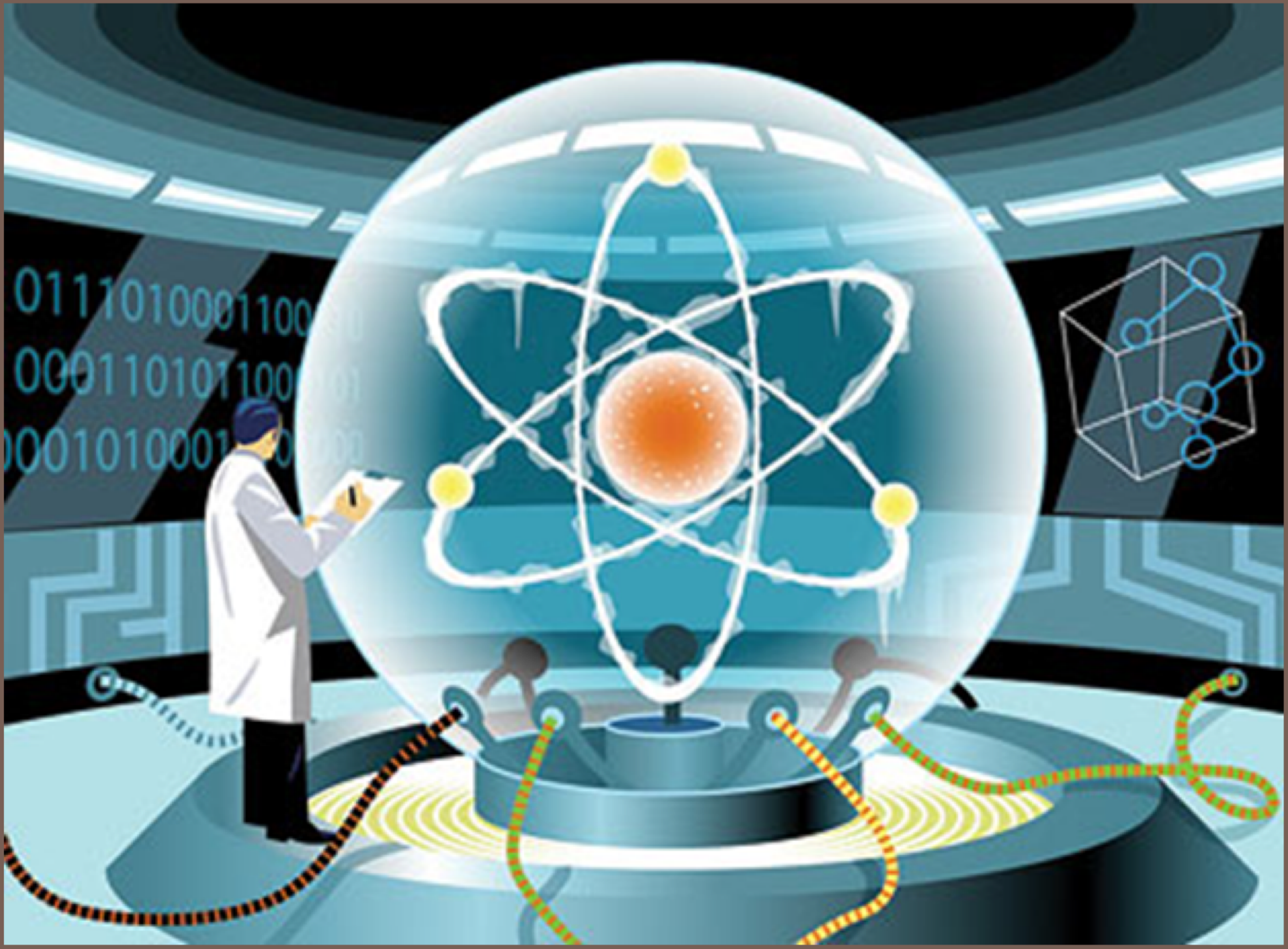

Variational Quantum Eigensolvers

Kenneth Brown, Duke University, ISCA 2018

Computational Challenge

Original Article

International Journal of
HIGH PERFORMANCE
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Scaling up Hartree–Fock calculations on Tianhe-2

Edmond Chow[1], Xing Liu[1], Sanchit Misra[2], Marat Dukhan[1], Mikhail Smelyanskiy[2], Jeff R. Hammond[2], Yunfei Du[3], Xiang-Ke Liao[3] and Pradeep Dubey[2]

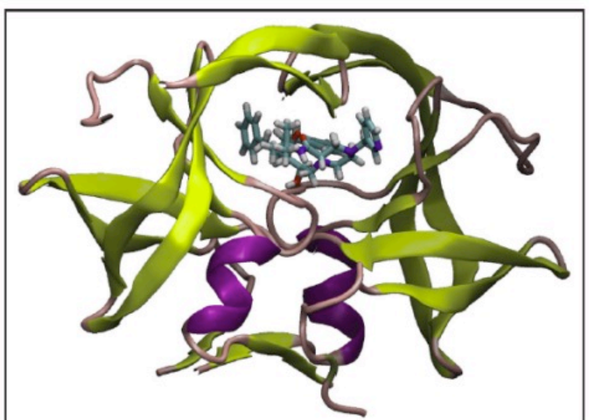


Figure 4. Indinavir bound to HIV-II protease (pdb code 1HSG).

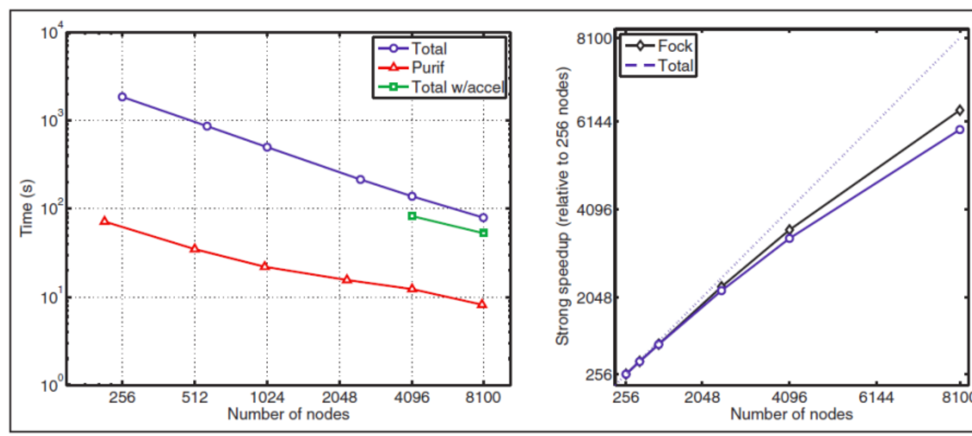
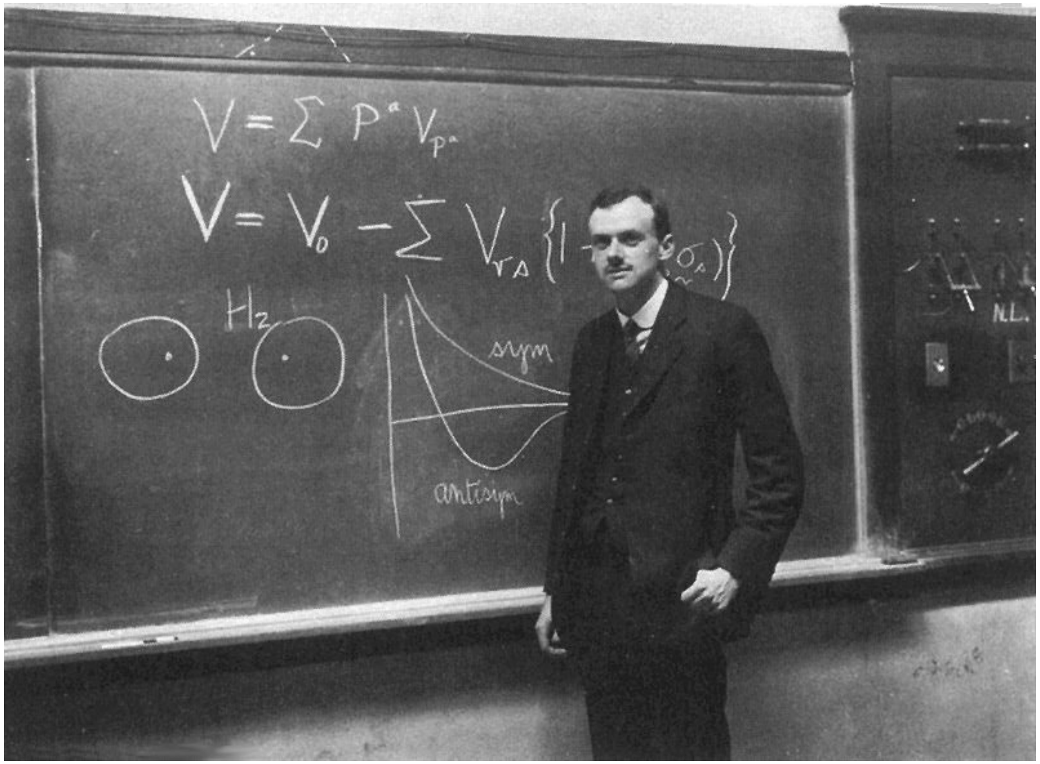


Figure 6. Timings and speedup for one SCF iteration for 1hsg_180 (27,394 basis functions) on Tianhe-2.

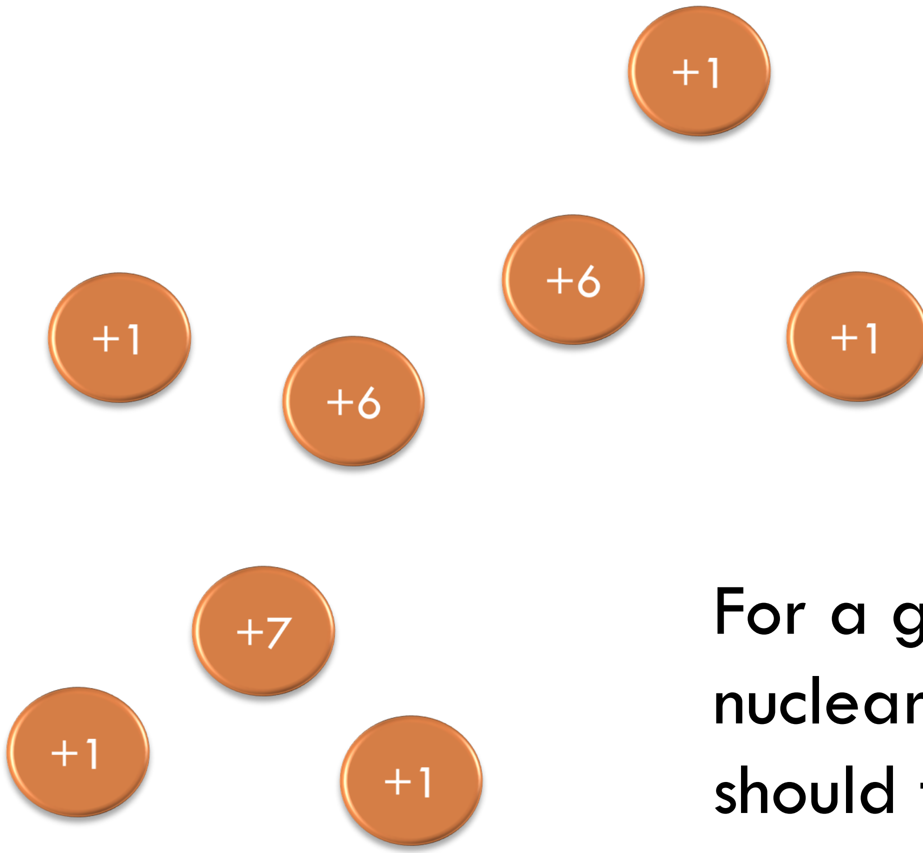
The problem with electrons



The underlying physical laws necessary for the mathematical theory of a large part of physics and the whole of chemistry are thus completely known, and the difficulty is only that the exact application of these laws leads to equations much too complicated to be soluble.

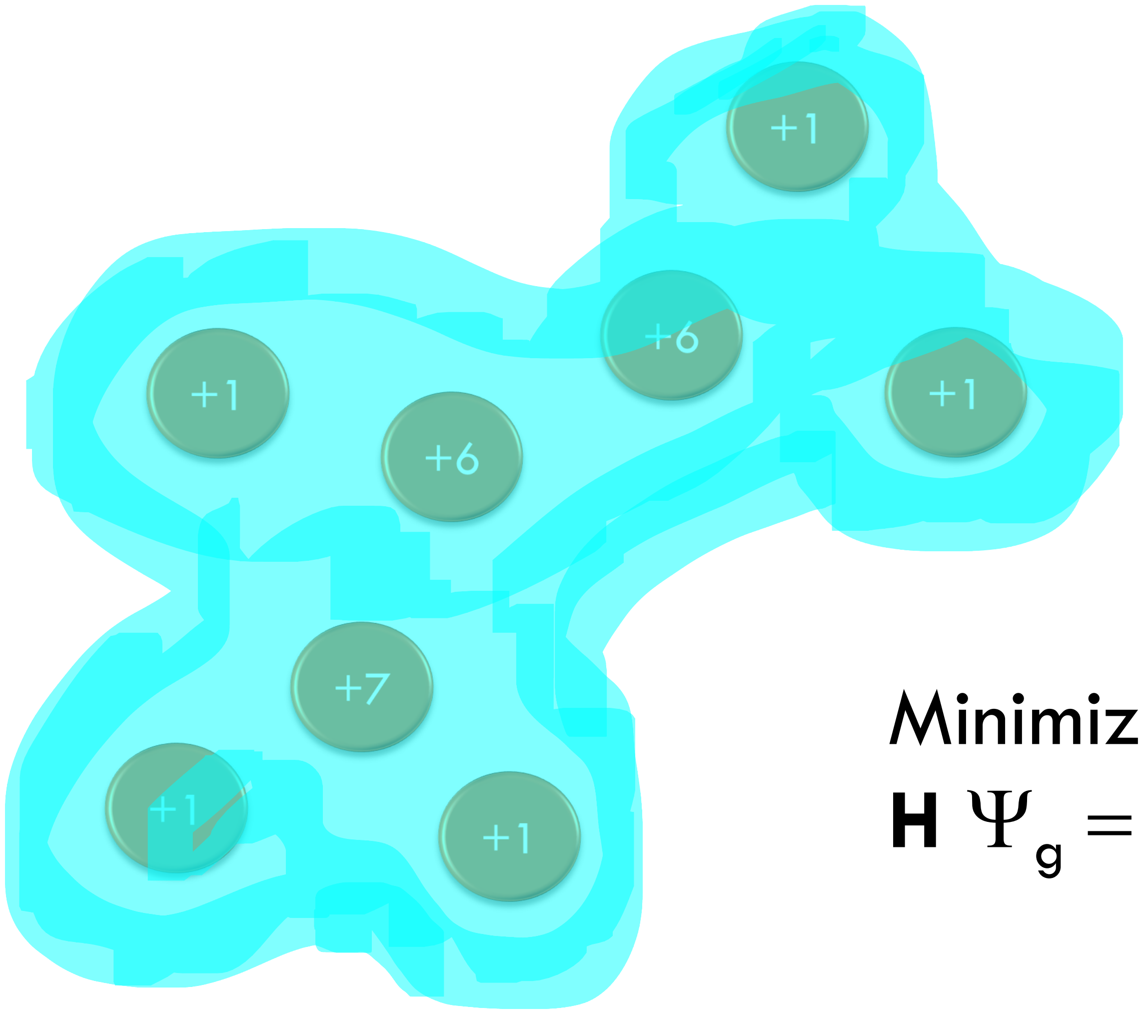
P.A.M. Dirac, Proc. R. Soc. A **123**, 714 (1929)

Where should the electrons go?



For a given location of nuclear charges, where should the electrons go?

Ground state wavefunction



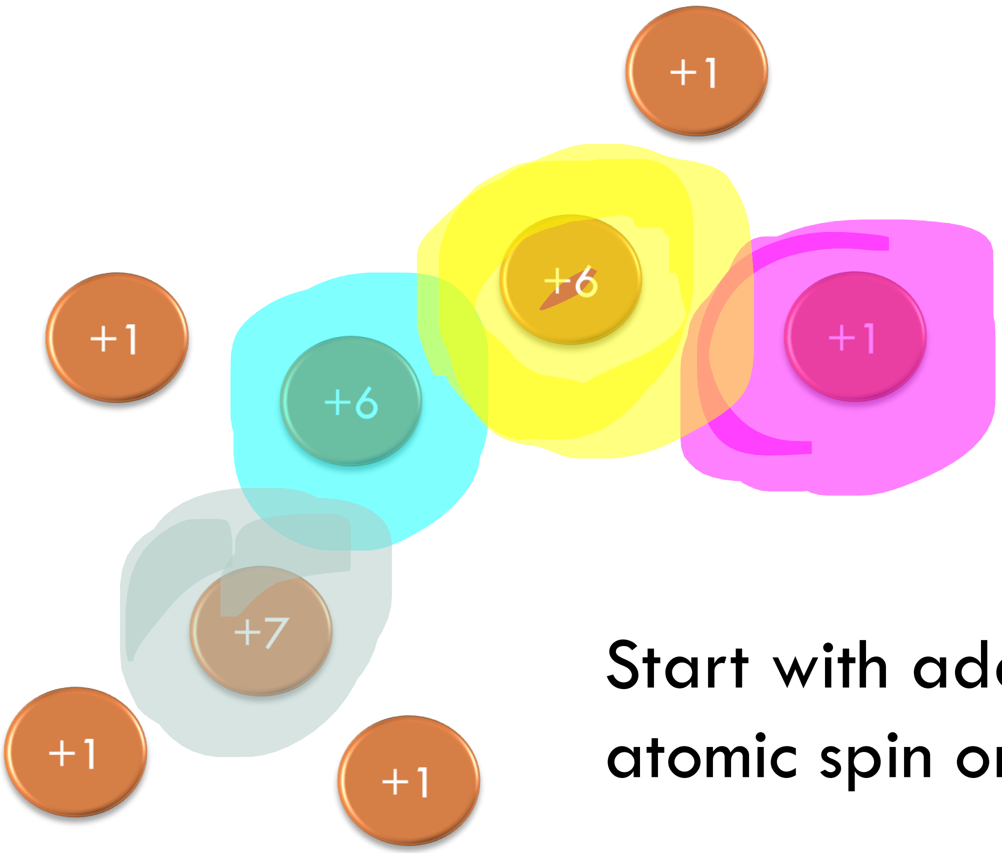
Minimize the energy

$$\mathbf{H}\,\Psi_g = E_g\,\Psi_g$$

Simple rules → Hard problem

- H is made from simple parts
  - Electrons have kinetic energy
  - Electrons repel each other
  - Electrons are attracted to nuclei
- Electrons have an additional property that if two switch addresses the wavefunction gains a – sign
  - Leads to Pauli exclusion principle
    - no two electrons have the same address
- How do we choose addresses?

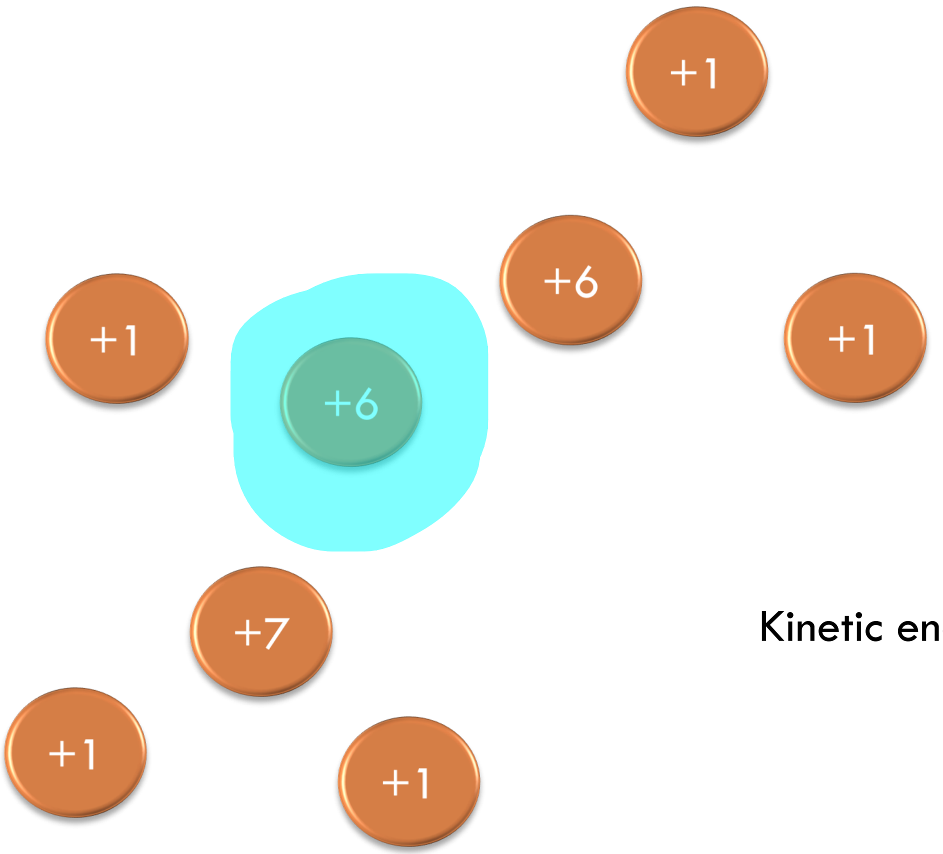
Start with something you know



Start with addresses we know, atomic spin orbitals.

Electrons hopping around

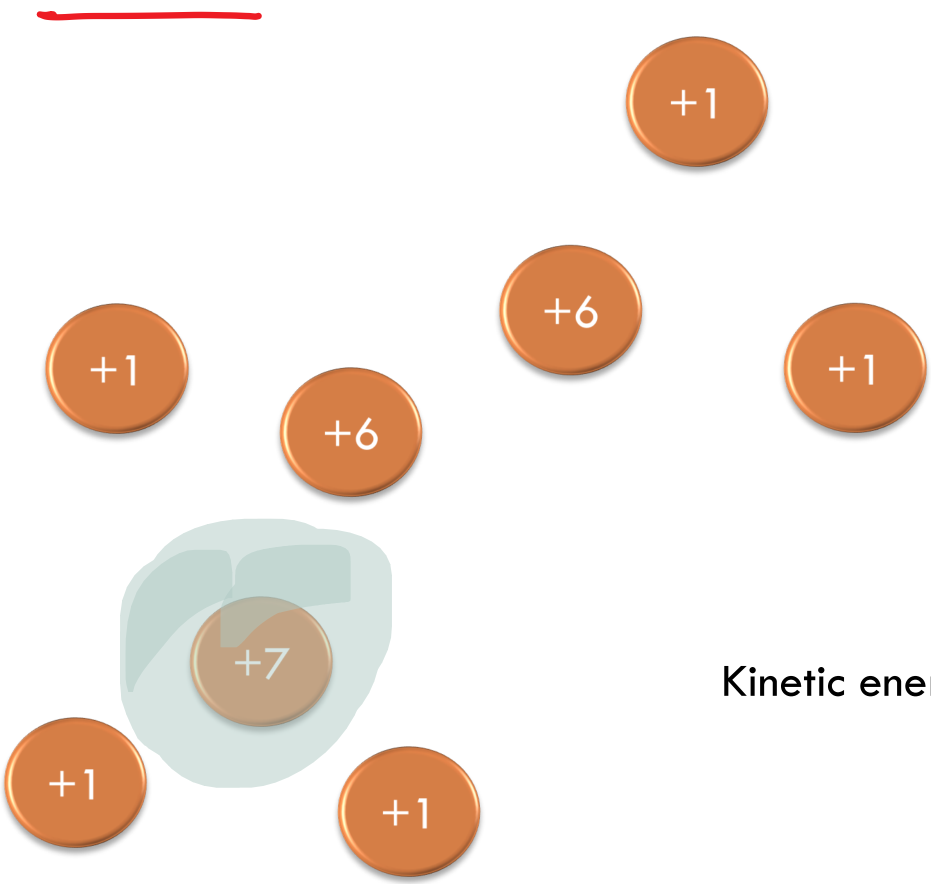
- $H = \sum h_{jk} b^{\dagger}_{j} b_{k} + \sum v_{jklm} b^{\dagger}_{j} b^{\dagger}_{k} b_{l} b_{m}$



Kinetic energy and attraction to nuclei

Electrons hopping around

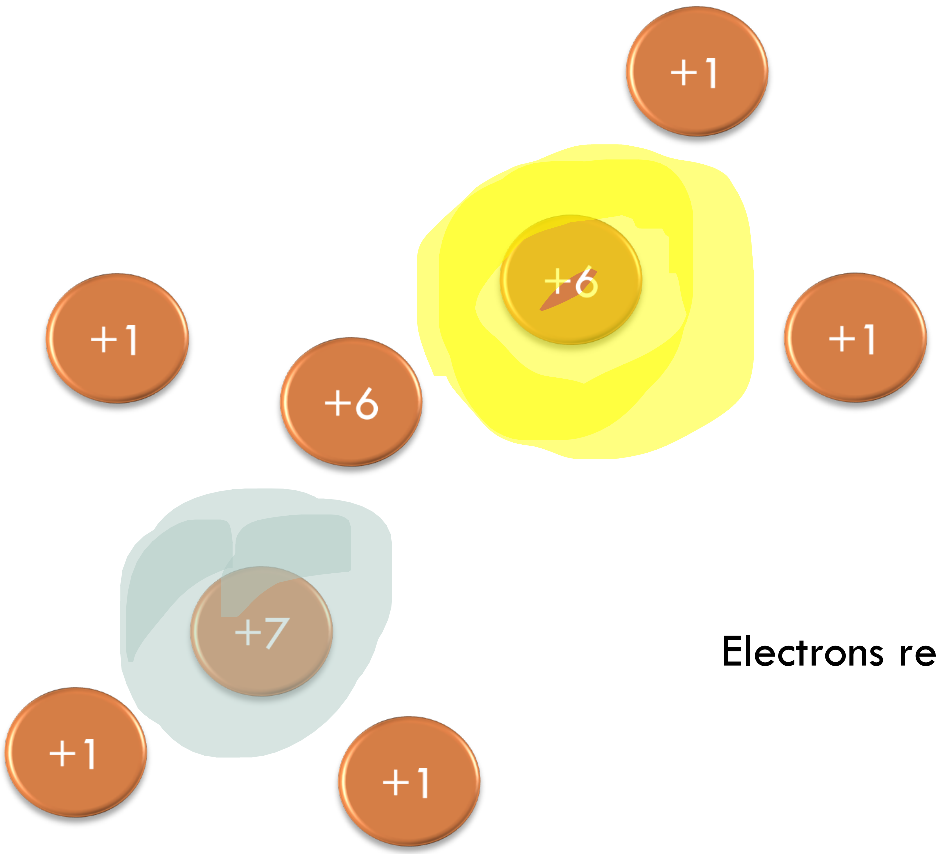
- $H = \sum h_{jk} b^\dagger_j b_k + \sum v_{jklm} b^\dagger_j b^\dagger_k b_l b_m$



Kinetic energy and attraction to nuclei

Electrons hopping around

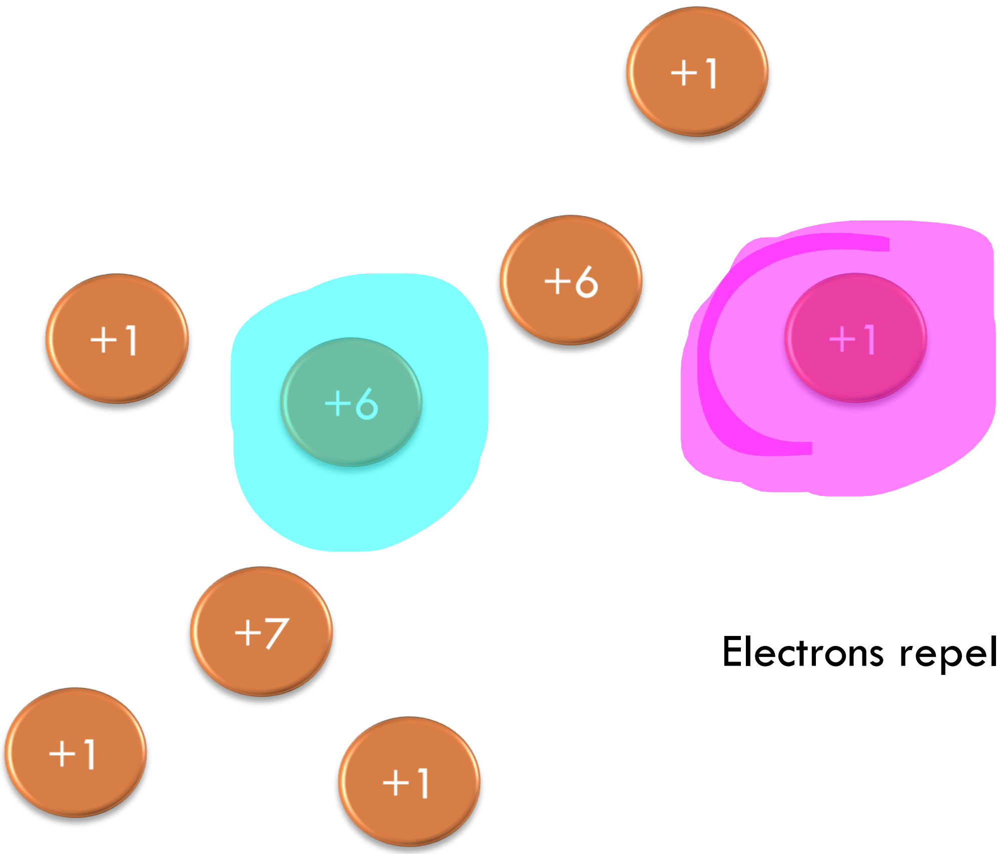
- $H = \sum h_{jk}\, b^\dagger_j c_k + \sum v_{jklm}\, b^\dagger_j b^\dagger_k b_l b_m$



Electrons repelling each other

Electrons hopping around

- $H= \sum h_{jk} b^{\dagger}_{j} b_{k} + \sum v_{jklm} b^{\dagger}_{j} b^{\dagger}_{k} b_{l} b_{m}$



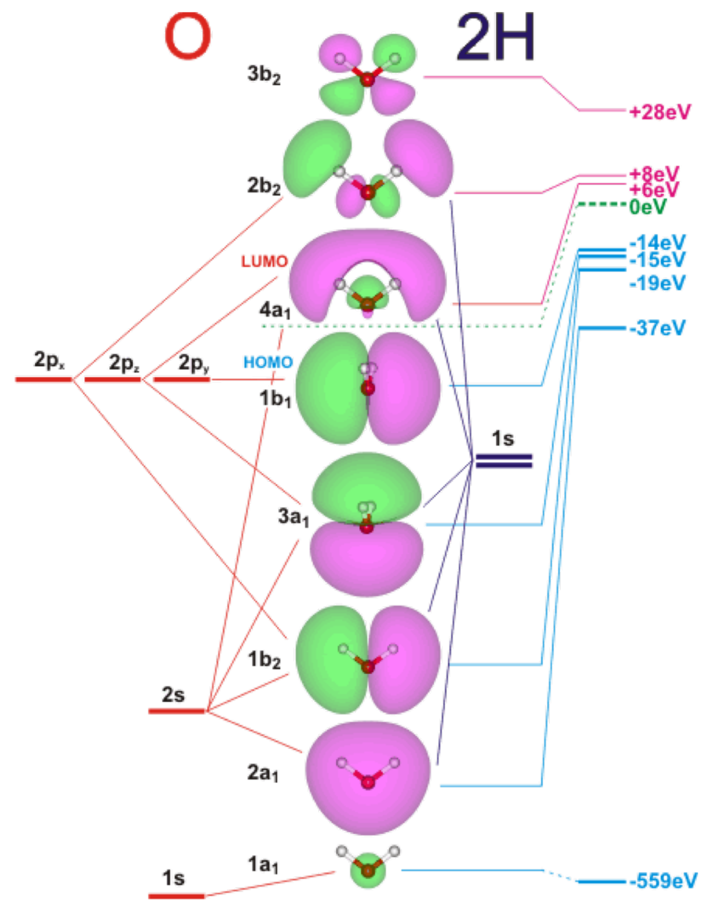
Electrons repelling each other

Good news and bad news

- Good news:
  - For m addresses only $m^4 + m^2$ terms in H
- Bad news:
  - For n electrons, there are m!/(n!)(m-n!) possible “classical” configurations
  - True ground state is described by superposition over all of these configurations: $\Psi_g = \Sigma c_k \phi_k$
- Mixed news:
  - While many molecules can be well approximated by a superposition over a small number of classical configurations, important classes of molecules and materials, such as catalysts and high T_c superconductors, cannot.

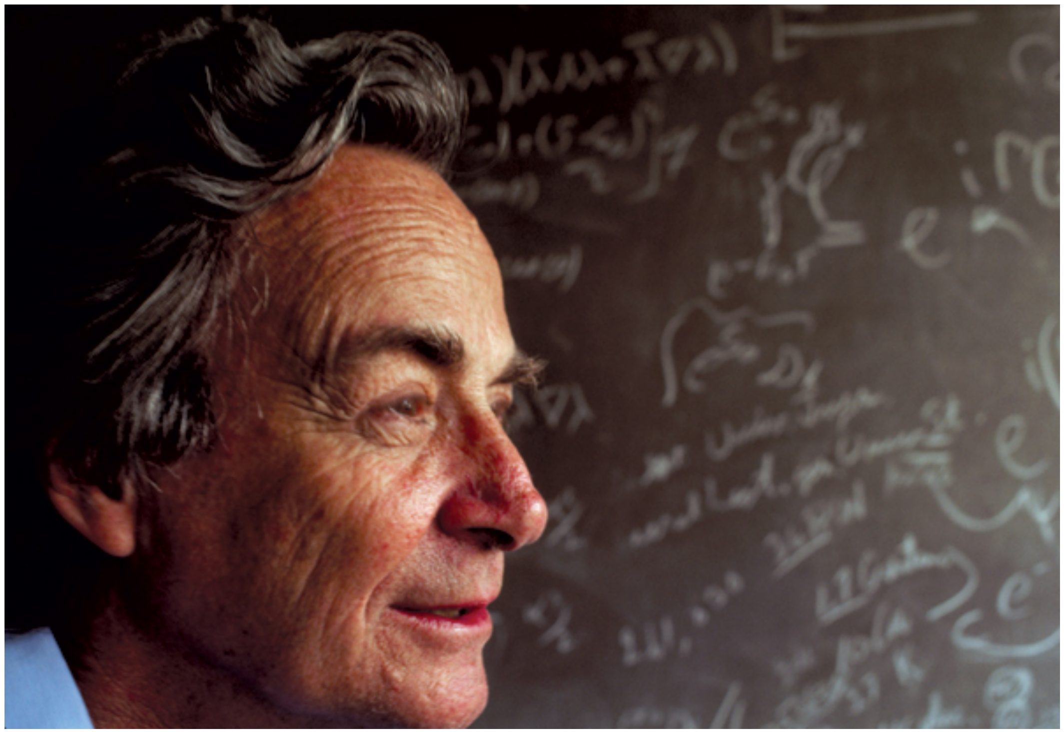
Molecules

- Water H_2O
- 2+6+2 electrons
- How many addresses?
  - **Simplest model: 14**
  - 3003 states
  - **cc-pVTZ model: 116**
  - 8×10^{23} states



- Classical Computer
  - Uses $>k^n$ electrons to represent the exact state of n electrons
- Molecule
  - Uses n electrons to represent n electrons

Disruptive Idea



"Let the computer itself be built of quantum mechanical elements which obey quantum mechanical laws."

R. Feynman, *Int. J. Theor. Phys.* **21**, 467 (1982)

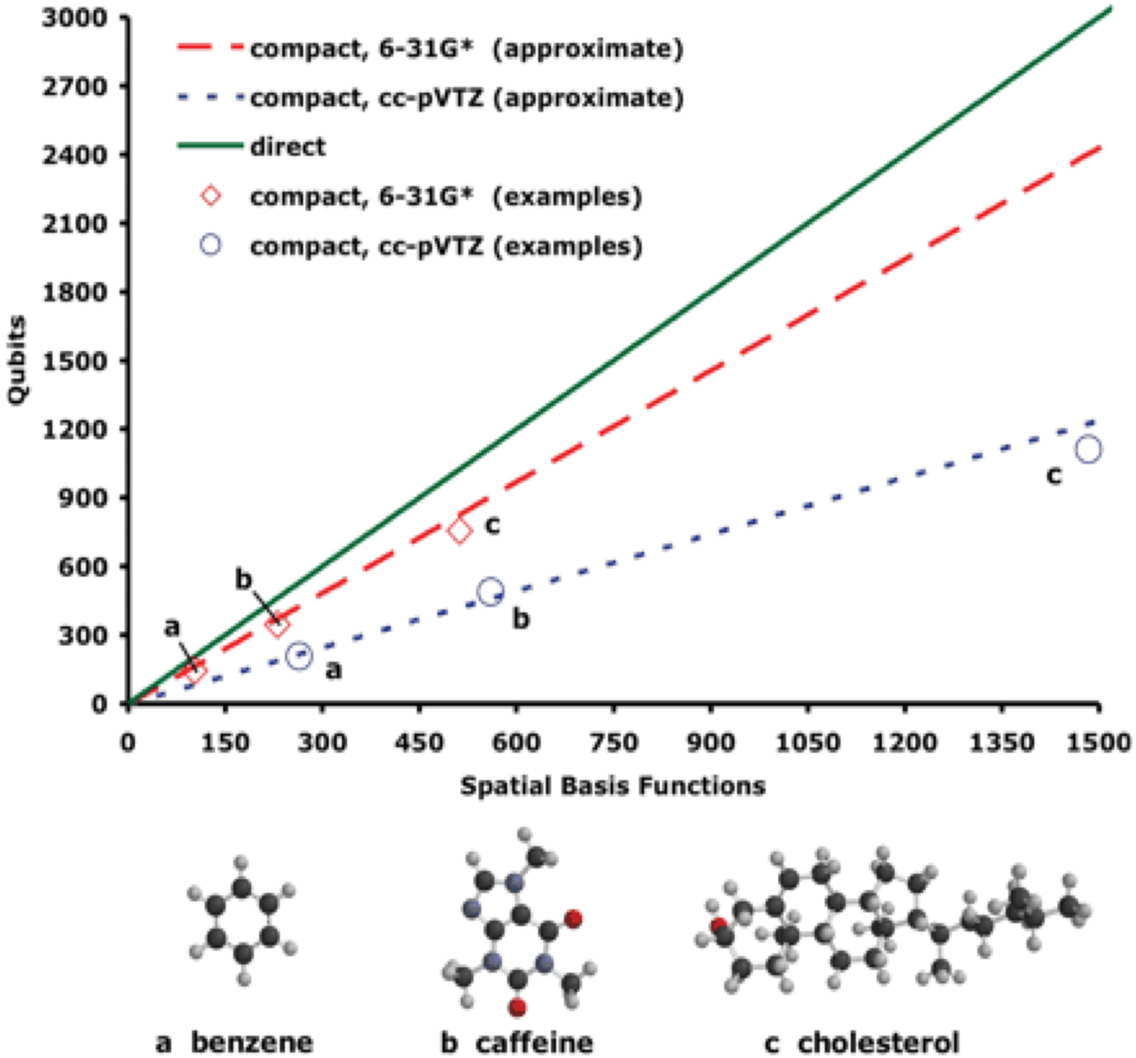
Extremely Disruptive Idea

N=PQ

Factoring numbers breaks the RSA encryption scheme.
Makes the internet even less safe. (HTTPS, etc.)

P.W. Shor, *Proc. of 35th FOCS*, 124 (1994)

Ground State Energy Estimation



D.S. Abrams and S. Lloyd,
Phys. Rev. Lett. **83**, 5162 (1999).

A. Aspuru-Guzik, A. Dutoi,
P. Love, and M. Head-Gordon
Science **309**, 1704 (2005).

Chemistry on a QC
Configurations are cheap

- Classical Computer
  - Uses >k^n electrons to represent the exact state of n electrons
- Molecule
  - Uses n electrons to represent n electrons
- Quantum Computer
  - Uses kn electrons to represent n electrons

Mapping Electrons to Qubits

$$\mathbf{H} = \sum_{p,q} h_{p,q} b_p^\dagger b_q + \sum_{p,q,r,s} h_{p,q,r,s} b_p^\dagger b_q^\dagger b_r b_s$$

- Jordan-Wigner

$$b_p^\dagger = (X - iY)_p Z_{p+1} Z_{p+2} Z_{p+3} \ldots Z_{n-1} Z_n$$

$$b_p^\dagger b_q + b_q^\dagger b_p = X_p Z_{p+1} \ldots Z_{q-1} X_q + Y_p Z_{p+1} \ldots Z_{q-1} Y_q$$

- Other maps (Bravyi-Kitaev, parity maps, ..)

Algorithms

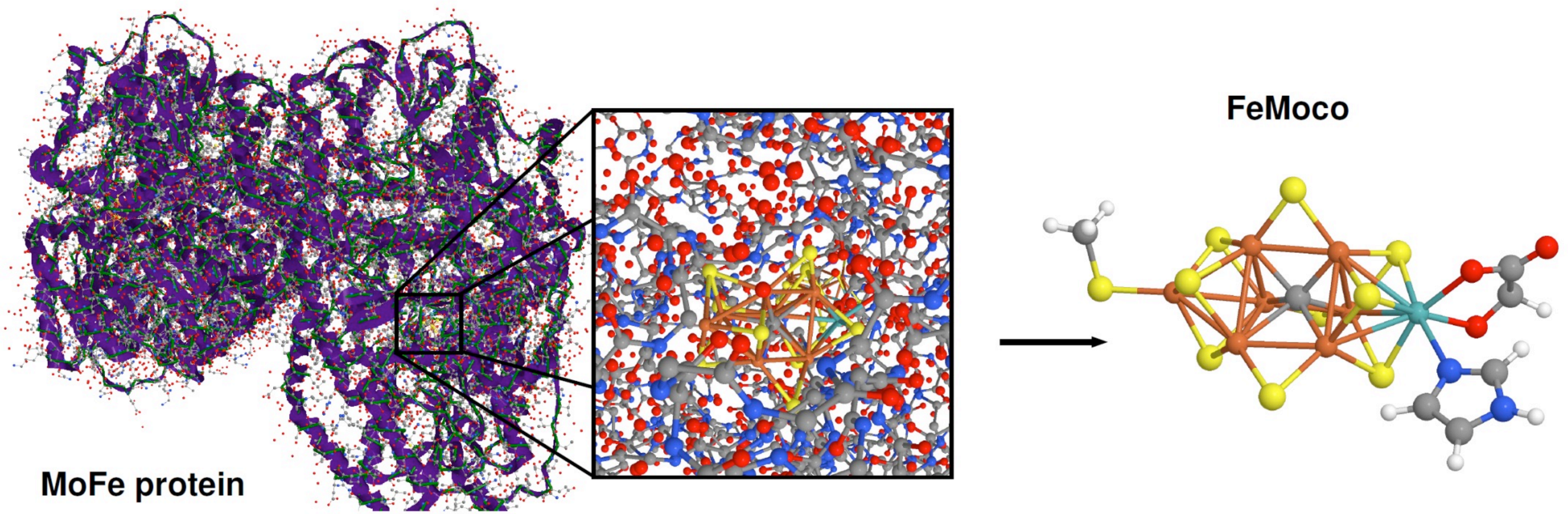
- **Quantum Phase Estimation**
  - Requires state preparation
  - **Measures the energy by applying controlled dynamics and using Quantum Fourier Transform to yield energy**
    - *Measurement circuit depth: Polynomial in the problem size*
  - Projects state to an eigenstate of the dynamics
- **Variational Quantum Eigensolver**
  - Requires state preparation
  - **Measures energy term by term**
    - *Measurement circuit depth: Constant in the problem size*
  - Update state preparation to minimize energy

QPE: Cost of generating U

Year	Reference	Basis	Algorithm	Oracle T Gates	PEA Queries	Total T Gates
2005	Aspuru-Guzik *et al.* [7]	Gaussians	Trotterization	$\mathcal{O}(\text{poly}(N/\epsilon))$	$\mathcal{O}(\text{poly}(N/\epsilon))$	$\mathcal{O}(\text{poly}(N/\epsilon))$
2010	Whitfield *et al.* [37]	Gaussians	Trotterization	$\mathcal{O}\left(N^4 \log\left(1/\epsilon\right)\right)$	$\mathcal{O}\left(\text{poly}\left(N/\epsilon\right)\right)$	$\mathcal{O}\left(\text{poly}\left(N/\epsilon\right)\right)$
2013	Wecker *et al.* [38]	Gaussians	Trotterization	$\mathcal{O}\left(N^4 \log\left(1/\epsilon\right)\right)$	$\mathcal{O}\left(N^6/\epsilon^{3/2}\right)$	$\mathcal{O}\left(\frac{N^{10}\log(1/\epsilon)}{\epsilon^{3/2}}\right)$
2014	McClean *et al.* [39]	Gaussians	Trotterization	$\mathcal{O}\left(\sim N^2 \log\left(1/\epsilon\right)\right)$	$\mathcal{O}\left(N^6/\epsilon^{3/2}\right)$	$\mathcal{O}\left(\sim \frac{N^{8}\log(1/\epsilon)}{\epsilon^{3/2}}\right)$
2014	Poulin *et al.* [40]	Gaussians	Trotterization	$\mathcal{O}\left(N^4 \log\left(1/\epsilon\right)\right)$	$\mathcal{O}\left(\sim N^2/\epsilon^{3/2}\right)$	$\mathcal{O}\left(\sim \frac{N^{6}\log(1/\epsilon)}{\epsilon^{3/2}}\right)$
2014	Babbush *et al.* [41]	Gaussians	Trotterization	$\mathcal{O}\left(N^4 \log\left(1/\epsilon\right)\right)$	$\mathcal{O}\left(\sim N/\epsilon^{3/2}\right)$	$\mathcal{O}\left(\sim \frac{N^{5}\log(1/\epsilon)}{\epsilon^{3/2}}\right)$
2015	Babbush *et al.* [42]	Gaussians	Taylorization	$\widetilde{\mathcal{O}}(N)$	$\mathcal{O}\left(\frac{N^4\log(N/\epsilon)}{\epsilon\log\log(N/\epsilon)}\right)$	$\widetilde{\mathcal{O}}(N^5/\epsilon)$
2016	Low *et al.* [25]	Gaussians	Qubitization	$\widetilde{\mathcal{O}}\left(N\right)$	$\mathcal{O}\left(\frac{N^4}{\epsilon} + \frac{\log(N/\epsilon)}{\epsilon\log\log(N/\epsilon)}\right)$	$\widetilde{\mathcal{O}}\left(N^5/\epsilon\right)$
2017	Babbush *et al.* [43]	Plane Waves	Taylorization	$\widetilde{\mathcal{O}}\left(N\right)$	$\mathcal{O}\left(\frac{N^{8/3}\log(N/\epsilon)}{\epsilon\log\log(N/\epsilon)}\right)$	$\widetilde{\mathcal{O}}(N^{11/3}/\epsilon)$
2017	Berry *et al.* [26]	Plane Waves	Qubitization	$\widetilde{\mathcal{O}}\left(N\right)$	$\mathcal{O}(N^{8/3}/\epsilon)$	$\widetilde{\mathcal{O}}(N^{11/3}/\epsilon)$
2018	Kivlichan *et al.* [44]	Plane Waves	Trotterization	$\mathcal{O}\left(N^2 + N\log N\log\left(1/\epsilon\right)\right)$	$\mathcal{O}\left(\sim N^{3/2}/\epsilon^{3/2}\right)$	$\mathcal{O}\left(\sim N^{7/2}/\epsilon^{3/2}\right)$
2018	This paper	Plane Waves	Qubitization	$\mathcal{O}\left(N + \log\left(1/\epsilon\right)\right)$	$\mathcal{O}\left(N^2/\epsilon\right)$	$\mathcal{O}\left(\frac{N^3+N^2\log(1/\epsilon)}{\epsilon}\right)$

Babbush et al. arXiv:1805.03662

Chemistry Application



Estimated number of gates for QPE: 10^{15}

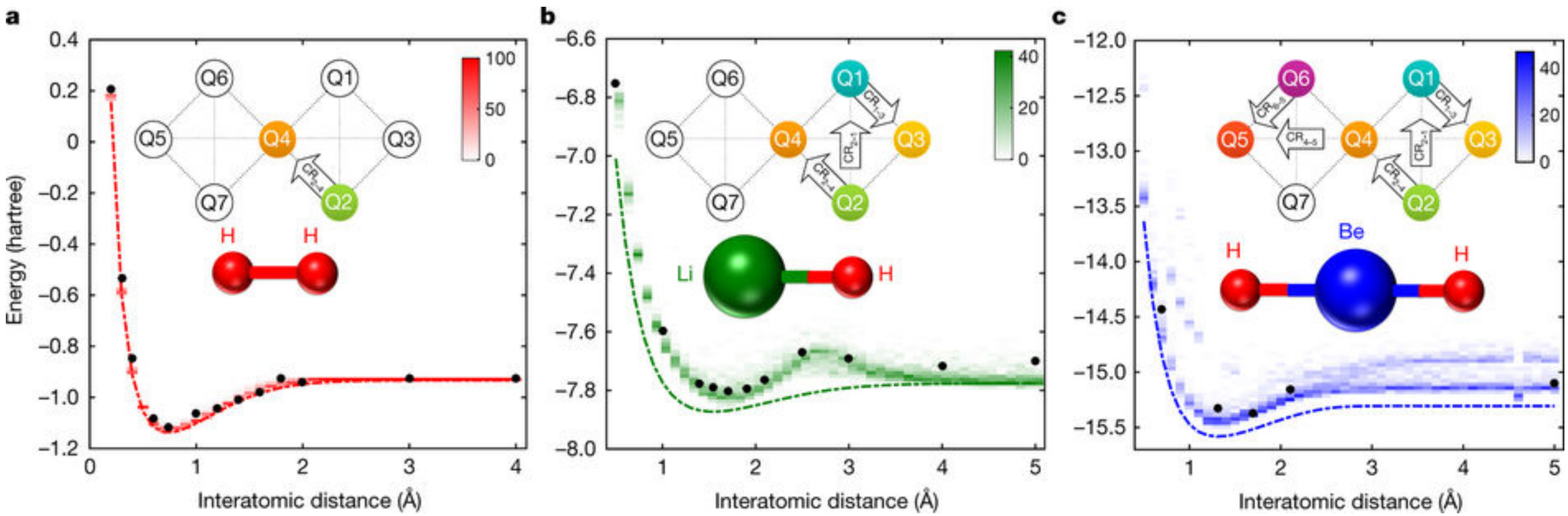
M. Reiher et al. PNAS **114**, *7555* (2017)

New methods: ~10^{12}

Current number of gates: 10^3

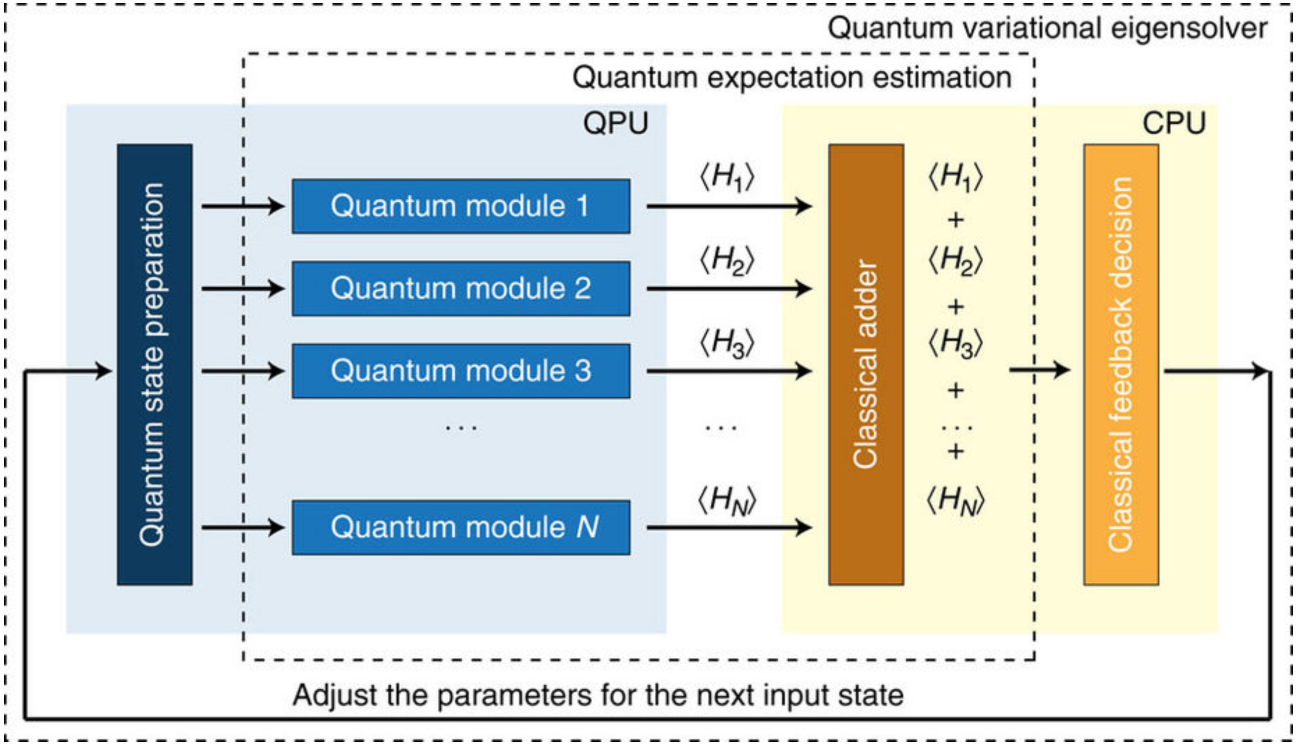
Based on error rate of 10^{-3}

Where is the field now?



IBM Superconductors: A. Kandala et al. Nature **549**, 242 (2017)

Variational Quantum Eigensolver



1. Start with a wavefunction ansatz
2. Minimize the sum of terms individually

Peruzzo et al. Nat. Commun. **5**, 4213 (2014)

Advantage: Smaller depth circuits

Disadvantage: Accuracy limited by sampling, no projection to the ground state

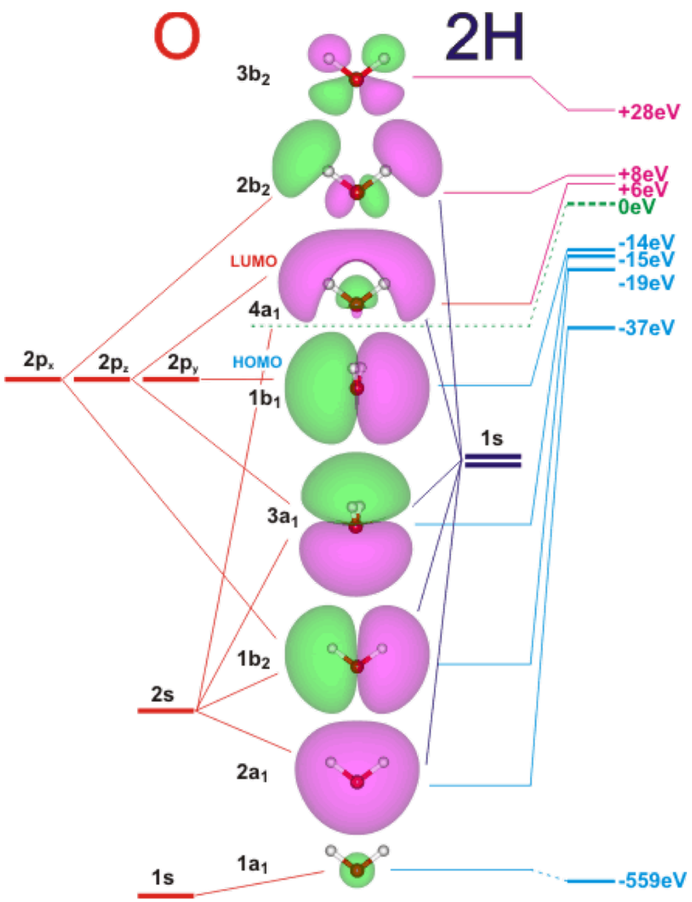
Unitary Coupled Cluster

$$|\Psi\rangle = e^{T-T^\dagger}|\Phi\rangle_{\text{ref}}$$

$$T = T_1 + T_2 + T_3 + \dots + T_N$$

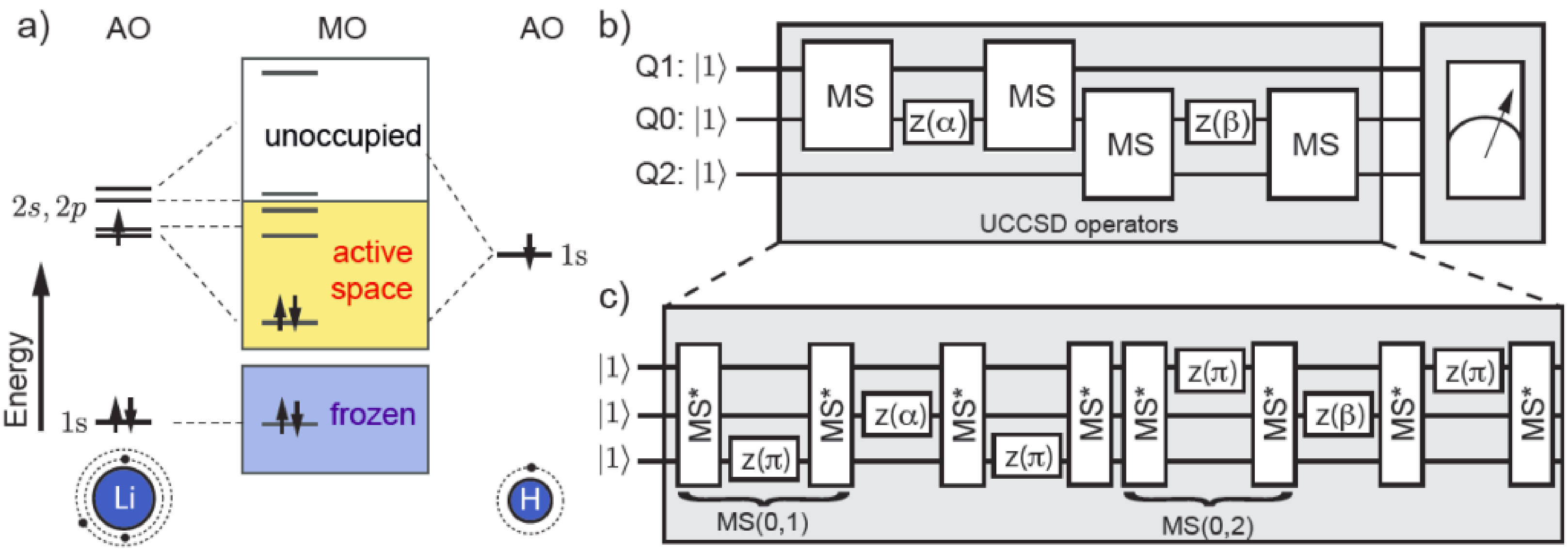
$$T_1 = \sum_{p,q} t_{p,q} b_p^\dagger b_q$$

$$T_2 = \sum_{p,q} t_{p,q,r,s} b_p^\dagger b_q^\dagger b_r b_s$$



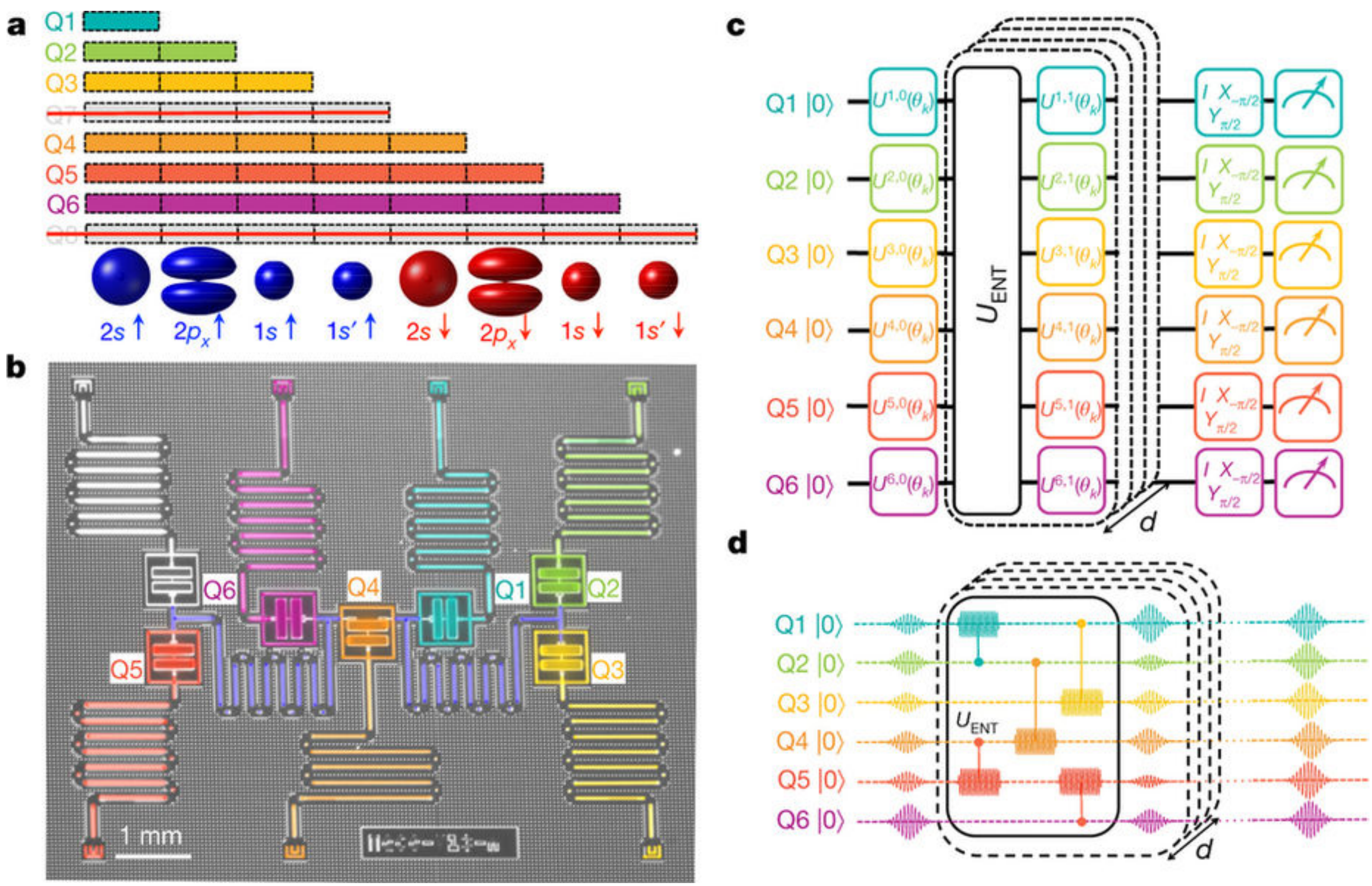
Peruzzo et al. Nat. Commun. **5**, 4213 (2014)

Ion Trap Implementation



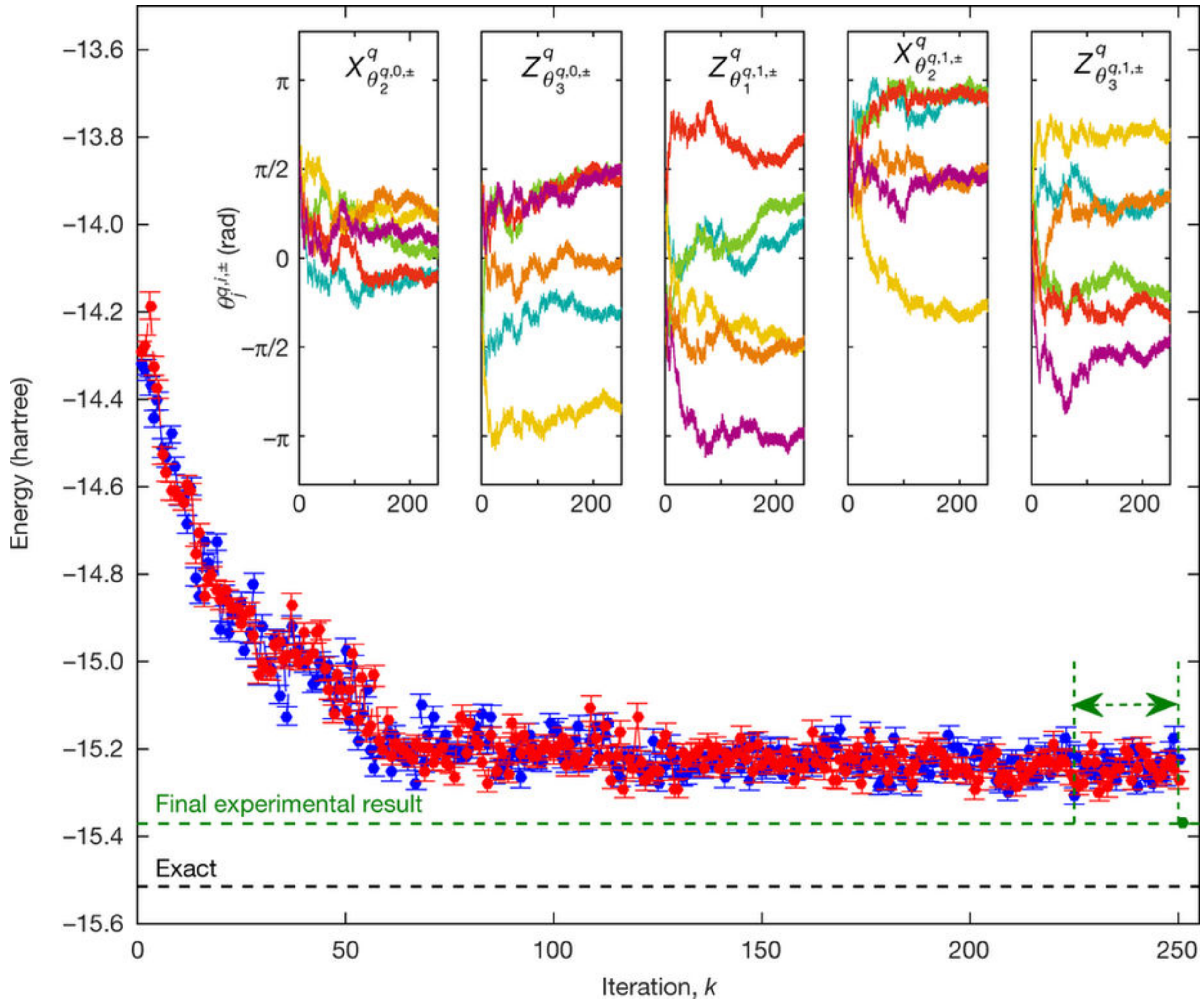
Hempel et al. arXiv:1803.10238

Machine Ansatz



A. Kandala et al. Nature **549**, 242 (2017)

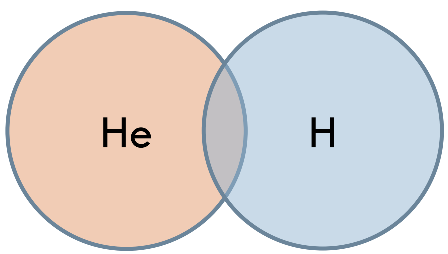
Example of convergence



A. Kandala et al. Nature **549,** 242 (2017)

State Space Reduction

HeH^+



4 spin-orbitals:

Is electron on He or H?

Is electron spin up or down?

4 qubits

Occupation of orbitals |He↑,He↓,H↑,H↓>

3 qubits

Hamiltonian preserves number of electrons and we are interested in the 2 electron problem.

Reduces to 6 states

|1100>,|1010>,|1001>,

|0110>,|0110>,|0011>

2 qubits

Hamiltonian preserves total spin and we are interested in one spin up and one spin down.

Reduces to 4 states

|1100>,|1001>, |0110>, |0011>