

# Higher-efficiency quantum algorithms for simulation of chemistry

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Annie Wei, Dean Southwood, Peter J. Love, Alán Aspuru-Guzik

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# Basis of talk

Second-quantized chemistry:

R. Babbush, D. W. Berry, **Ian D. Kivlichan**, A. Y. Wei, P. J. Love and A. Aspuru-Guzik, *New Journal of Physics* **18**, 033032, arXiv:1506.01020 (2016)

Configuration interaction:

R. Babbush, D. W. Berry, **Ian D. Kivlichan**, A. Y. Wei, P. J. Love and A. Aspuru-Guzik, arXiv:1506.01029 (2015)

# Overview

## 1 Why chemistry?

- What chemistry problem are we solving?
- Why should you care?

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- The integrals that appear (and a trick to evaluate integrals exponentially faster on a quantum computer)

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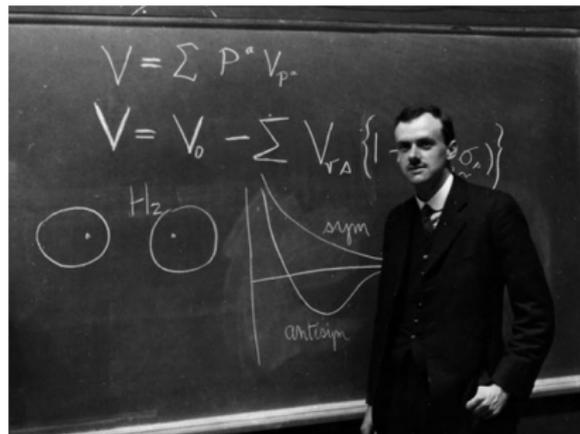
- The integrals that appear (and a trick to evaluate integrals exponentially faster on a quantum computer)

## 4 New quantum algorithm for chemistry simulation in configuration interaction

- Sparsity of the chemistry Hamiltonian and a 1-sparse coloring

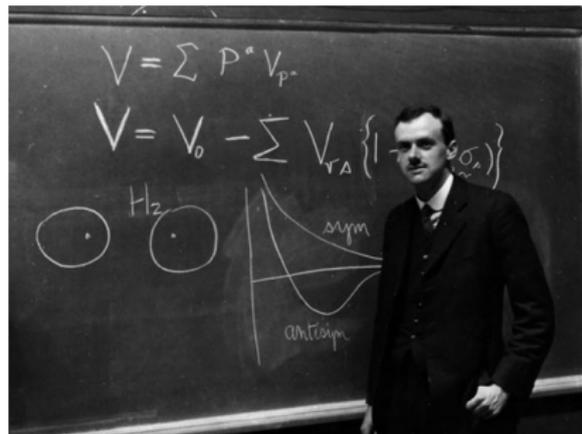
# The electronic structure problem

The 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.



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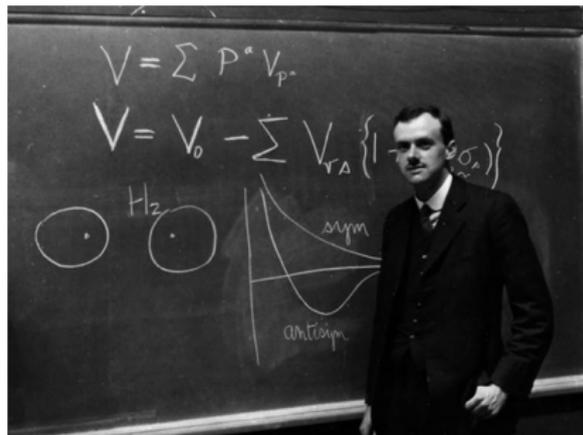
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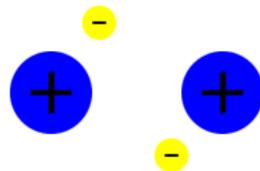
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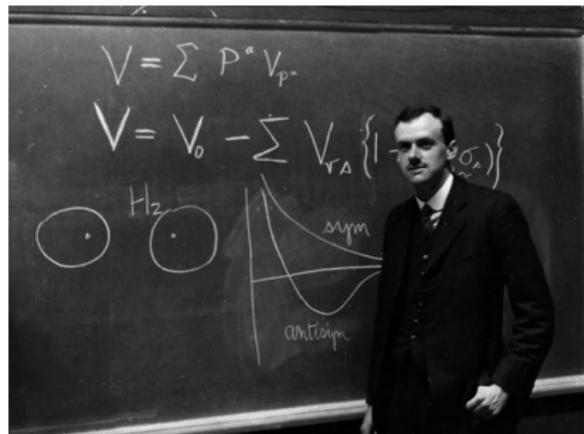
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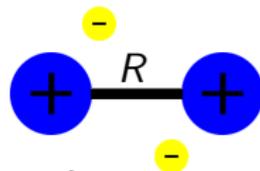
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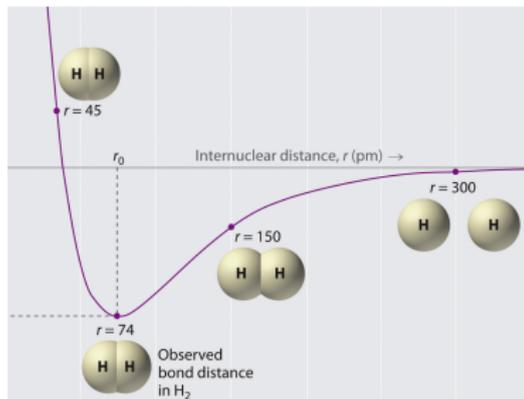


- Clamp nuclei under the Born-Oppenheimer approximation

$$|\Psi\rangle = |\psi\rangle_{\text{elec}} |\psi\rangle_{\text{nuc}} \Rightarrow H = T_{\text{elec}} + V_{\text{nuc-elec}} + V_{\text{elec-elec}}$$

# Why is the electronic structure problem important?

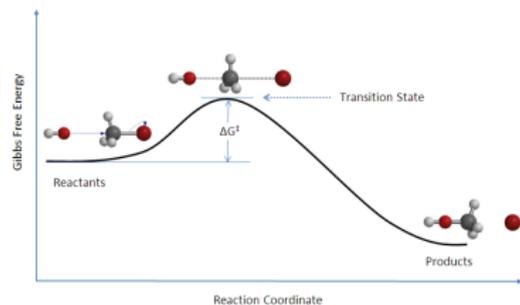
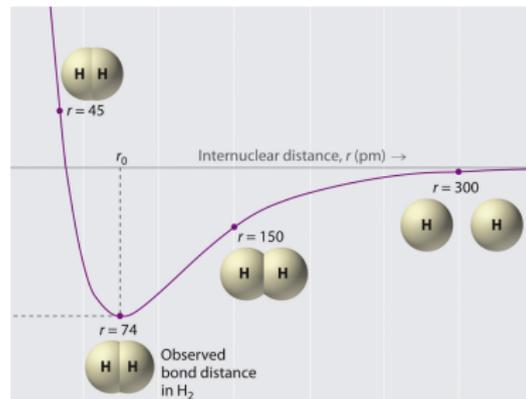
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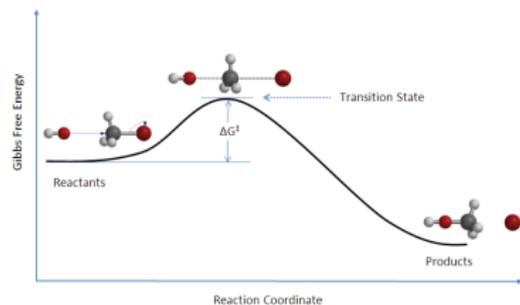
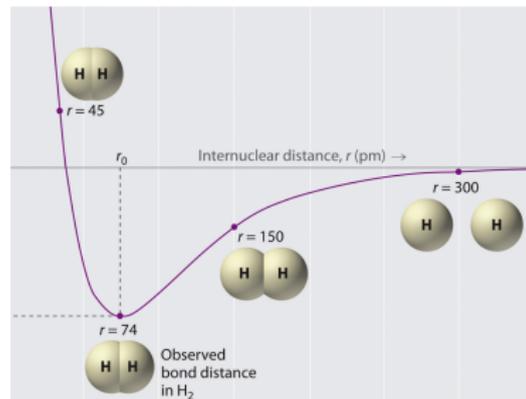


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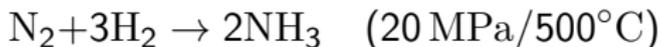


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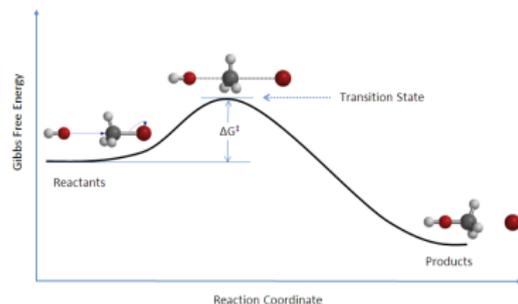
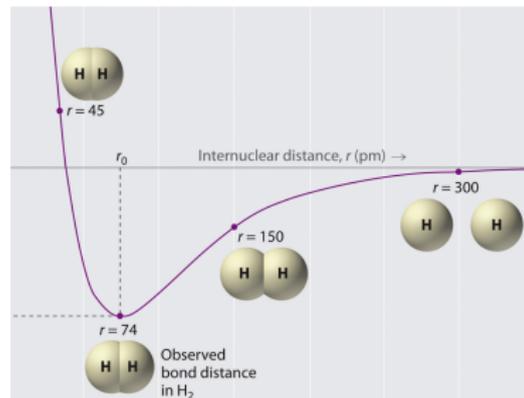
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5% of natural gas, 2% of energy!

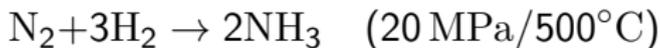


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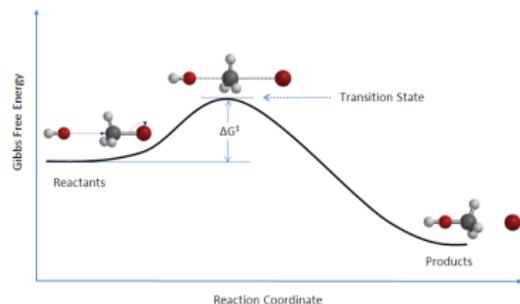
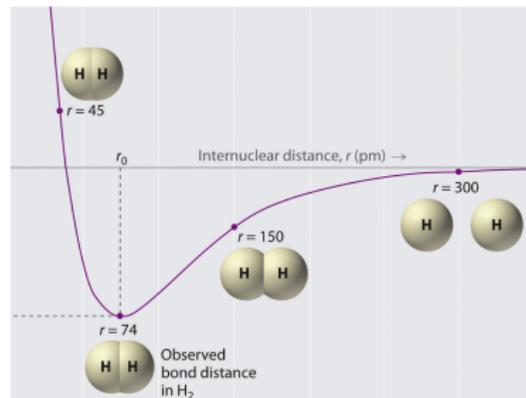
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- We can't do this classically: but could with a  $\sim 100$ -qubit quantum computer



# The canonical quantum chemistry algorithm<sup>1</sup>

- 1 Write Hamiltonian in qubit basis as sum of local terms,

$$H = \sum_{pq} h_{pq} a_p^\dagger a_q + \frac{1}{2} \sum_{pqrs} h_{pqrs} a_p^\dagger a_q^\dagger a_r a_s \equiv \sum_{\gamma} H_{\gamma}$$

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- ③ Use Trotterization to implement molecular evolution operator,

$$e^A e^B \neq e^{A+B} \quad e^{-iHt} = \lim_{r \rightarrow \infty} \left( \prod_{\gamma} e^{-iH_{\gamma} t/r} \right)^r$$

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- ④ Use phase estimation to measure the phase from time-evolution

$$e^{-iHt} |\psi\rangle = \sum_k \langle k|\psi\rangle e^{-iE_k t} |k\rangle \quad \text{Prob}(E_0 | \psi) = |\langle\psi|0\rangle|^2$$

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- 10/2014: Babbush *et al.*, chemical origin of errors<sup>5</sup>, numerics indicating  $\sim N^4 Z_{\max}^3$  gates

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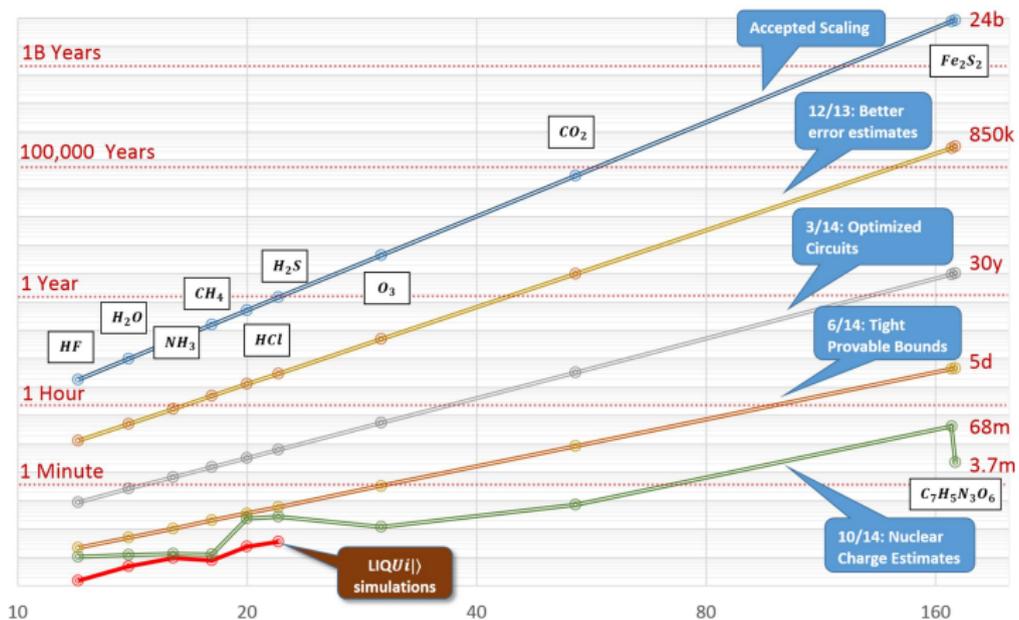
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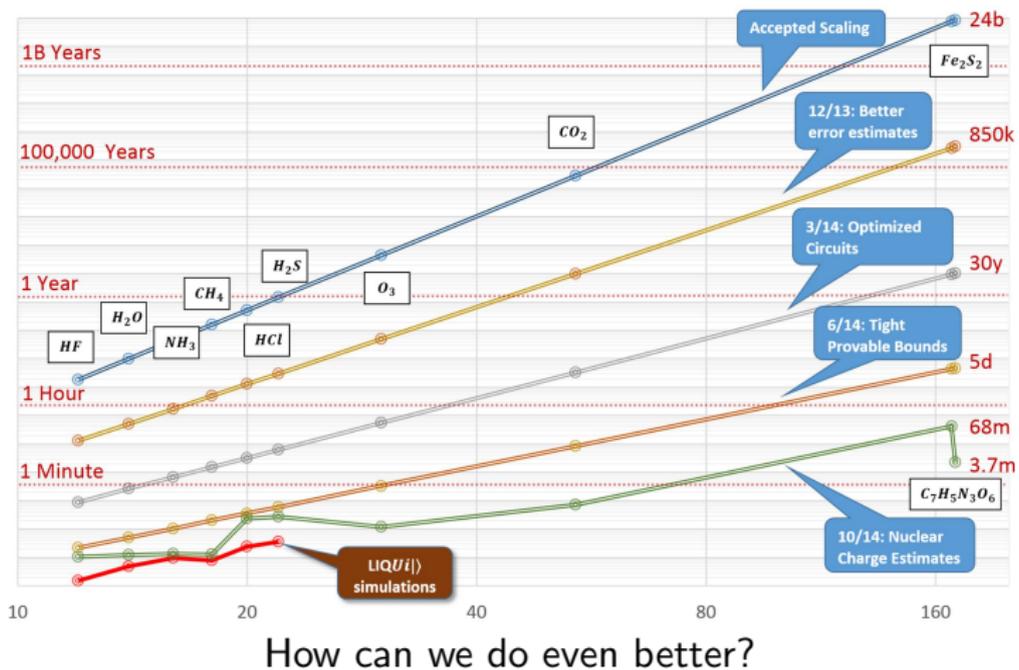
<sup>5</sup>R. Babbush *et al.*, Phys. Rev. A **91**, 022311 (2015).

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<sup>2</sup>Dave Wecker, Microsoft Research. Used with permission

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# Truncated Taylor series simulation

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# Truncated Taylor series simulation

- Berry, Childs, Cleve, Kothari, Somma<sup>3</sup>: approximate the time-evolution operator with a *truncated Taylor expansion* rather than Trotter-Suzuki decomposition
- Deterministic algorithm for simulating *sparse Hamiltonians* super-polynomially more precisely
  - $\tilde{O}(nd^2t \log(1/\epsilon))$  for a  $d$ -sparse  $n$ -qubit Hamiltonian
  - Compare accuracy scaling  $\epsilon$  with Lie-Trotter-Suzuki  $\text{poly}(1/\epsilon)$

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- 2 Divide into  $r \geq \sum_{\gamma} |W_{\gamma}| t$  segments
- 3 *Apply approximate time-evolution operator as truncated Taylor series*  $\tilde{U}_r \approx e^{-iHt/r}$  to initial state,  $r$  times (nasty part)

# The approximate time-evolution operator

- Expand  $e^{-iHt/r}$  as a Taylor series of these complex coefficients  $W_\gamma$  and unitaries  $H_\gamma$ , truncated to order  $K = \frac{\log(r/\epsilon)}{\log \log(r/\epsilon)}$ , i.e.

$$\tilde{U}_r = \sum_{k=0}^K \frac{(-iHt/r)^k}{k!} = \sum_{k=0}^K \sum_{\gamma_1, \dots, \gamma_K} \frac{(-it/r)^k}{k!} W_{\gamma_1} \dots W_{\gamma_K} H_{\gamma_1} \dots H_{\gamma_K}$$

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- Initialize ancilla register with amplitudes  $\sim$ square roots of Taylor series coefficients
- Use ancilla register to control when we apply products of  $H_\gamma$
- Use *oblivious amplitude amplification* to “extract” state time-evolved by  $t/r$ . Repeat  $r$  times

# Rest of the talk

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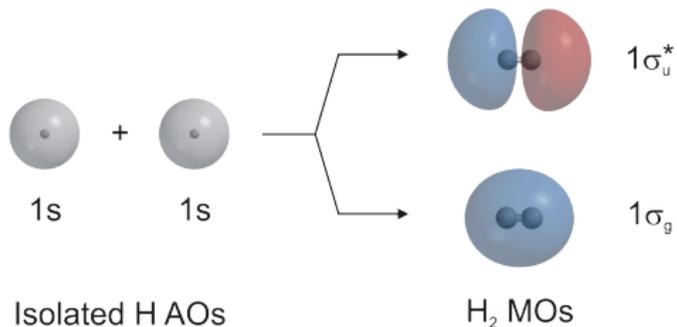
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    - Evaluate integrals on-the-fly  $\rightarrow \tilde{O}(N^5)$
  - 2 Chemistry in configuration interaction (first-quantized)
    - Decomposition of the configuration interaction matrix (Hamiltonian in that basis)  $\rightarrow \tilde{O}(\eta^2 N^3)$

# The second-quantized representation

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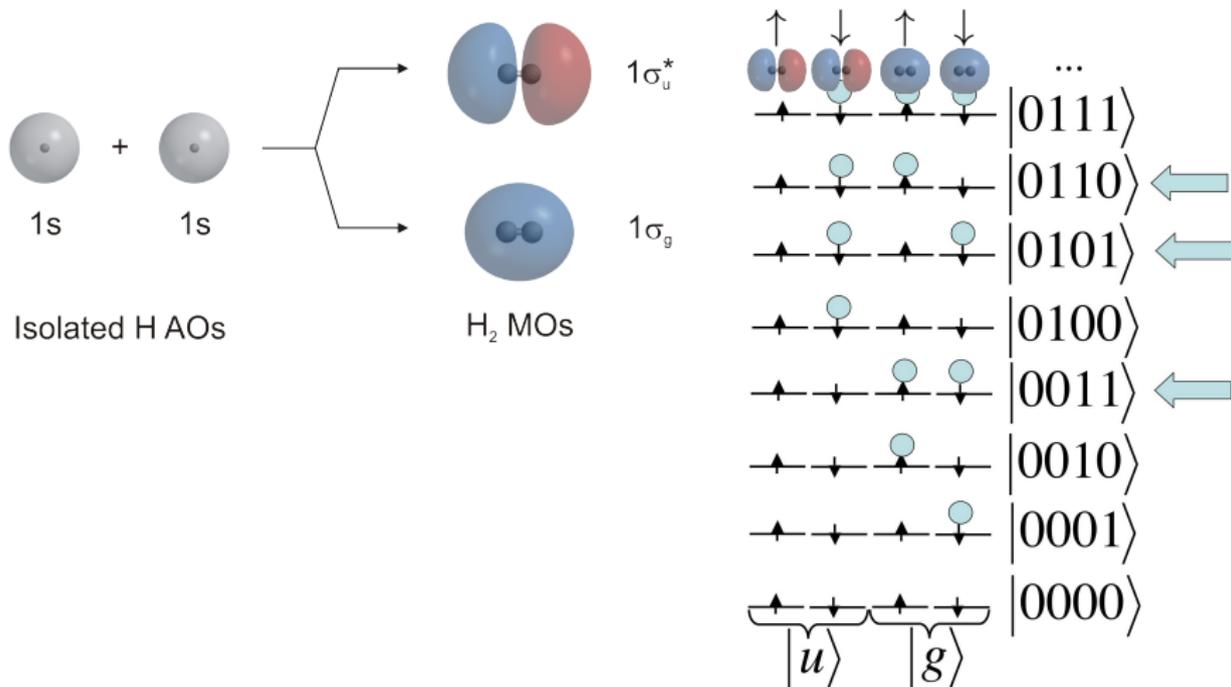
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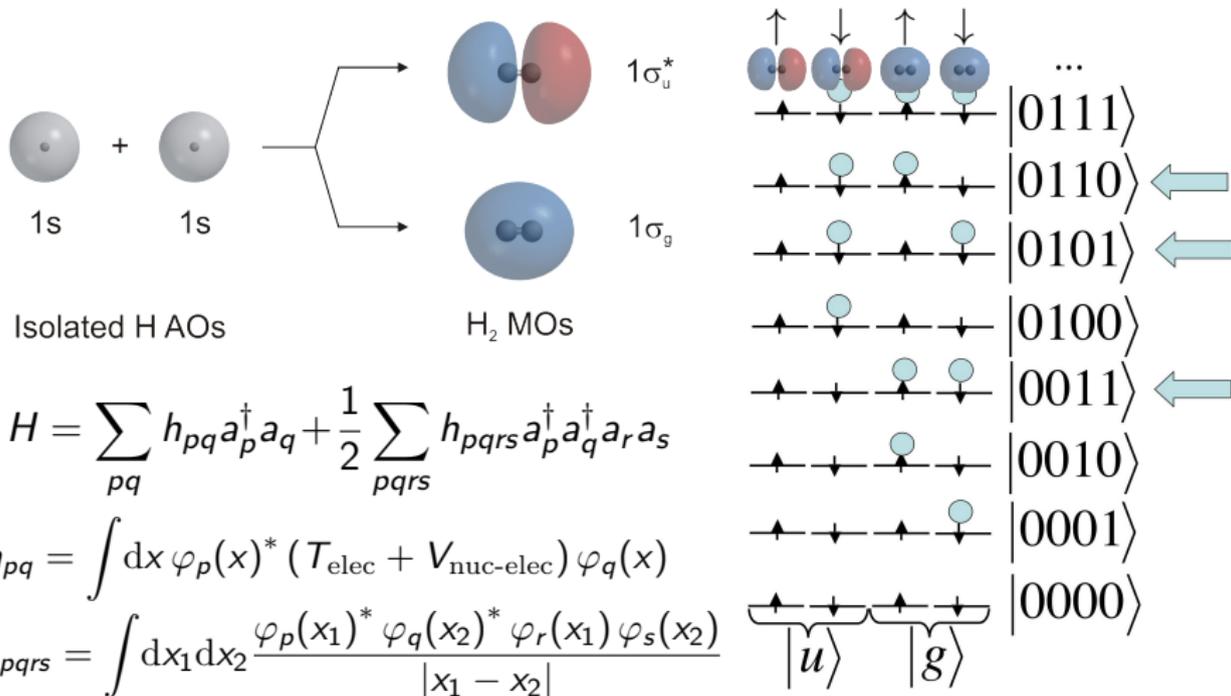
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# How can we improve second quantization?

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- 1 can be mapped to a linear combination of unitaries using Jordan-Wigner (decompose into Pauli operators on qubits),
- 2 the weights on each tensor product are given by integrals

$$h_{pq} = \int d\vec{r} \varphi_p(\vec{r})^* (T_{\text{elec}} + V_{\text{nuc-elec}}) \varphi_q(\vec{r}) \text{ or}$$
$$h_{pqrs} = \int d\vec{r}_1 d\vec{r}_2 \frac{\varphi_p(\vec{r}_1)^* \varphi_q(\vec{r}_2)^* \varphi_r(\vec{r}_1) \varphi_s(\vec{r}_2)}{|\vec{r}_1 - \vec{r}_2|}$$

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But then have to store them,  $O(N^4)$  to access
- Instead, general-purpose trick to evaluate in only  $O(\log(1/\epsilon))$ :
  - Assume  $\exists$  black box for the integrand
  - Restrict to finite volume and break into Riemann sum,

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- Break up  $\frac{V}{n_{\text{points}}} w_\gamma(\vec{z}_\rho)$  into a sum of signs  $w_{\gamma,m}(\vec{z}_\rho) = \pm 1$ ,  
determined by comparison with integrand  $w_\gamma(\vec{z})$
- Sum approximates integral, but only  $O(\log(V/\epsilon))$  to compute to  
precision  $\epsilon$

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- Finite volume OK, can choose  $\varphi_i$  significant on  $V = O(\log N)$
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- Worst thing to evaluate is 6-D integrals  $h_{pqrs}$ , still  $O(\log N)$
- Can evaluate  $\varphi_i$  in logarithmic time to get  $w_{\gamma,m}(\vec{z}_\rho)$ . Can be done coherently, then use truncated Taylor series for evolution
- However, evaluating  $N$  of them brings cost to  $\tilde{O}(N)$

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How can we do *even better*?

# The configuration interaction (CI) representation

First quantization: instead of encoding occupation (second quantization), limit to valid states:

$$|\alpha\rangle = |\alpha_1, \alpha_2, \dots, \alpha_n\rangle,$$

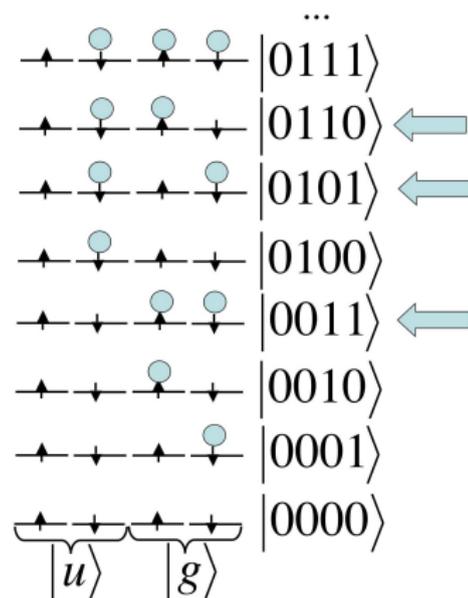
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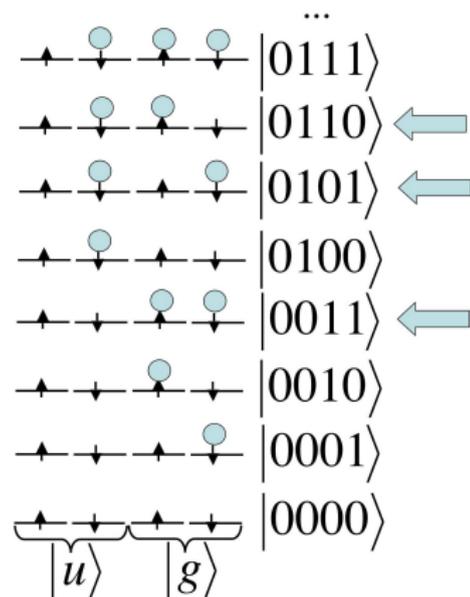
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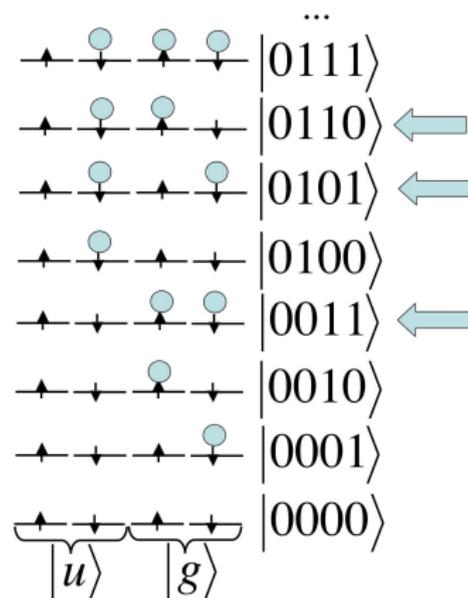
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How to simulate?  $\rightarrow$  1-sparse coloring



# Sparse matrices

$$\begin{pmatrix} 1.0 & 0 & 5.0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 3.0 & 0 & 0 & 0 & 0 & 11.0 & 0 \\ 0 & 0 & 0 & 0 & 9.0 & 0 & 0 & 0 \\ 0 & 0 & 6.0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 7.0 & 0 & 0 & 0 & 0 \\ 2.0 & 0 & 0 & 0 & 0 & 10.0 & 0 & 0 \\ 0 & 0 & 0 & 8.0 & 0 & 0 & 0 & 0 \\ 0 & 4.0 & 0 & 0 & 0 & 0 & 0 & 12.0 \end{pmatrix}$$

2-sparse:  $\leq 2$  non-zero entries per row/column.

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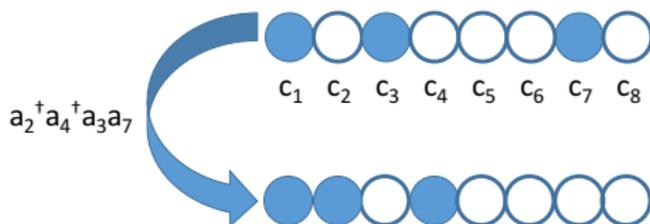
Sparsity of chemistry? 1-sparse coloring?

# Sparsity of the Hamiltonian

- Straightforward:  $a_i^\dagger a_j^\dagger a_k a_l$  terms in the Hamiltonian have the most non-zero matrix elements

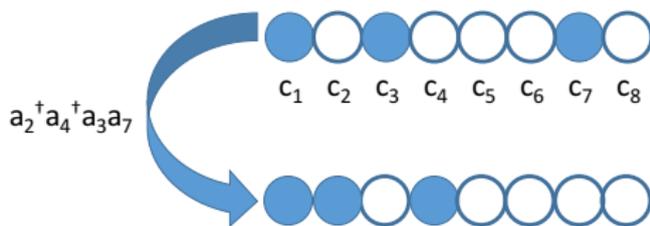
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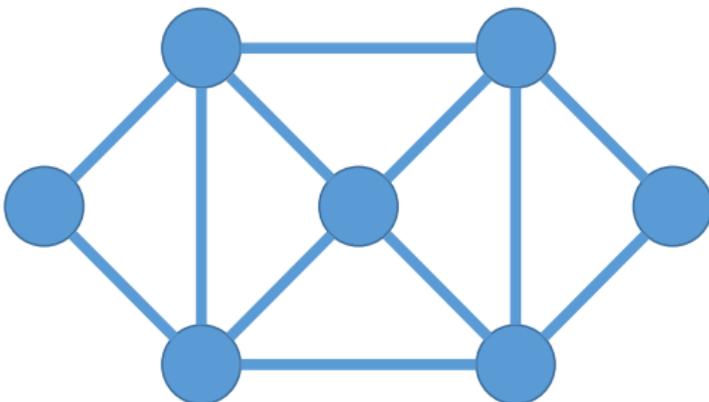


- $\implies$  any state can be connected by the Hamiltonian to  $O(\eta^2 N^2)$  other states: this is its sparsity
- $\implies$  trivial application  $\tilde{O}(nd^2 t \log(1/\epsilon)) = \tilde{O}(\eta^4 N^5 t \log(1/\epsilon))$

# Edge colorings

Say I give you this degree 4 graph (each vertex is connected to at most four others).

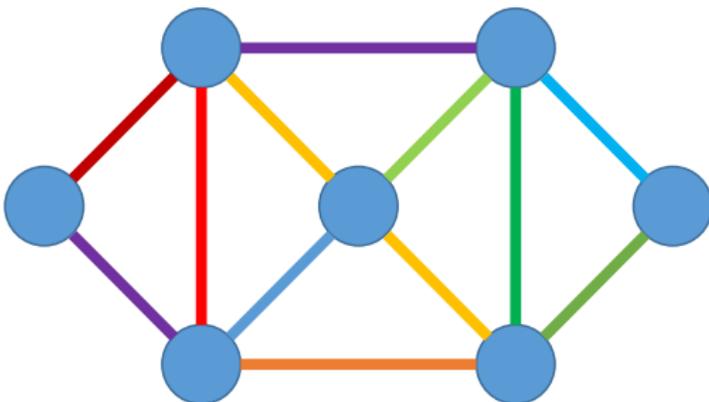
Can you color edges such that each vertex has at most one edge of any color?



# Edge colorings

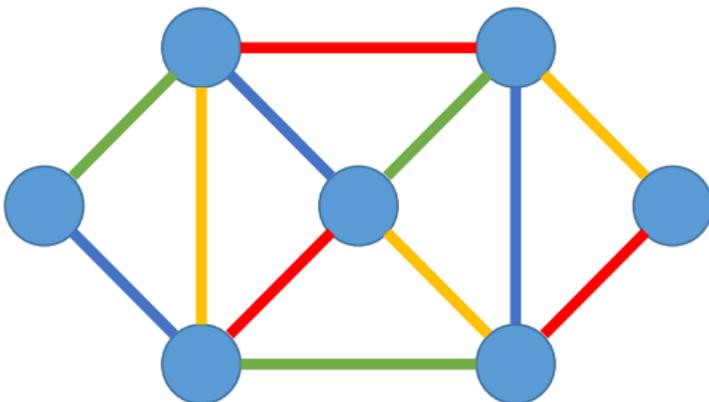
Here's a way to do it: if there are  $v$  vertices, choose  $vd$  colors and assign one to each edge!

This is the  $\tilde{O}(d^2)$  if we trivially applied the truncated Taylor series algorithm to chemistry.



# Edge colorings

∃ coloring that uses only  $d$  colors: just intractable to find.  
And even once found, can't necessarily be applied...  
Does such a coloring exist for the chemistry Hamiltonian?  
How might we find + apply it?



# CI algorithm

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- Cost:  $\tilde{O}(N)$  for  $N$  SOs from integrals  $\implies \tilde{O}(rN) = \tilde{O}(\eta^2 N^3)$

# Take-home messages

- 1 Can solve interesting and industrially relevant problems (electronic structure in chemistry) with quantum computers
- 2 A lot of work has been done in last two years on algorithms using Lie-Trotter-Suzuki (rigorous  $\tilde{O}(N^8 t / \epsilon^{o(1)})$ ), but can do *even better* using new Taylor series techniques

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- 3 Tricks:
  - Evaluating integrals on-the-fly and working with linear combinations of them (general-purpose trick)
  - Sparse colorings using structure of the chemistry Hamiltonian

# Acknowledgements

Collaborators: Ryan Babbush (Google—talk at 2:40 PM), Dominic Berry (Macquarie), Annie Wei (Harvard), Peter Love (Tufts), Alán Aspuru-Guzik (Harvard)



**Australian Government**

**Australian Research Council**



# Thanks for listening! 😊

Second-quantized chemistry:

R. Babbush, D. W. Berry, **Ian D. Kivlichan**, A. Y. Wei, P. J. Love and  
A. Aspuru-Guzik, *New Journal of Physics* **18**, 033032, arXiv:1506.01020 (2016)

Configuration interaction:

R. Babbush, D. W. Berry, **Ian D. Kivlichan**, A. Y. Wei, P. J. Love and  
A. Aspuru-Guzik, arXiv:1506.01029 (2015)

New paper on the complexity of simulating many-body physics / chemistry in real space (truncated Taylor series + surprising finite-difference approximations):

**Ian D. Kivlichan**, N. Wiebe, R. Babbush, and A. Aspuru-Guzik, arXiv:1608.05696 (2016)

# Mapping a fermionic algebra into qubits

$$H = \sum_{pq} h_{pq} a_p^\dagger a_q + \frac{1}{2} \sum_{pqrs} h_{pqrs} a_p^\dagger a_q^\dagger a_r a_s \text{ not a qubit Hamiltonian}$$

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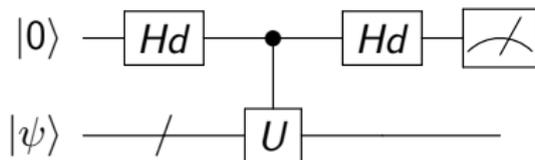
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**The Jordan-Wigner transformation is  $O(N)$ -local**

# Kitaev's quantum phase estimation algorithm<sup>4</sup>

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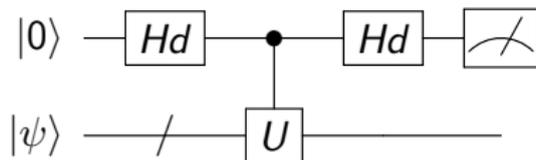
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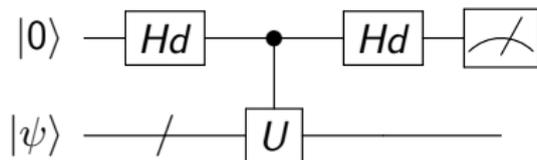
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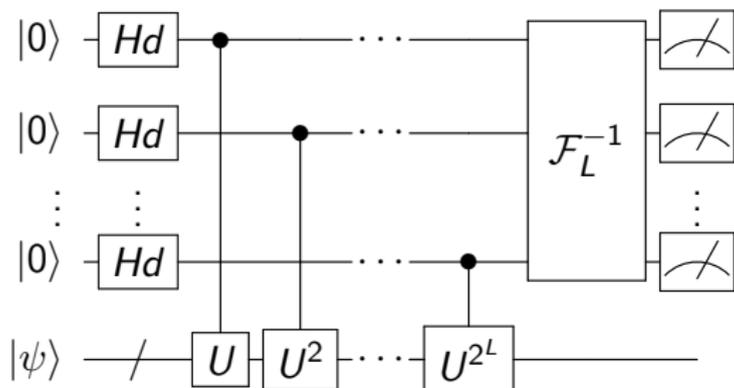
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Instead use inverse QFT



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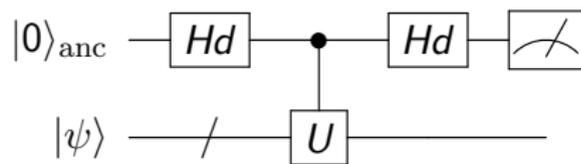
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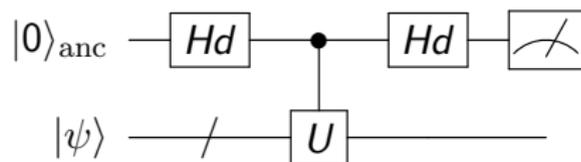
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