# New Directions in quantum simulation of quantum chemistry

Peter Love, Jake Seeley, Martin Richard, Sarah Sofia
Haverford College
with
Ken Brown, Mauricio Gutiérrez
Georgia Tech
Kelly Stevens, Gregory Mohler, Jared Huggins
Georgia Tech Research Institute (GTRI)
Jarrod McClean, Ryan Babbush, Alan Aspuru-Guzik
Harvard

# AREAS OF INTEREST

Physical Simulation Applications:

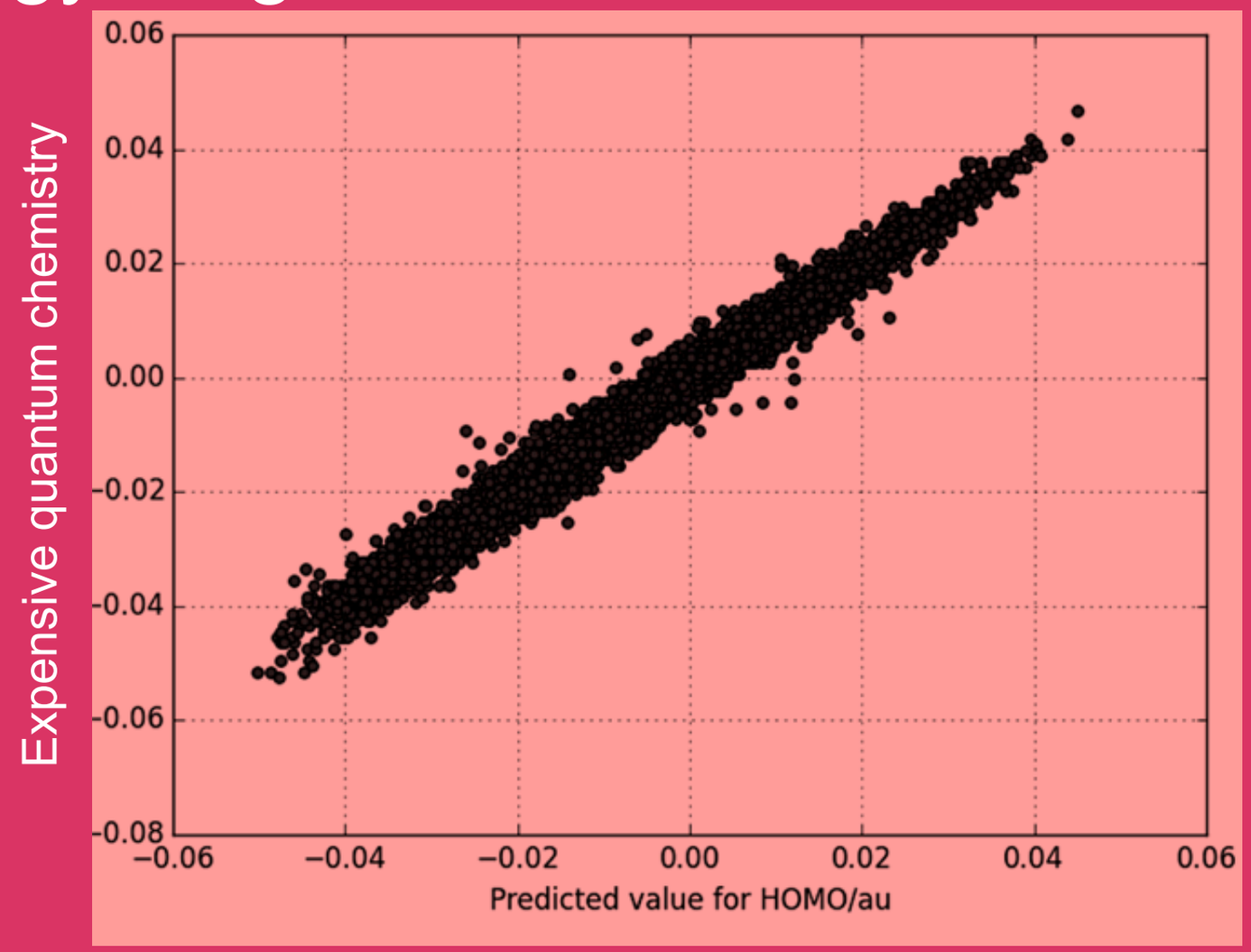
- Quantum computers are known to have advantages for the simulation of physical systems.
- Can we advance the state of the art in algorithms?
- Can we find new applications of interest to DOE?

Data Science applications:

- Quantum computers have shown key algorithmic advantages (e.g. solving linear systems)
- Can quantum computers be used in **data science?**
- Can we advance the state of the art in algorithms?
- Can we find new applications of interest to DOE?

# Multilayer perceptron applied to energy: Organic Photovoltaics

"Quantum manufacturing" (De Felice)



# Research questions / excellent summary

Scott Aaronson

So in summary, how excited should we be about the new quantum machine learning algorithms? To whatever extent we care about quantum computing at all, I'd say we should be excited indeed: HHL and its offshoots represent real advances in the theory of quantum algorithms, and in a world with quantum computers, they'd probably find practical uses. But along with the excitement, we ought to maintain a sober understanding of what these algorithms would and wouldn't do: an understanding that the original papers typically convey, but that often gets lost in secondhand accounts.

The new algorithms provide a general template, showing how quantum computers *might* be used to provide exponential speedups for central problems like clustering, pattern-matching, and principal component analysis. But for each intended application of the template, one still needs to invest a lot of work to see whether (a) the application satisfies all of the algorithm's "fine print," and (b) once we include the fine print, there's *also* a fast classical algorithm that provides the same information. This makes the quantum machine learning algorithms quite different from (say) Shor's factoring algorithm. Having spent half my life in quantum computing research, I still find it miraculous that the laws of quantum physics let us solve *any* classical problems exponentially faster than today's computers seem able to solve them. So maybe it shouldn't surprise us that, in machine learning like anywhere else, Nature will still make us work for those speedups.

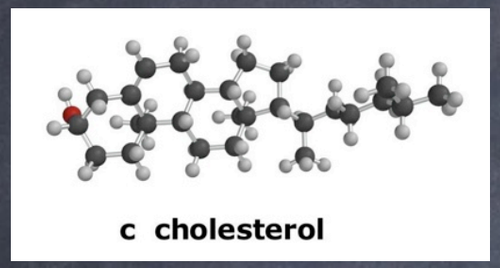
http://www.scottaaronson.com/papers/qml.pdf

# What is Quantum Simulation?

## One quantum system pretending to be another

- Lab system can do initialization, evolution, measurement
- Want to compute $\langle\psi|\hat{A}|\psi\rangle$ for state $|\psi\rangle$, observable $\hat{A}$
- Initialize lab system in some state
- Control laboratory system to produce state representing $|\psi\rangle$
- Measure some set of observables (e.g qubit states 0,1) to obtain information about $\hat{A}$
- Lab system = quantum computer: quantum simulation algorithms
- If lab system = target system: we call that experiment!

# Chemistry on a quantum computer




Map fermions to Qubits

State preparation

Phase eestimation

Digital readout

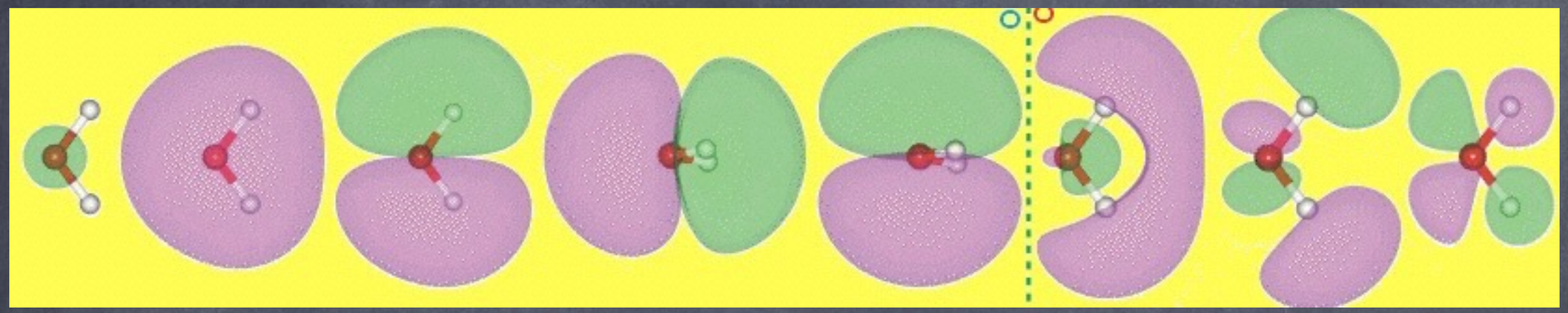
E=??

KEY STEPS REQUIRE TIME EVOLUTION

Mapping + Trotter

Simulated Quantum Computation of Molecular Energies" Alan Aspuru-Guzik, Anthony Dutoi, Peter J. Love, Martin Head-Gordon, Science, **309**, 5741, (2005)

# Electronic Structure



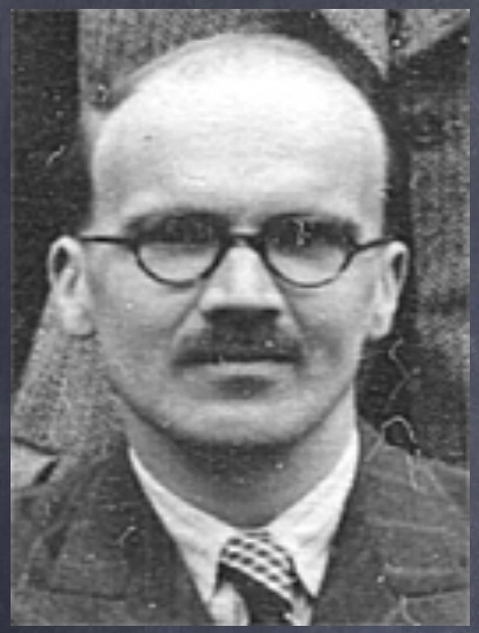
Fermionic anticommutation relations

$$\{a_j, a_k\} = 0 \qquad \{a_j^\dagger, a_k^\dagger\} = 0 \qquad \{a_j, a_k^\dagger\} = \delta_{jk} 1$$

Molecular electronic Hamiltonian

$$H = \sum_{i,j} h_{ij} a_i^\dagger a_j + \frac{1}{2} \sum_{i,j,k,l} h_{ijkl} a_i^\dagger a_j^\dagger a_k a_l$$

# A Quantum Computer for Chemistry?



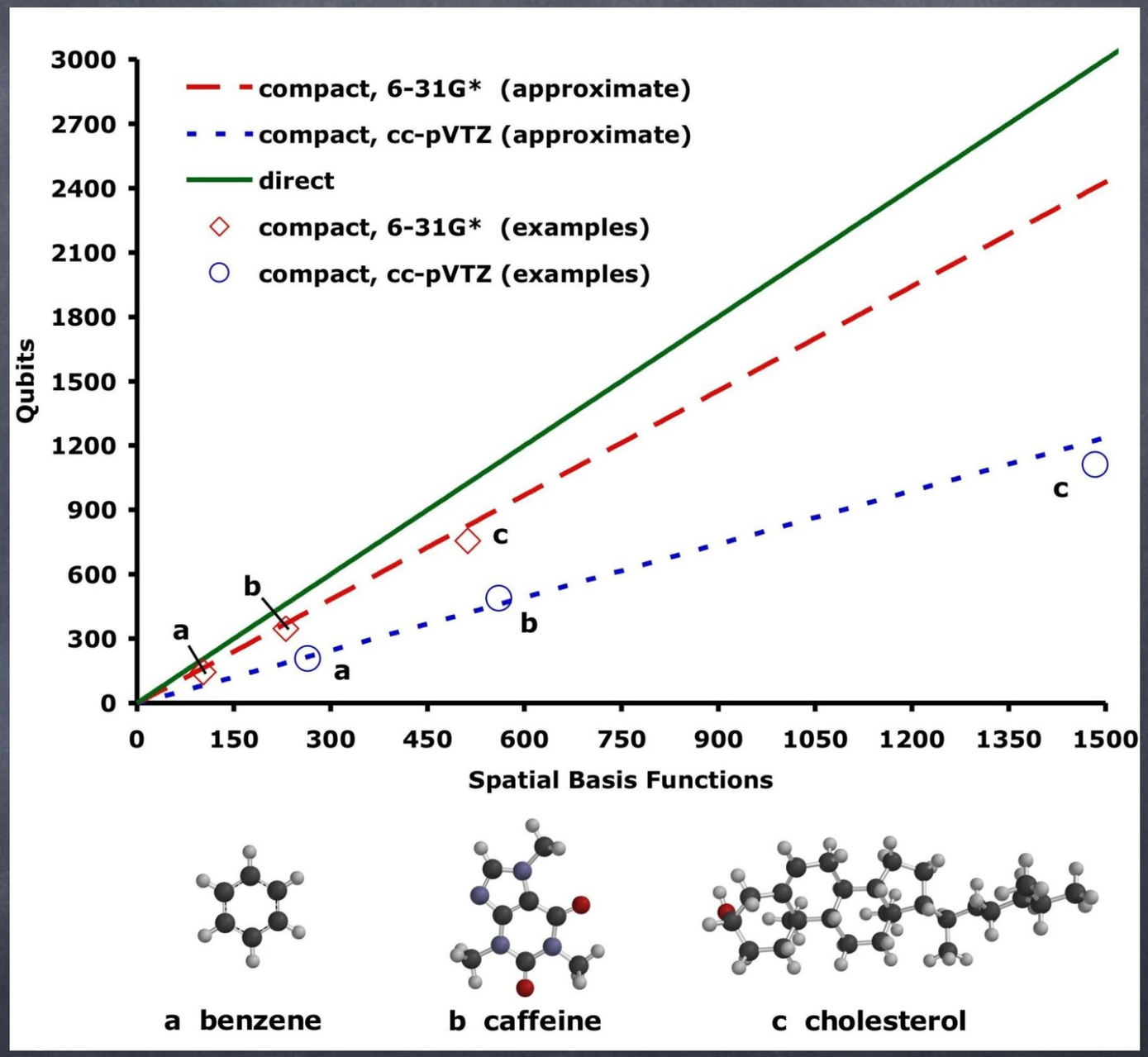
Electronic wave functions

II. A calculation for the ground state of the beryllium atom

By S. F. Boys, *Theoretical Chemistry Department, University of Cambridge**

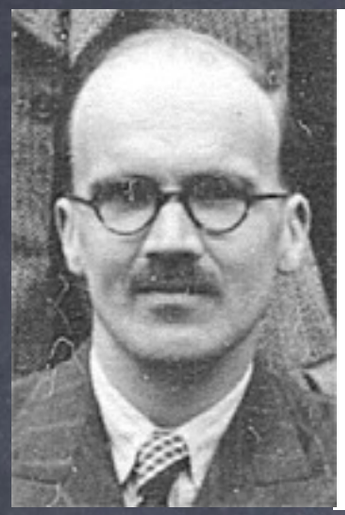
(*Communicated by Sir Alfred Egerton, F.R.S.—Received* 31 *August* 1949)

An approximate wave function expressed in terms of exponential functions, spherical harmonics, etc., with numerical coefficients has been calculated for the ground state of the beryllium atom. Judged by the energy criterion this gives a more accurate result than the Hartree result which was the best previously known. This has been calculated as a trial of a fresh method of calculating atomic wave functions. A linear combination of Slater determinants is treated by the variational method. The results suggest that this will provide a more powerful and convenient method than has previously been available for atoms with more than two electrons.




Simulated Quantum Computation of Molecular Energies, Alan Aspuru-Guzik, Anthony Dutoi, Peter J. Love, Martin Head-Gordon, Science, 309, 5741, (2005)

J. T. Seeley, M. Richard, P. J. Love J. Chem. Phys. **137**, 224109 (2012)



Electronic wave functions

I. A general method of calculation for the stationary states of any molecular system

By S. F. Boys, *Theoretical Chemistry Department, University of Cambridge**

(*Communicated by Sir Alfred Egerton, F.R.S.—Received* 31 *August* 1949)

| Year | Calculation | Citation | Qubits |
|---|---|---|---|
| 1933 | $H_2$ | H. M. James, A. S. Coolidge JCP **1**, 825 | 1 |
| 1950 | Be | S. F. Boys Proc Roy Soc **201** 125 | 3,4 |
| 1952 | He | G. R. Taylor, R. G. Parr PNAS **38** 154 | 2 |
| 1955 | He | H Shull, P.-O. Lowdin JCP **23** 1565 | 2,3 |
| 1956 | BH, $H_2O$ | S. F. Boys, G. B. Cook, C. M. Reeves, I. Shavitt, Nature **178** 1207 | 5,7 |
| 1957 | LiH, $BeH^+$ | J. Miller et al. JCP **27** 1385 | 3-5 |
| 1960 | Be | R. E. Watson, Phys. Rev. **119** 170 | 6 |
| 1960 | $CH_2$ | J. M. Foster, S. F. Boys, RMP **32** 305 | 19 |
| 1963 | $H_2$ | S. Hagstrom, H. Shull, RMP **35** 624 | 3-6 |
| 1966 | HeH, $Li_2$ | C. F. Bender, E. R. Davidson, JPC **70** 2675 | 3 |
| 1967 | $H_2O$ | R Mcweeny, K. A. Ohno, Proc. Roy. Soc **A255**, 367 | 10 |
| 1968 | Be | C. F. Bunge, Phys. Rev. **168**, 92 | 11 |
| 1970 | $H_2O$ | R. P. Hosteny et al Chem. Phys. Lett. **7**, 325 | 23 |

## Can quantum chemistry be performed on a small quantum computer?

Dave Wecker,[1] Bela Bauer,[2] Bryan K. Clark,[2,3] Matthew B. Hastings,[2,1] and Matthias Troyer[4]

[1] *Quantum Architectures and Computation Group, Microsoft Research, Redmond, WA 98052, USA*
[2] *Station Q, Microsoft Research, Santa Barbara, CA 93106-6105, USA*
[3] *Kavli Institute for Theoretical Physics, University of California, Santa Barbara, CA 93106, USA*
[4] *Theoretische Physik, ETH Zurich, 8093 Zurich, Switzerland*

As quantum computing technology improves and quantum computers with a small but non-trivial number of $N \geq 100$ qubits appear feasible in the near future the question of possible applications of small quantum computers gains importance. One frequently mentioned application is Feynman's original proposal of simulating quantum systems, and in particular the electronic structure of molecules and materials. In this paper, we analyze the computational requirements for one of the standard algorithms to perform quantum chemistry on a quantum computer. We focus on the quantum resources required to find the ground state of a molecule twice as large as what current classical computers can solve exactly. We find that while such a problem requires about a ten-fold increase in the number of qubits over current technology, the required increase in the number of gates that can be coherently executed is many orders of magnitude larger. This suggests that for quantum computation to become useful for quantum chemistry problems, drastic algorithmic improvements will be needed.

arXiv:1312.1695v1

Phase estimation gives long skinny algorithms

Qubit requirements grounds for optimism

Gate requirements grounds for pessimism

## The Trotter Step Size Required for Accurate Quantum Simulation of Quantum Chemistry

David Poulin,[1] M. B. Hastings,[2,3] Dave Wecker,[3] Nathan Wiebe,[3] Andrew C. Doherty,[4] and Matthias Troyer[5]

[1] *Département de Physique, Université de Sherbrooke, Québec, Canada*
[2] *Station Q, Microsoft Research, Santa Barbara, CA 93106-6105, USA*
[3] *Quantum Architectures and Computation Group, Microsoft Research, Redmond, WA 98052, USA*
[4] *Centre for Engineered Quantum Systems, School of Physics, The University of Sydney, Sydney, NSW 2006, Australia*
[5] *Theoretische Physik, ETH Zurich, 8093 Zurich, Switzerland*

(Dated: June 20, 2014)

The simulation of molecules is a widely anticipated application of quantum computers. However, recent studies [1, 2] have cast a shadow on this hope by revealing that the complexity in gate count of such simulations increases with the number of spin orbitals $N$ as $N^8$, which becomes prohibitive even for molecules of modest size $N \sim 100$. This study was partly based on a scaling analysis of the Trotter step required for an ensemble of random artificial molecules. Here, we revisit this analysis and find instead that the scaling is closer to $N^6$ in worst case for real model molecules we have studied, indicating that the random ensemble fails to accurately capture the statistical properties of real-world molecules. Actual scaling may be significantly better than this due to averaging effects. We then present an alternative simulation scheme and show that it can sometimes outperform existing schemes, but that this possibility depends crucially on the details of the simulated molecule. We obtain further improvements using a version of the coalescing scheme of [1]; this scheme is based on using different Trotter steps for different terms. The method we use to bound the complexity of simulating a given molecule is efficient, in contrast to the approach of [1, 2] which relied on exponentially costly classical exact simulation.

## Chemical Basis of Trotter-Suzuki Errors in Quantum Chemistry Simulation

Ryan Babbush,[1] Jarrod McClean,[2] Dave Wecker,[1] Alán Aspuru-Guzik,[2] and Nathan Wiebe[1]

[1] *Quantum Architectures and Computation Group, Microsoft Research, Redmond, WA 98052*
[2] *Department of Chemistry and Chemical Biology, Harvard University, Cambridge, MA 02138*

(Dated: February 6, 2015)

Although the simulation of quantum chemistry is one of the most anticipated applications of quantum computing, the scaling of known upper bounds on the complexity of these algorithms is daunting. Prior work has bounded errors due to Trotterization in terms of the norm of the error operator and analyzed scaling with respect to the number of spin orbitals. However, we find that these error bounds can be loose by up to sixteen orders of magnitude for some molecules. Furthermore, numerical results for small systems fail to reveal any clear correlation between ground state error and number of spin orbitals. We instead argue that chemical properties, such as the maximum nuclear charge in a molecule and the filling fraction of orbitals, can be decisive for determining the cost of a quantum simulation. Our analysis motivates several strategies to use classical processing to further reduce the required Trotter step size and to estimate the necessary number of steps, without requiring additional quantum resources. Finally, we demonstrate improved methods for state preparation techniques which are asymptotically superior to proposals in the simulation literature.

## Improving Quantum Algorithms for Quantum Chemistry

M. B. Hastings,[1,2] Dave Wecker,[2] Bela Bauer,[1] and Matthias Troyer[3]

[1] *Station Q, Microsoft Research, Santa Barbara, CA 93106-6105, USA*
[2] *Quantum Architectures and Computation Group, Microsoft Research, Redmond, WA 98052, USA*
[3] *Theoretische Physik, ETH Zurich, 8093 Zurich, Switzerland*

We present several improvements to the standard Trotter-Suzuki based algorithms used in the simulation of quantum chemistry on a quantum computer. First, we modify how Jordan-Wigner transformations are implemented to reduce their cost from linear or logarithmic in the number of orbitals to a constant. Our modification does not require additional ancilla qubits. Then, we demonstrate how many operations can be parallelized, leading to a further linear decrease in the parallel depth of the circuit, at the cost of a small constant factor increase in number of qubits required. Thirdly, we modify the term order in the Trotter-Suzuki decomposition, significantly reducing the error at given Trotter-Suzuki timestep. A final improvement modifies the Hamiltonian to reduce errors introduced by the non-zero Trotter-Suzuki timestep. All of these techniques are validated using numerical simulation and detailed gate counts are given for realistic molecules.

Brilliant, careful optimization of trotterization

# Algorithms and Improvements

Map — Prepare — Evolve — Measure

Adiabatic simulation

| | | | | |
|---|---|---|---|---|
| ~~Second Quantized~~ + | ~~Jordan Wigner~~ | ~~Adiabatic Preparation~~ | ~~Trotterization to CNOT circuits~~ | ~~Phase estimation and logical readout~~ |
| Sparse Simulation methods | Bravyi Kitaev | Unitary Coupled Cluster | Choose physical elementary gates | Quantum variational Hamiltonian estimation |

# Replacing Jordan-Wigner

# Occupation number basis and Jordan-Wigner transformation

- Qubit Creation and annihilation operators:

$$a_j^\dagger \equiv \hat{\mathcal{Q}}_j^+ \otimes \hat{\mathcal{Z}}_{j-1}^{\rightarrow} \quad a_j \equiv \hat{\mathcal{Q}}_j^- \otimes \hat{\mathcal{Z}}_{j-1}^{\rightarrow}$$

- Where:

$$\hat{\mathcal{Q}}^+ = |1\rangle\langle 0| = \frac{1}{2}(\sigma^x - i\sigma^y) \quad \hat{\mathcal{Q}}^- = |0\rangle\langle 1| = \frac{1}{2}(\sigma^x + i\sigma^y)$$

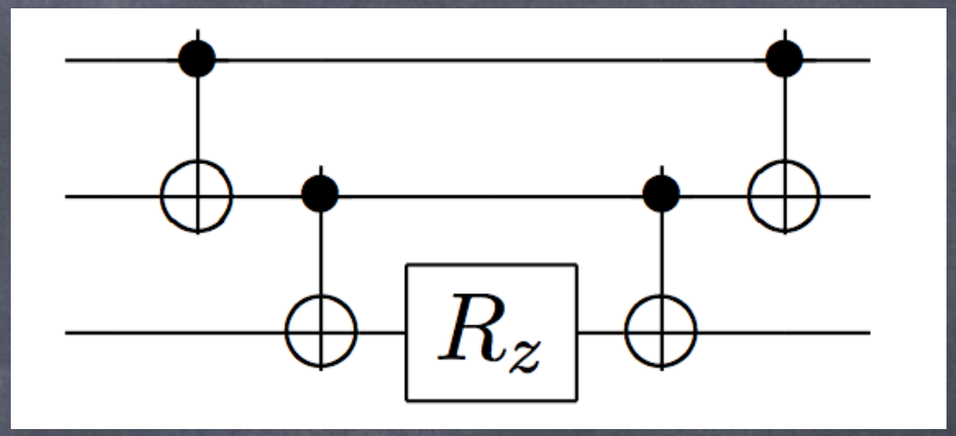
$$\hat{\mathcal{Z}}_i^{\rightarrow} \equiv \sigma_i^z \otimes \sigma_{i-1}^z \otimes \cdots \sigma_1^z \otimes \sigma_0^z$$

P. Jordan and E. Wigner, *Z. Phys*. 47, 631 (1928). R. Somma, G. Ortiz, J.E.Gubernatis, E. Knill, R. Laflamme, “Simulating physical phenomena by quantum networks”, *Phys Rev. A* 65, 042323 (2002).

# Strings and ladders

- Exponentiating products of Pauli-Z matrices:

$$e^{i(\sigma^z \otimes \sigma^z \otimes \sigma^z)}$$




These ladders are hard to implement and are O(n) long in JW for CNOT but O(1) for n-qubit Molmer-Sorenson gates

From transistor to trapped-ion computers for quantum chemistry
M.-H. Yung, J. Casanova, A. Mezzacapo, J. McClean, L. Lamata, A. Aspuru-Guzik, E. Solano, arXiv:1307.4326

# The parity basis

- Make parity local - store parity in the qubits

$$p_j = \sum_{s=0}^{j} l_s$$

- Parity is local! But occupancy is non-local

$$a_j^\dagger \equiv \hat{\mathcal{X}}_{j+1}^{\leftarrow} \otimes \hat{\mathcal{P}}_j^{+} \quad a_j \equiv \hat{\mathcal{X}}_{j+1}^{\leftarrow} \otimes \hat{\mathcal{P}}_j^{-}$$

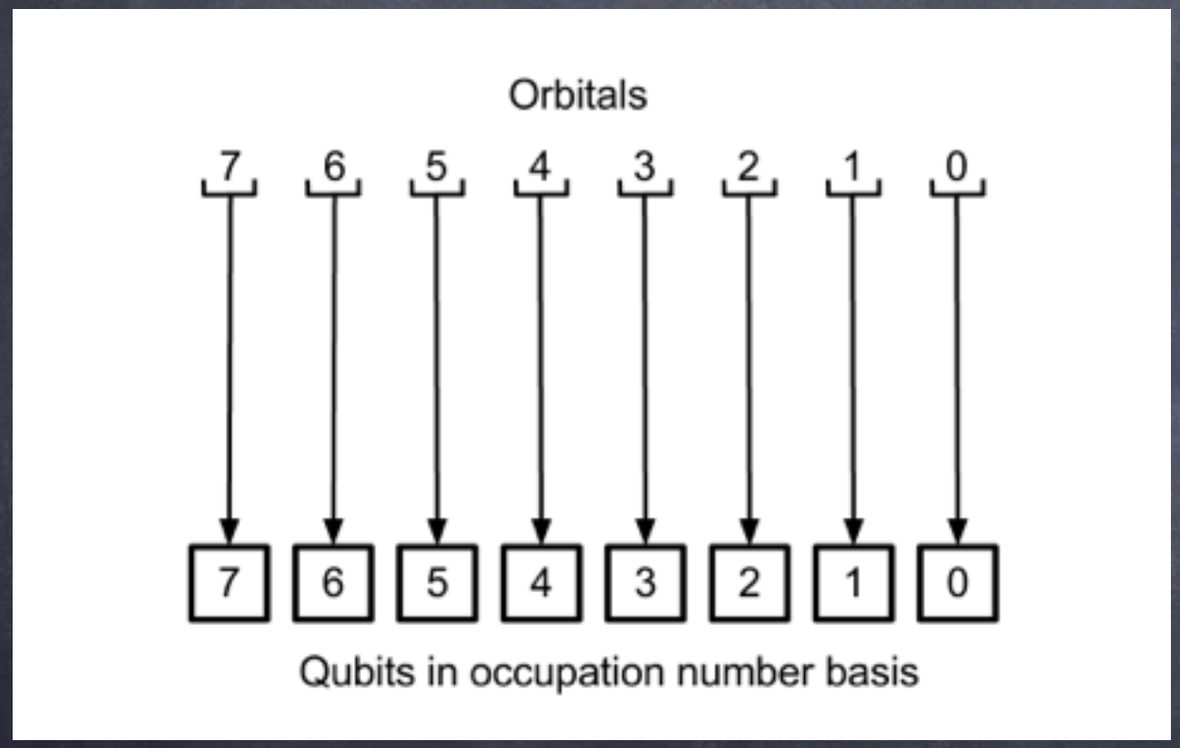
$$\hat{\mathcal{P}}_j^{\pm} \equiv \hat{\mathcal{Q}}_j^{\pm} \otimes |0\rangle\langle 0|_{j-1} - \hat{\mathcal{Q}}_j^{\mp} \otimes |1\rangle\langle 1|_{j-1}$$

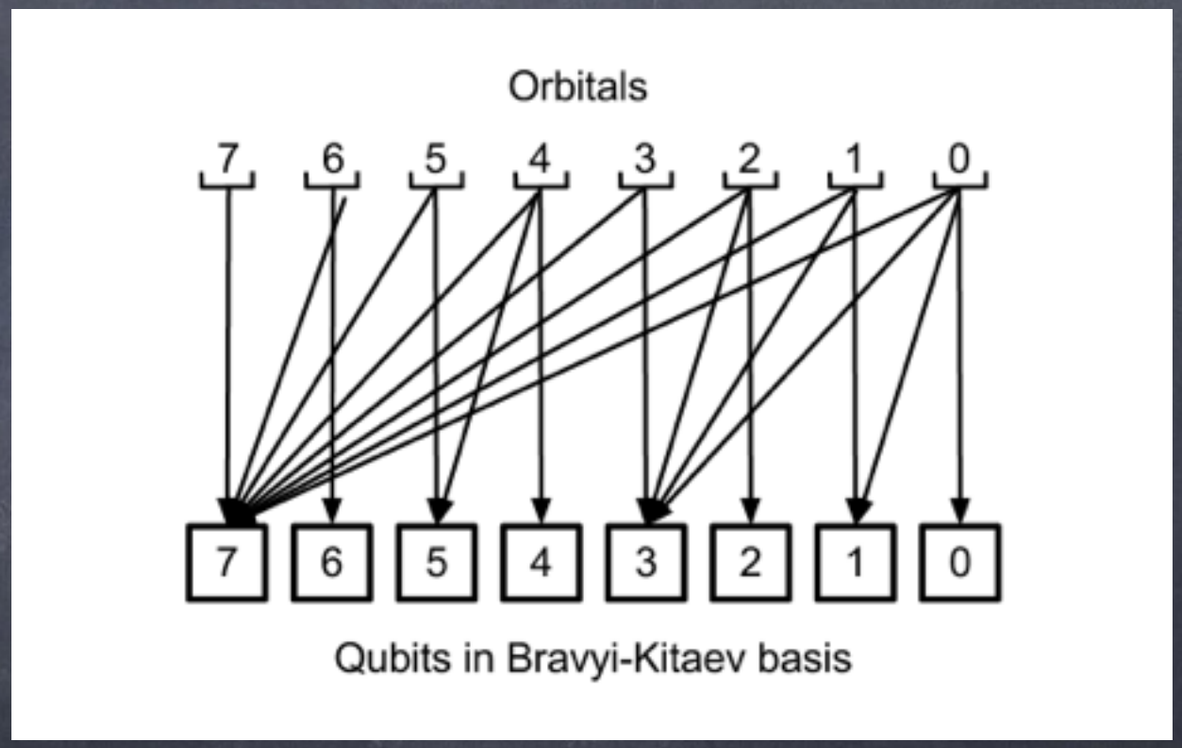
$$\hat{\mathcal{X}}_i^{\leftarrow} \equiv \sigma_{n-1}^x \otimes \sigma_{n-2}^x \otimes \cdots \sigma_{i+1}^x \otimes \sigma_i^x$$

S. Bravyi and A. Yu. Kitaev, “Fermionic quantum computation”, *Annals of Physics, **298** 210-226 2002*

# The Bravyi-Kitaev basis

- Strike a happy medium between local occupancy and local parity




Old basis

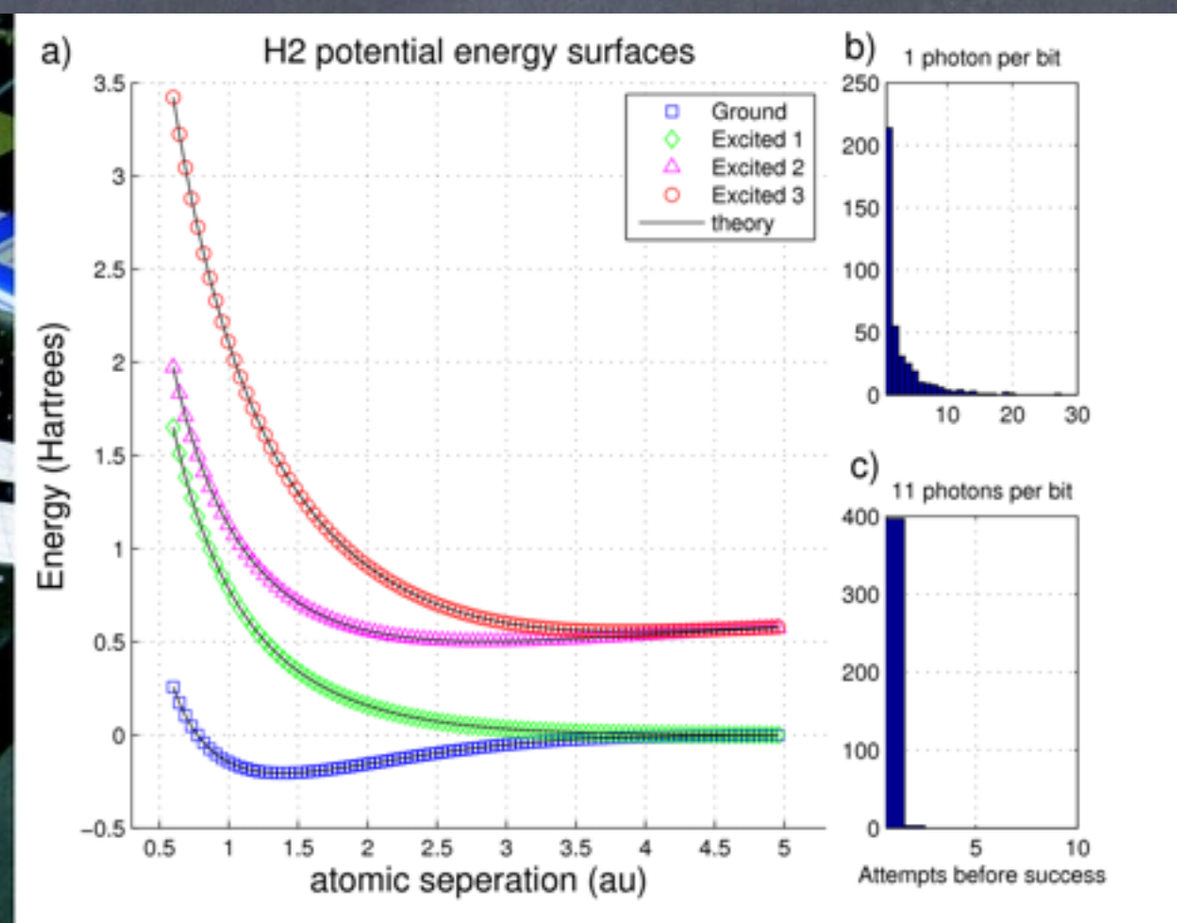
New basis

S. Bravyi and A. Yu. Kitaev, "Fermionic quantum computation", Annals of Physics, **298** 210-226 (2002), J. T. Seeley, M. Richard, P. J. Love J. Chem. Phys. **137**, 224109 (2012)

# An example: $H_2$ in a minimal basis

$$|\chi_0\rangle = |\psi_g\rangle|\alpha\rangle \quad |\chi_1\rangle = |\psi_g\rangle|\beta\rangle \quad |\chi_2\rangle = |\psi_u\rangle|\alpha\rangle \quad |\chi_3\rangle = |\psi_u\rangle|\beta\rangle$$

For this example n = 4




B. P Lanyon, J. D Whitfield, G. G Gillett, M. E Goggin, M. P Almeida, I Kassal, J. D Biamonte, M Mohseni, B. J Powell, M Barbieri, A Aspuru-Guzik, A. G White, Towards Quantum Chemistry on a Quantum Computer, Nature Chemistry, **2**, 106, 2010

# A Tale of Two Transformations

- The Jordan-Wigner spin Hamiltonian for $H_2$

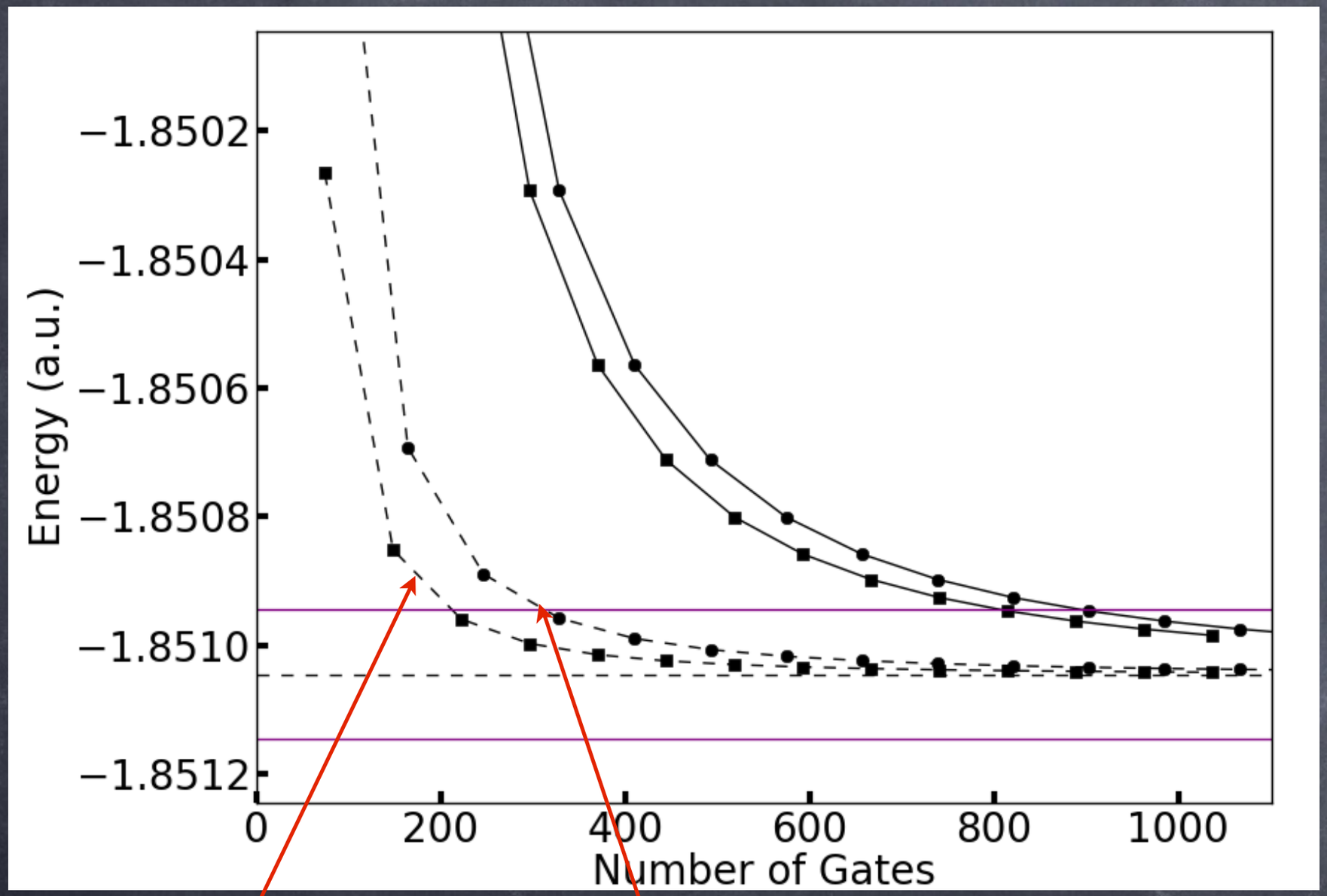
$$-0.8175\,\mathbf{1} + 0.1725\,\sigma_0^z + 0.1725\,\sigma_1^z - 0.22\,\sigma_2^z - 0.22\,\sigma_3^z + 0.1675\,\sigma_1^z\sigma_0^z + 0.12\,\sigma_2^z\sigma_0^z + 0.165\,\sigma_2^z\sigma_1^z + 0.165\,\sigma_3^z\sigma_0^z + 0.12\,\sigma_3^z\sigma_1^z + 0.175\,\sigma_3^z\sigma_2^z - 0.0225\,\sigma_3^x\sigma_2^x\sigma_1^x\sigma_0^x - 0.0225\,\sigma_3^x\sigma_2^x\sigma_1^y\sigma_0^y - 0.0225\,\sigma_3^x\sigma_2^y\sigma_1^x\sigma_0^y + 0.0225\,\sigma_3^x\sigma_2^y\sigma_1^y\sigma_0^x + 0.0225\,\sigma_3^y\sigma_2^x\sigma_1^x\sigma_0^y - 0.0225\,\sigma_3^y\sigma_2^x\sigma_1^y\sigma_0^x - 0.0225\,\sigma_3^y\sigma_2^y\sigma_1^x\sigma_0^x - 0.0225\,\sigma_3^y\sigma_2^y\sigma_1^y\sigma_0^y$$

- The Bravyi-Kitaev spin Hamiltonian for $H_2$

$$-0.8175\,\mathbf{1} + 0.1725\,\sigma_0^z + 0.1675\,\sigma_1^z - 0.22\,\sigma_2^z + 0.1725\,\sigma_1^z\sigma_0^z + 0.12\,\sigma_2^z\sigma_0^z + 0.175\,\sigma_3^z\sigma_1^z - 0.0225\,\sigma_2^x\sigma_0^x - 0.0225\,\sigma_2^y\sigma_0^y + 0.0225\,\sigma_2^x\sigma_1^z\sigma_0^x + 0.0225\,\sigma_2^y\sigma_1^z\sigma_0^y + 0.165\,\sigma_2^z\sigma_1^z\sigma_0^z + 0.12\,\sigma_3^z\sigma_2^z\sigma_0^z - 0.0225\,\sigma_3^z\sigma_2^x\sigma_0^x - 0.0225\,\sigma_3^z\sigma_2^y\sigma_0^y - 0.22\,\sigma_3^z\sigma_2^z\sigma_1^z + 0.0225\,\sigma_3^z\sigma_2^x\sigma_1^z\sigma_0^x + 0.0225\,\sigma_3^z\sigma_2^y\sigma_1^z\sigma_0^y + 0.165\,\sigma_3^z\sigma_2^z\sigma_1^z\sigma_0^z$$

- These two Hamiltonians are isospectral.
- Let's compare the computational cost of simulating them

# Accuracy vs cost




Chemical accuracy

Second order trotter Bravyi-Kitaev

Second order trotter Jordan Wigner

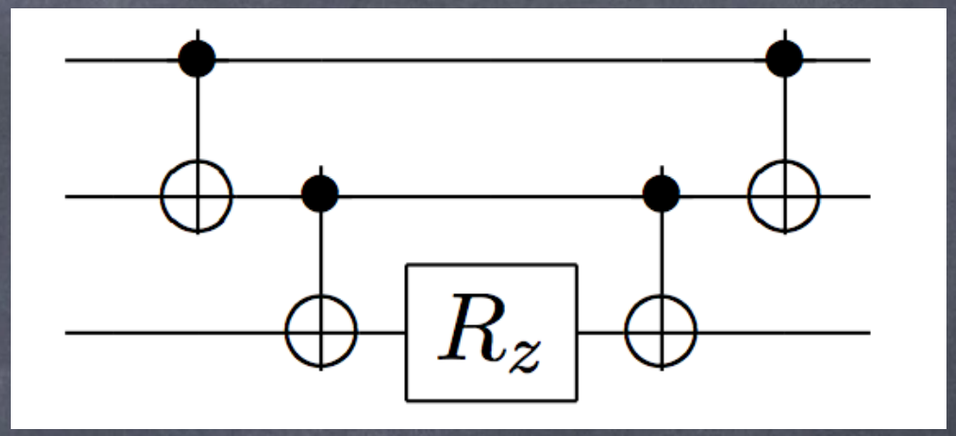
222 vs 328 gates

# Special Purpose Hardware: Ion Traps

# Strings and ladders

- Exponentiating products of Pauli-Z matrices:

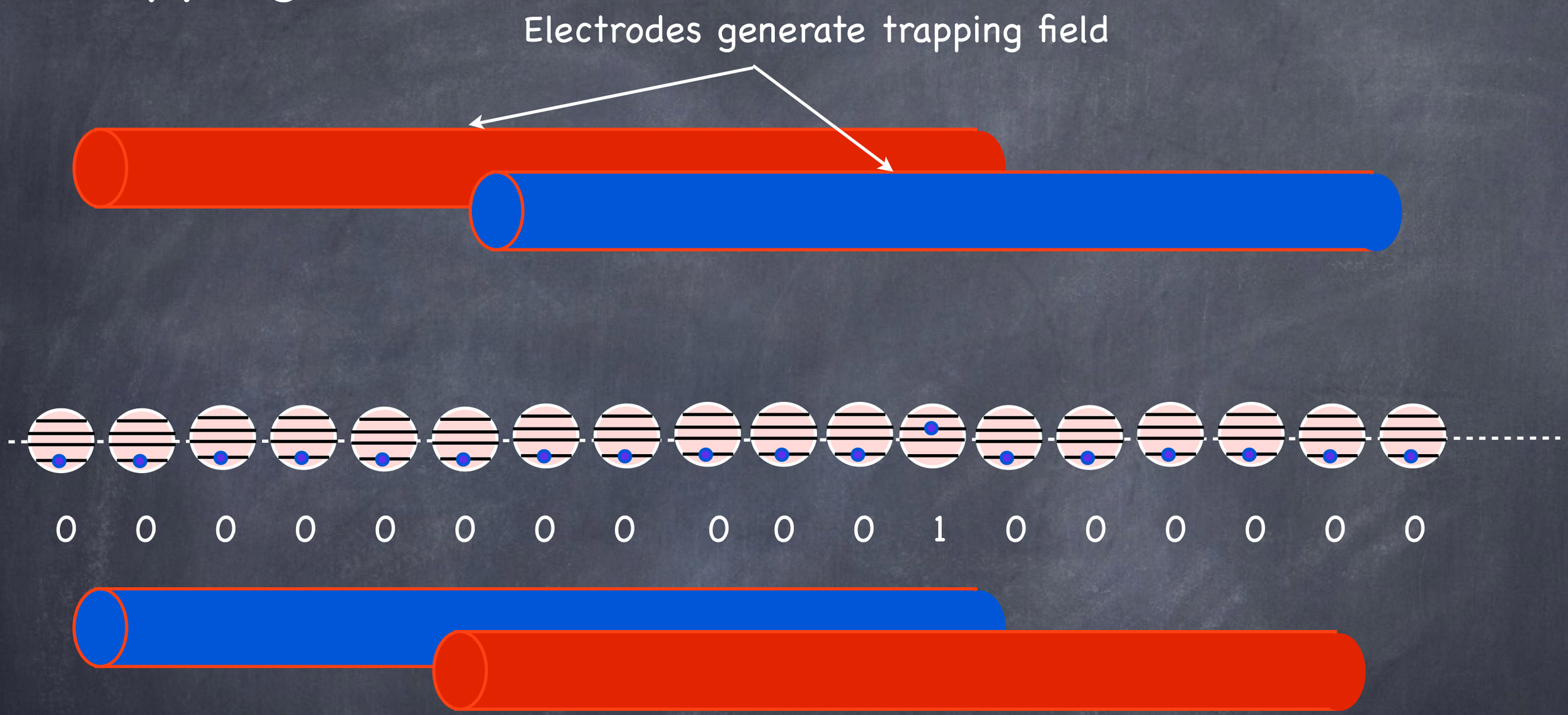
$$e^{i(\sigma^z \otimes \sigma^z \otimes \sigma^z)}$$




These ladders are hard to implement and are O(log n) long in BK for CNOT but O(1) for log n qubit Molmer-Sorenson gates

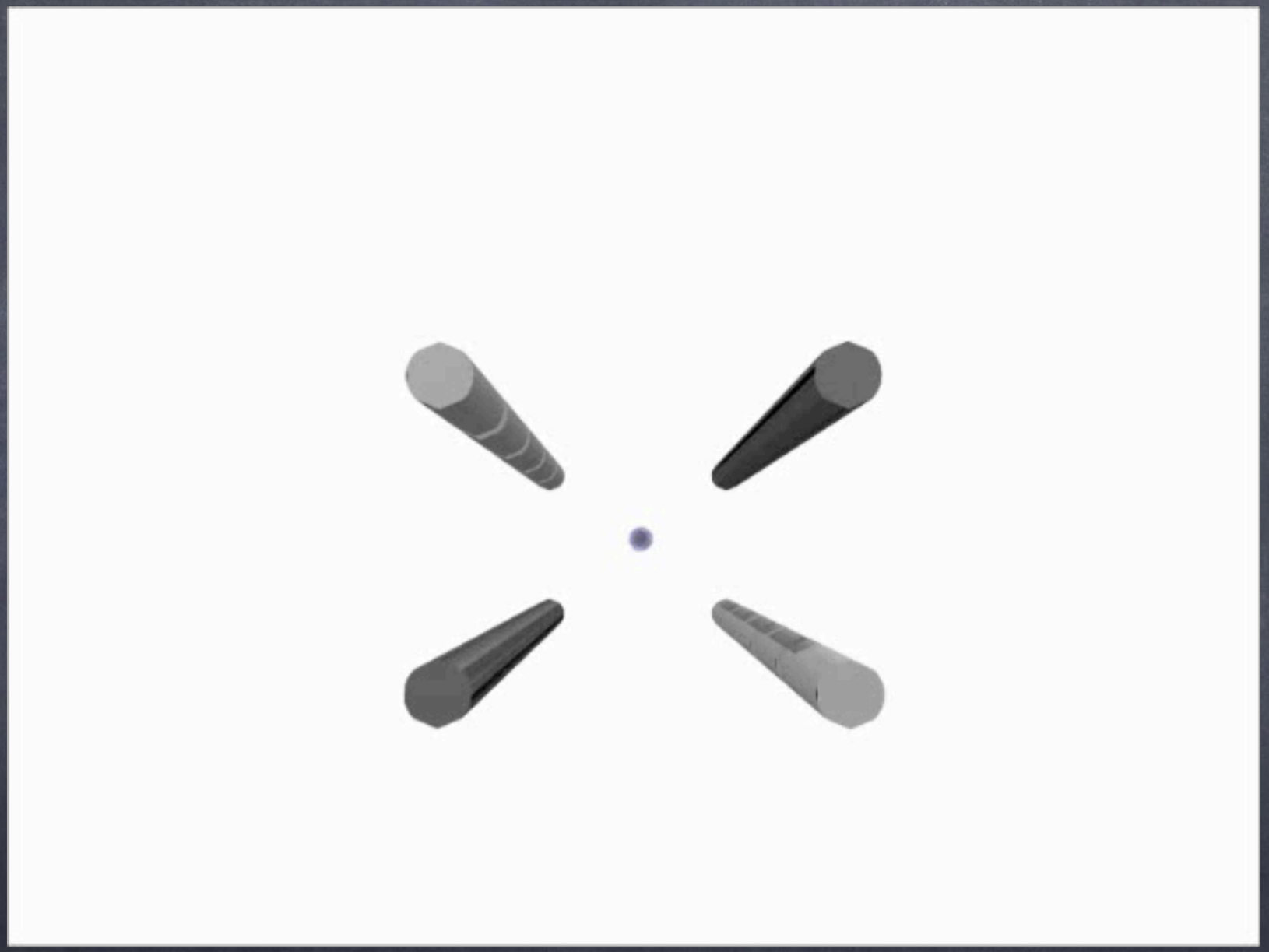
Scalable!

# Trapping Ions




From transistor to trapped-ion computers for quantum chemistry
M.-H. Yung, J. Casanova, A. Mezzacapo, J. McClean, L. Lamata, A. Aspuru-Guzik, E. Solano, arXiv:1307.4326

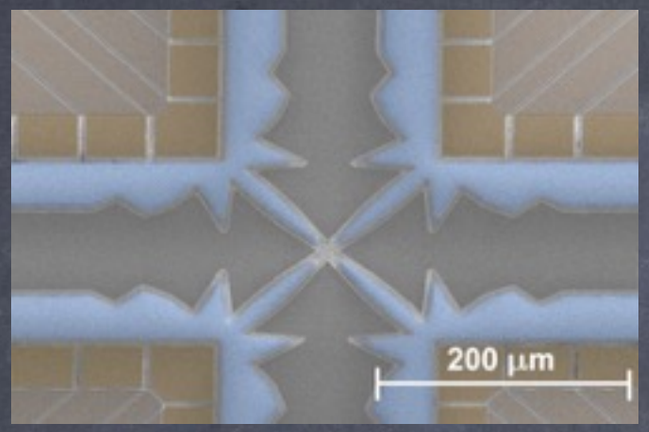
# Fabricating Surface Traps



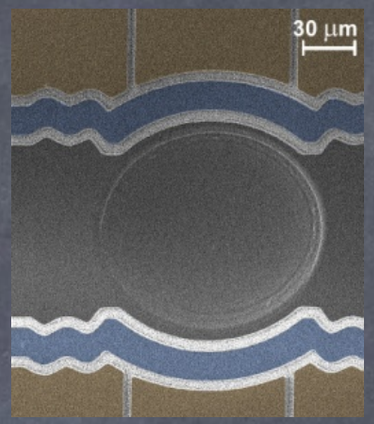
Movie credit: Georgia Tech Research Institute (GTRI)

# Components for scalable ion traps

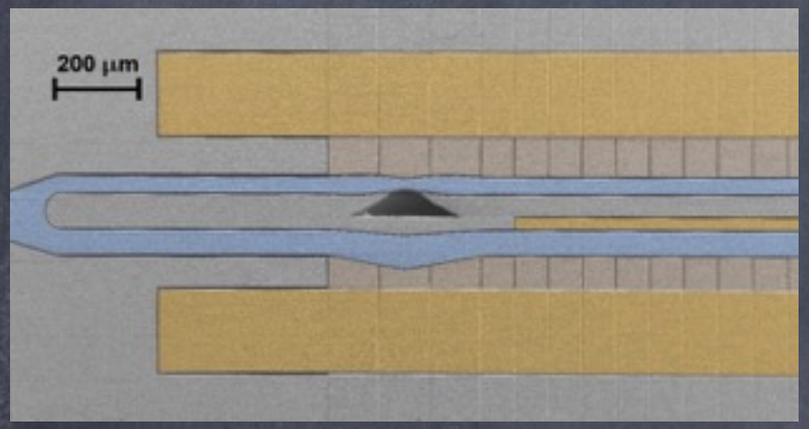
Junctions

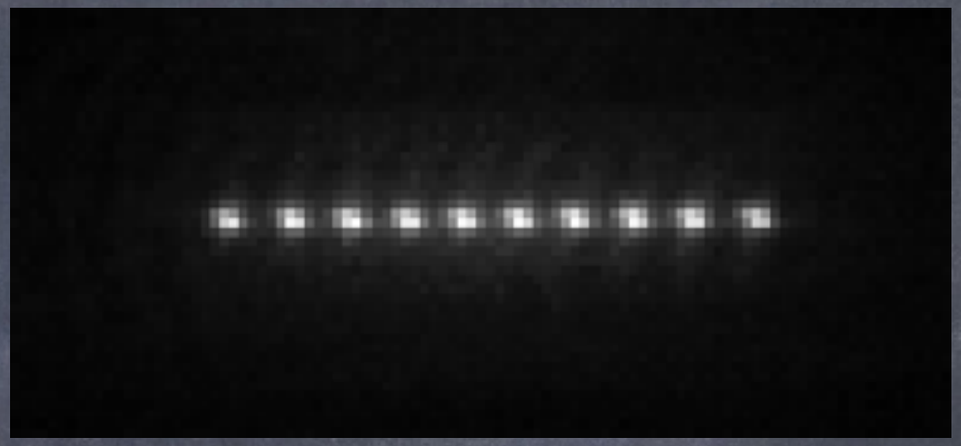



Mirror

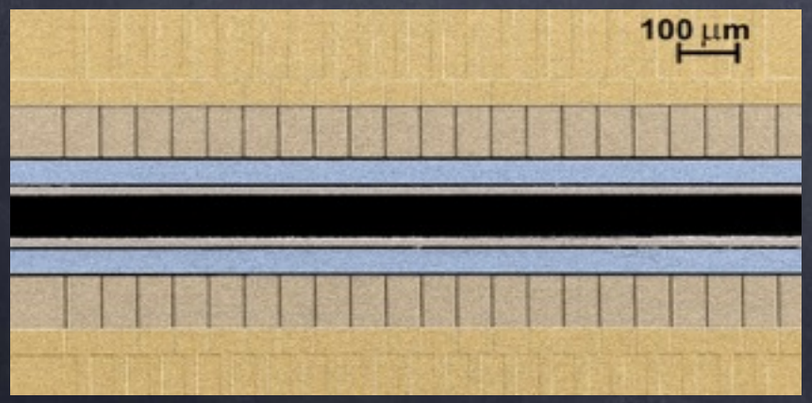


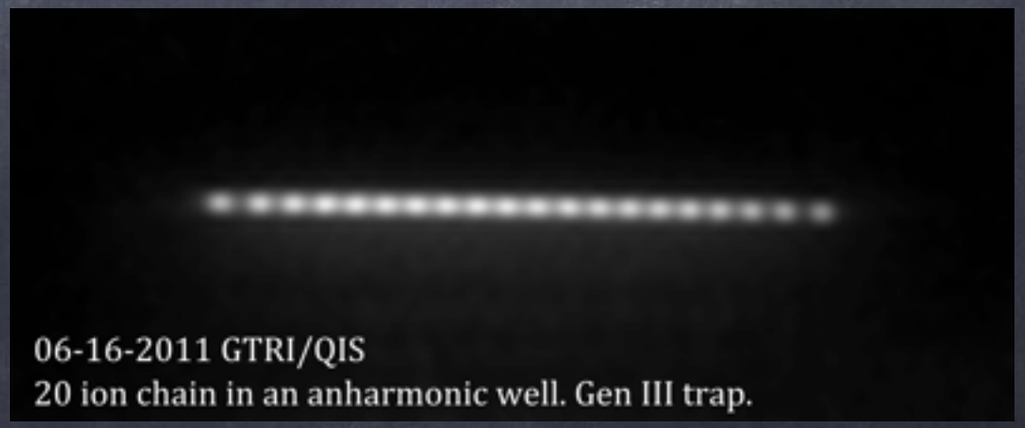

Gen II linear trap



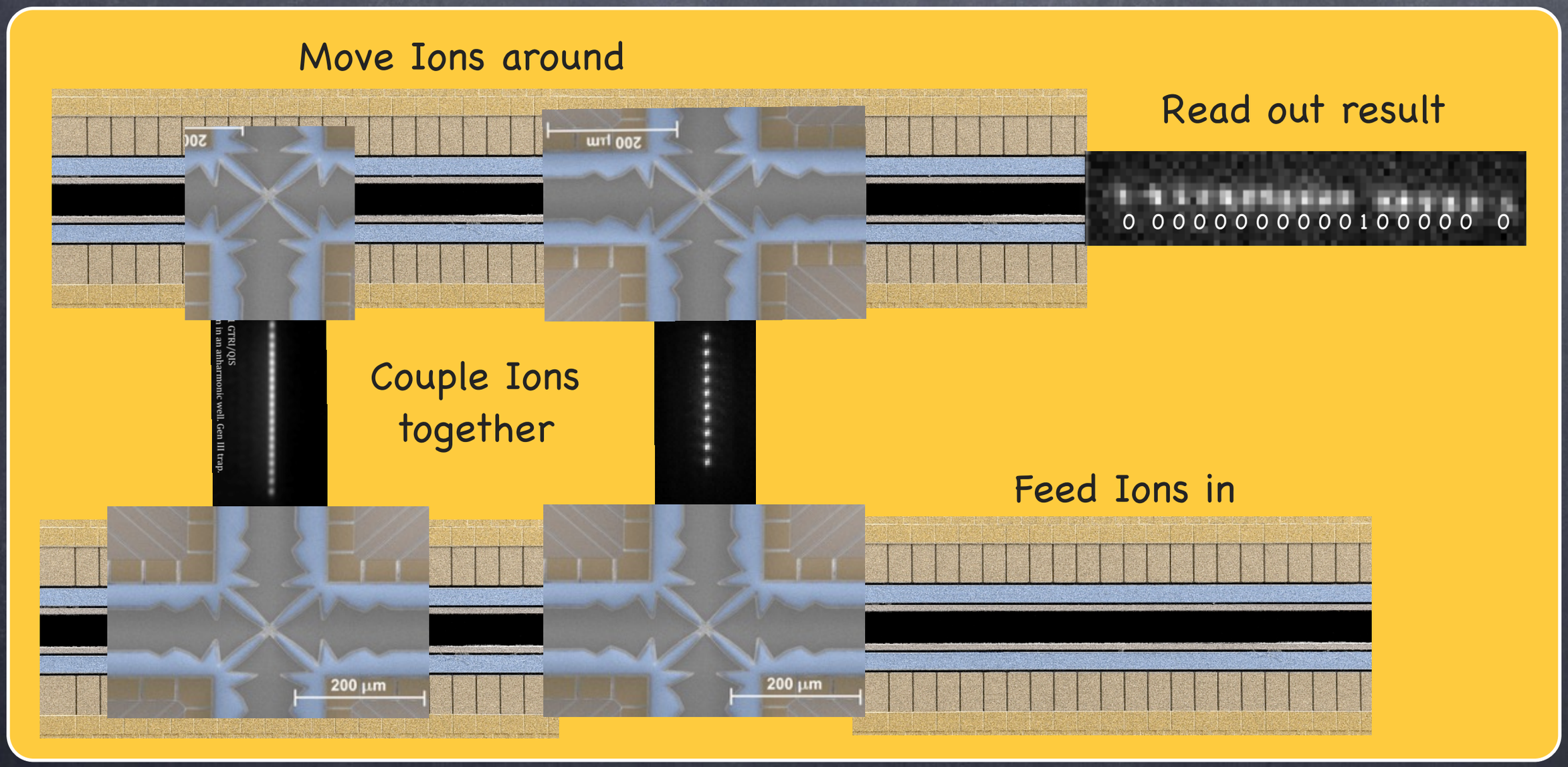
Gen III linear trap



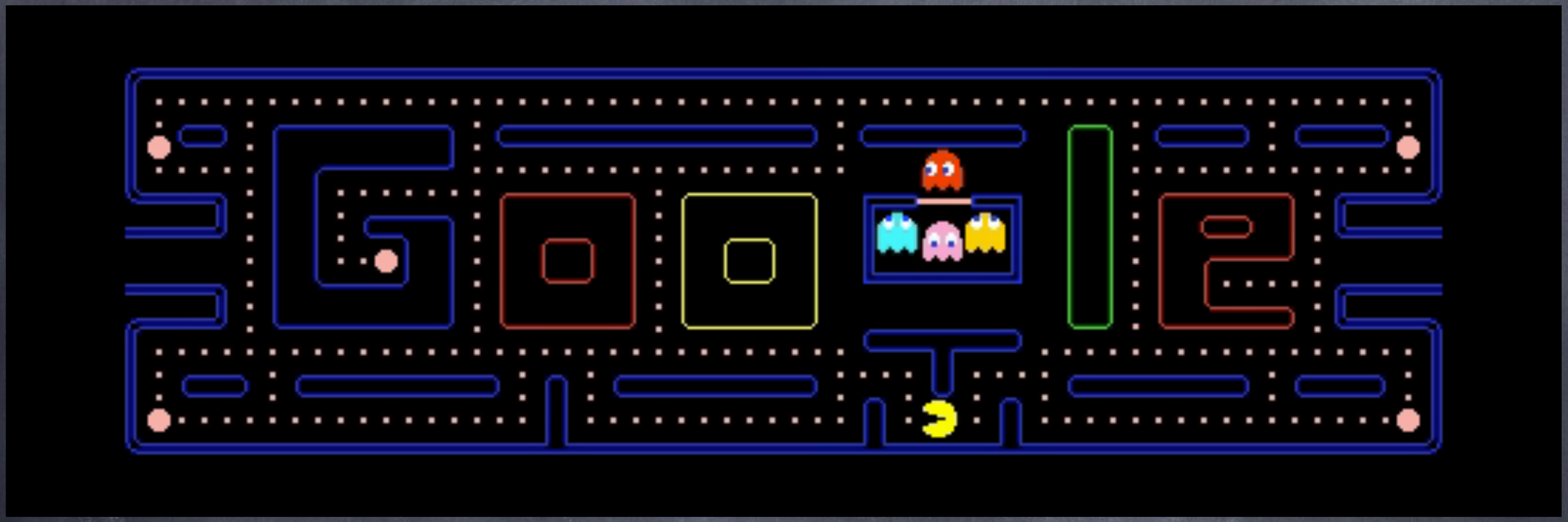




S. C. Doret et al. New J. Phys. 14, 073012 (2012),
J. T. Merrill et al, New J. Phys. 13, 103005 (2011)

# What should we build?

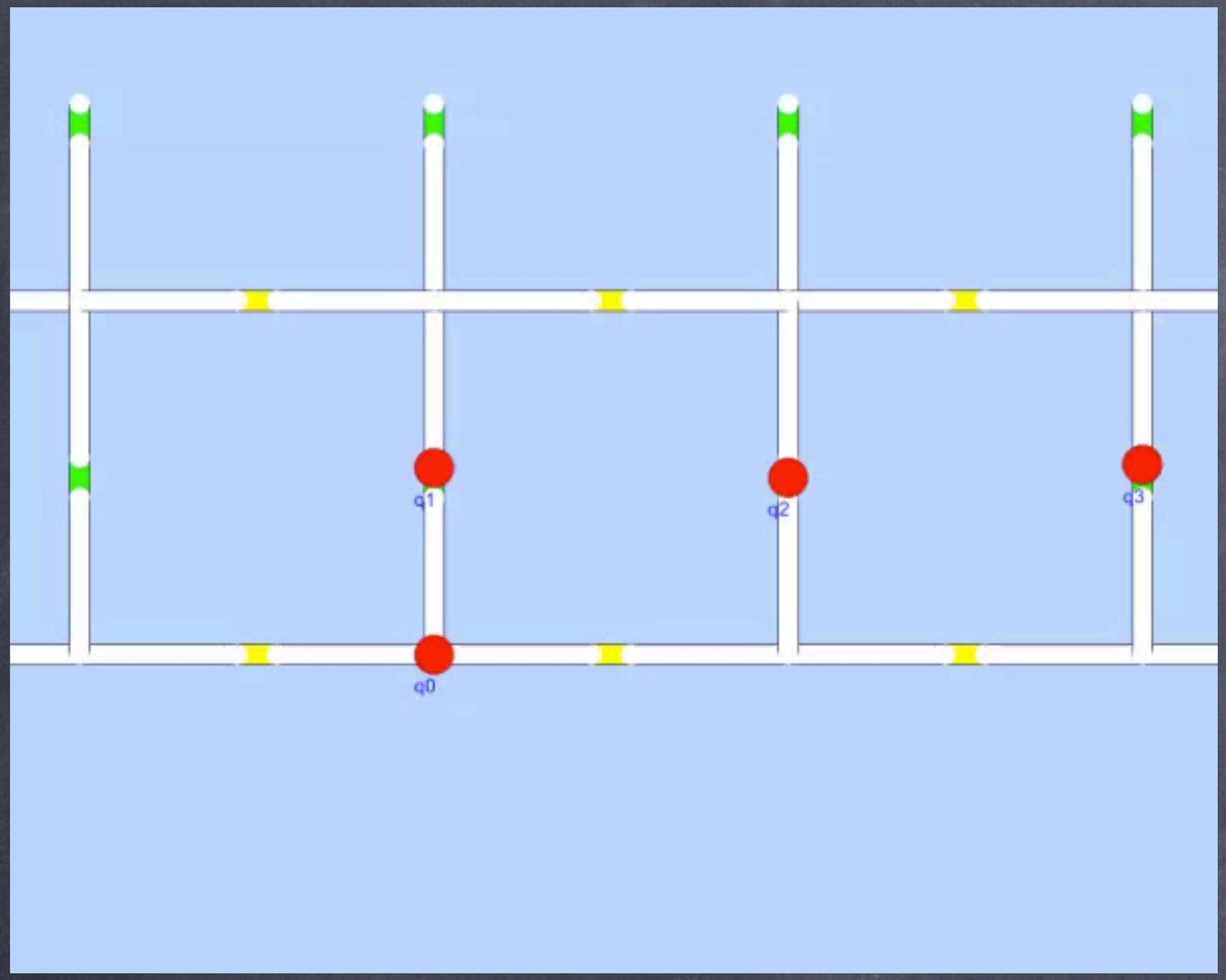


# The Pac Man Quantum Computer



Research Problem - what is the best Pac Man Maze for Chemical calculations?

Answer implied by : J. T. Seeley, M. Richard, P. J. Love J. Chem. Phys. **137**, 224109 (2012)

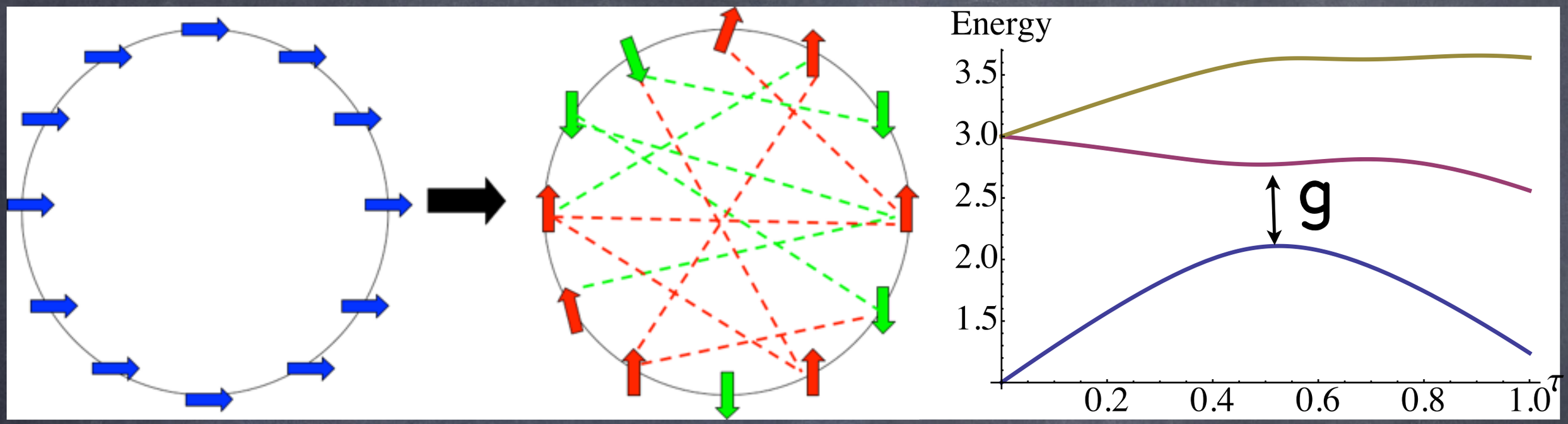



# Preliminary Results

- Bravyi-Kitaev makes Molmer-Sorensen simulation of interacting fermions SCALABLE
- Motivates development of M-S gates on surface trap

# Special Purpose Hardware: Adiabatic

# The Adiabatic Model

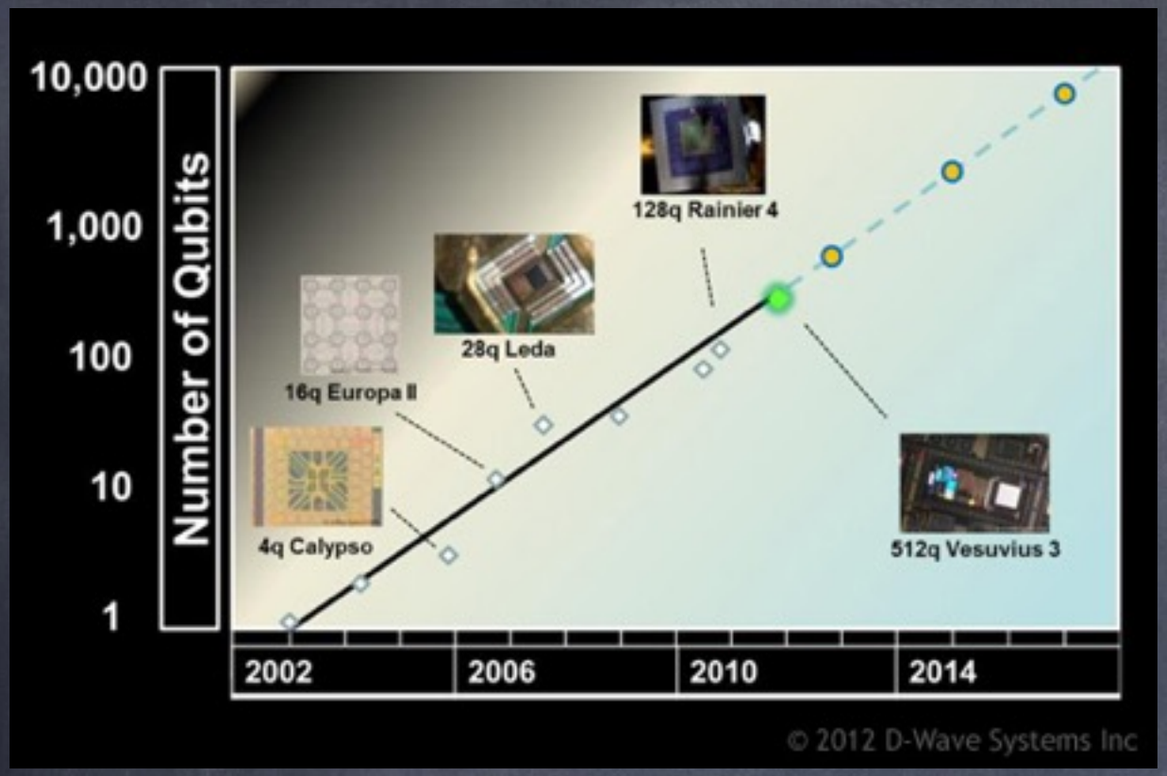


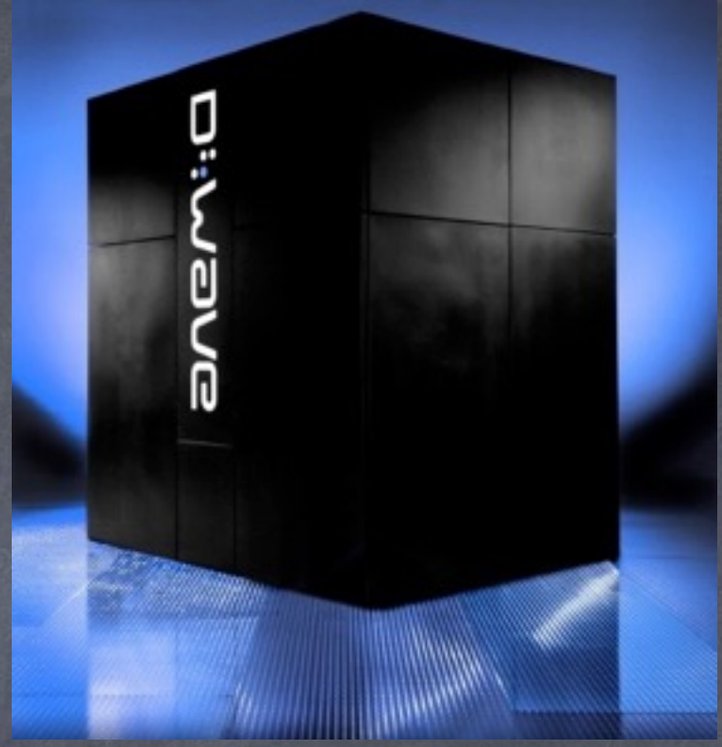

$$H_i = g\sum_i X_i \rightarrow (1-s)H_i + sH_f \rightarrow H_f = \sum_{\langle i,j\rangle} J_{ij} Z_i Z_j + \sum_i h_i Z_i$$

$$T \gg \max_s \frac{|\langle 1;s|\,\dot{H}(s)\,|0;s\rangle|}{g^2}$$

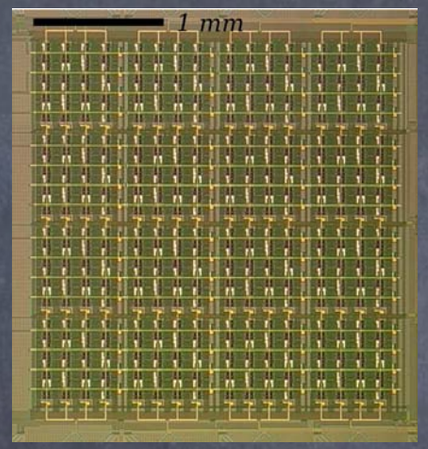
Quantum Computation by Adiabatic Evolution, Edward Farhi, Jeffrey Goldstone, Sam Gutmann, Michael Sipser, quant-ph/0001106v1

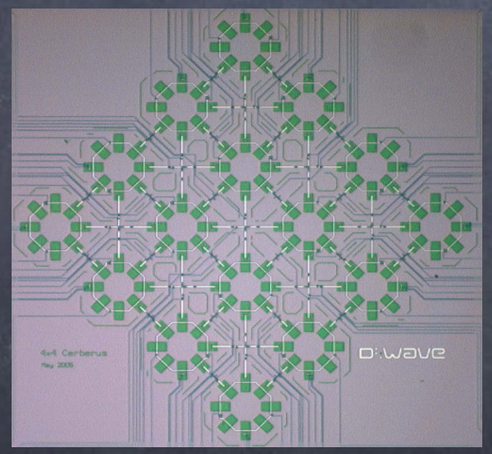
# The Rise of the Machines



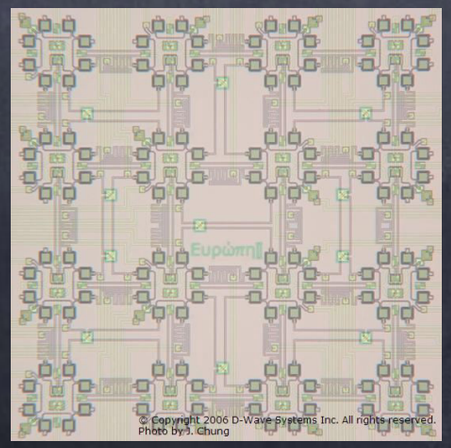




2011

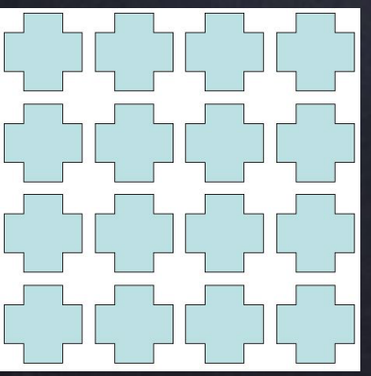



2007




2005

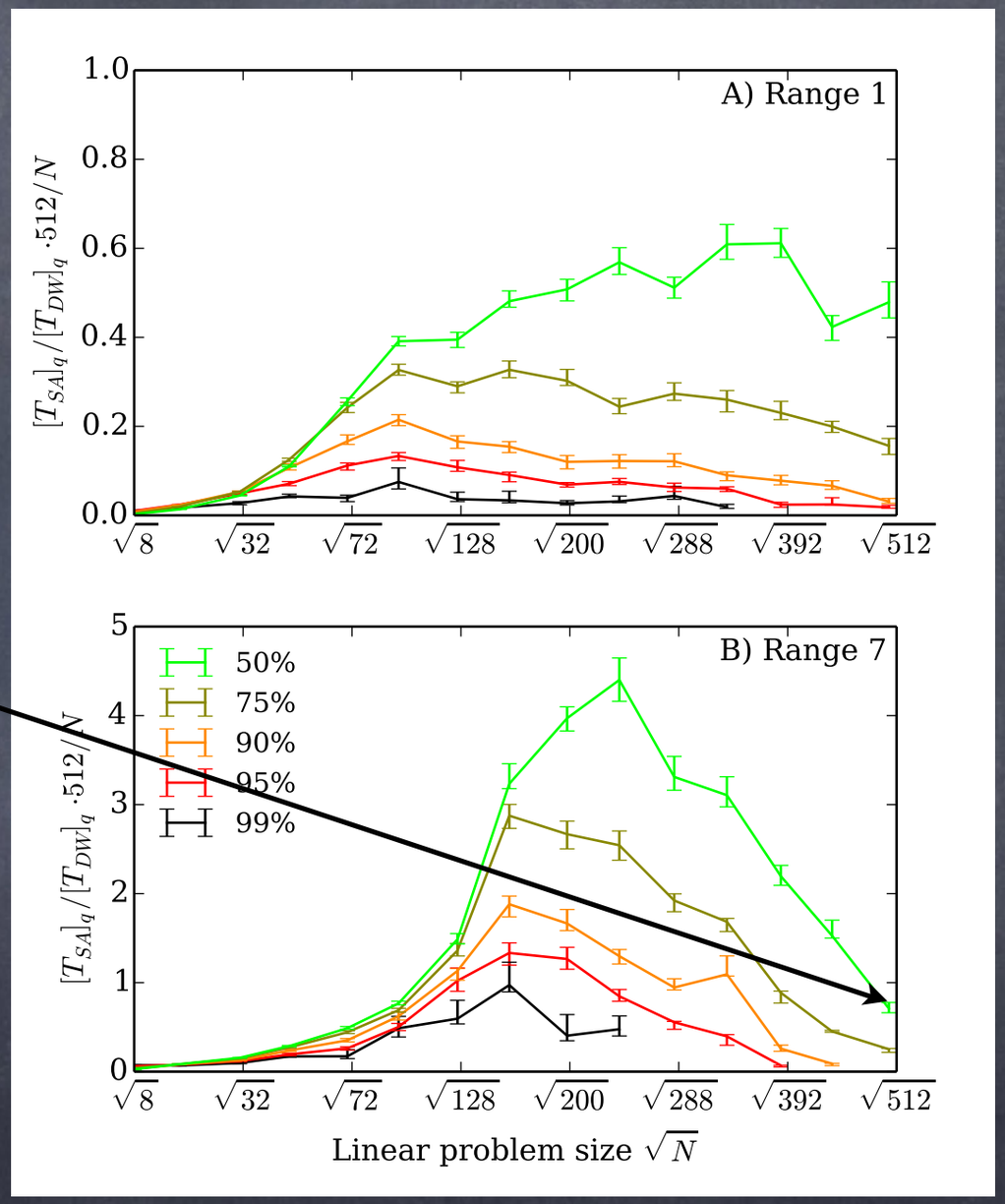


# ...and their fall?

**Defining and detecting quantum speedup**

Troels F. Rønnow,[1] Zhihui Wang,[2] Joshua Job,[3] Sergio Boixo,[4] Sergei V. Isakov,[5] David Wecker,[6] John M. Martinis,[7] Daniel A. Lidar,[8] and Matthias Troyer*[1]

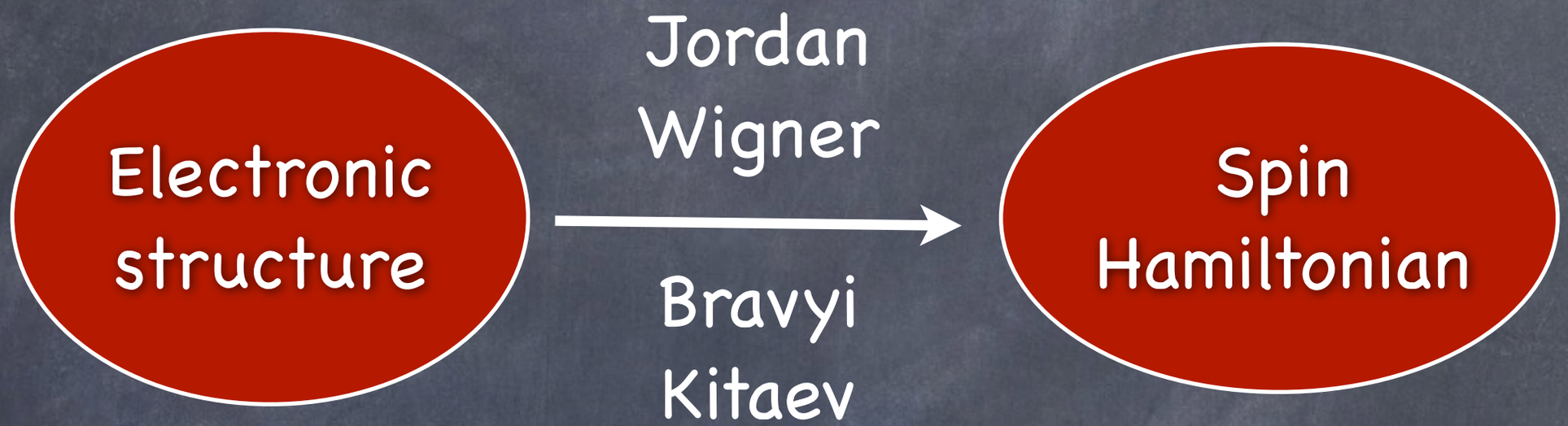
Speedup absent for large problems (BAD)




arXiv:1401.2910v1

"Comparing the performance of the device on random spin glass instances with limited precision to simulated classical and quantum annealers, we find no evidence of quantum speedup when the entire data set is considered, and obtain inconclusive results when comparing subsets of instances on an instance-by-instance basis."

Could we develop a useful device for simulation from this?

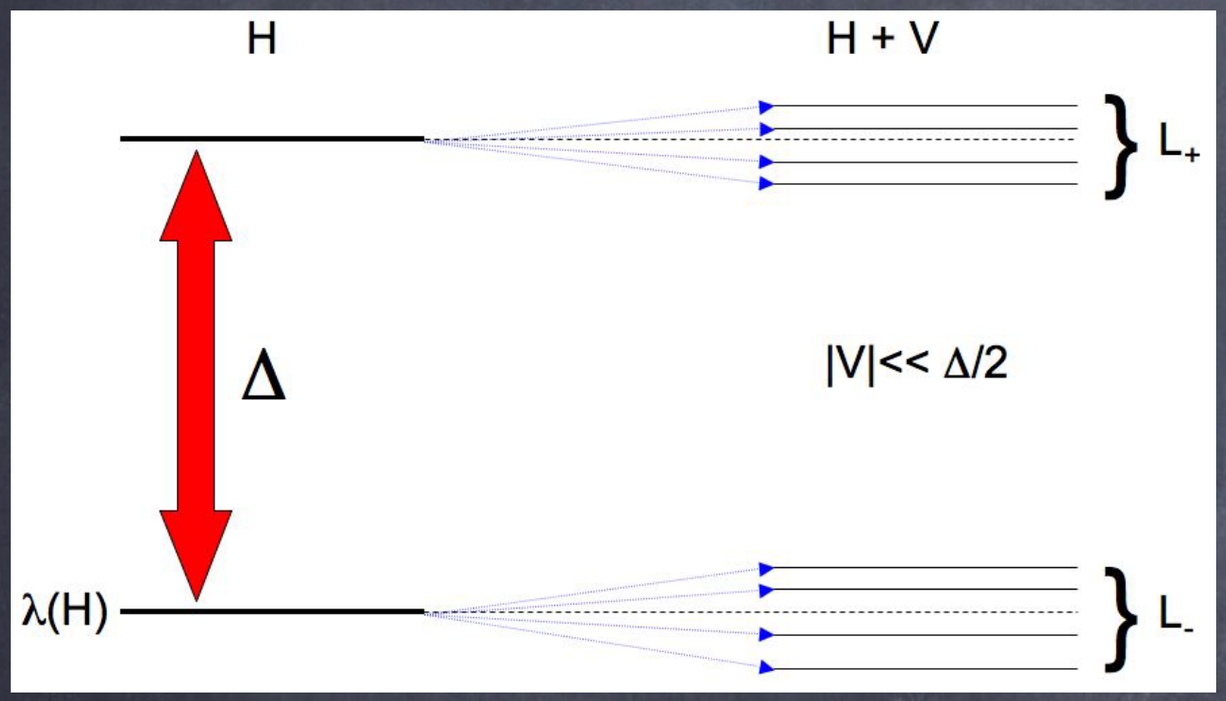


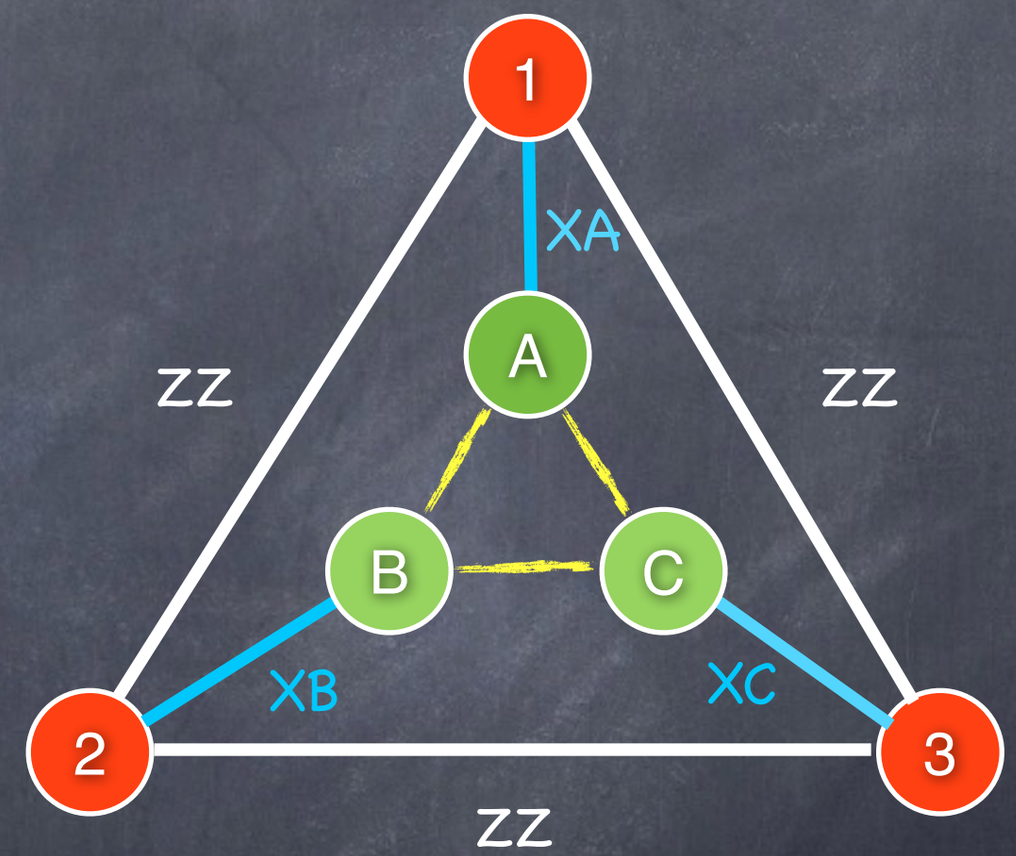

Can we build an adiabatic device for these spin Hamiltonians, instead of the classical Ising model?

Two problems 1) Not Ising form -non-ZZ couplings
2) Not two local - have high weight operators

# Gadgets

Generate k-local interactions in an effective Hamiltonian at kth order in perturbation theory using k-ancilla



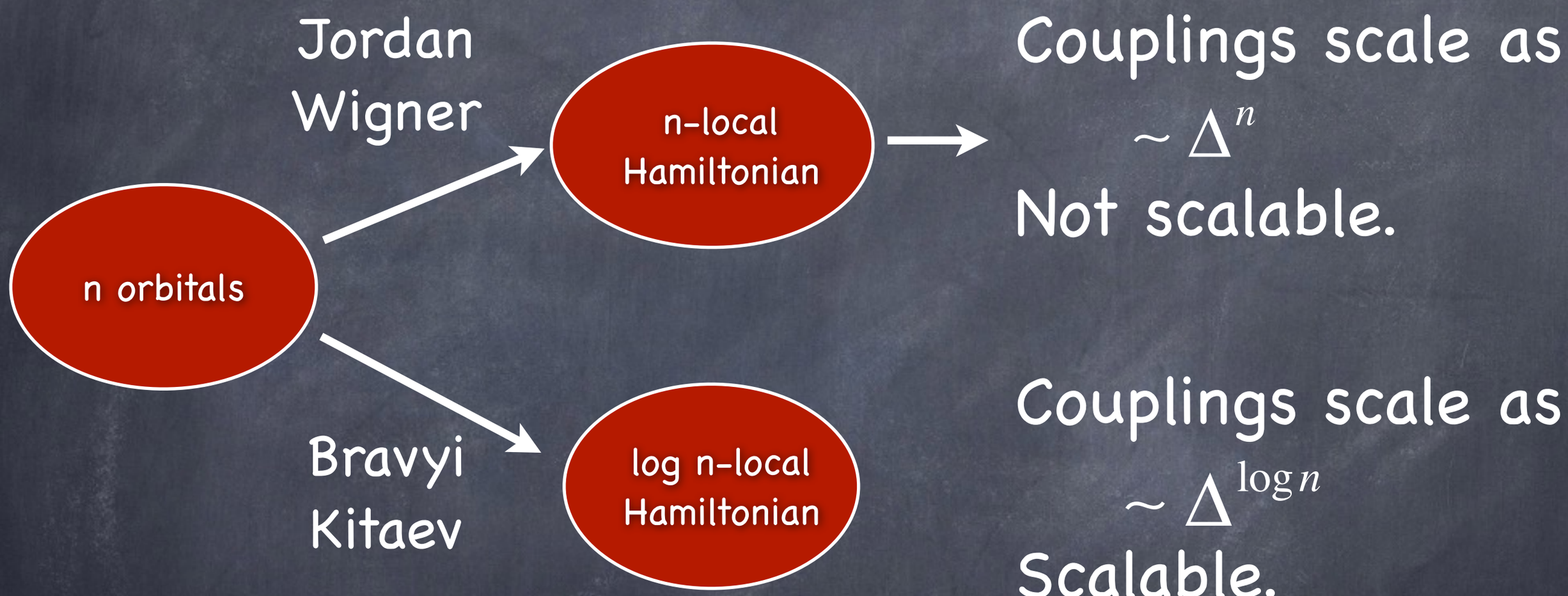

$$H_T = A \bullet B \bullet C$$

$$H_{anc} = -\Delta\left(Z_1 \otimes Z_2 + Z_1 \otimes Z_3 + Z_2 \otimes Z_3\right)$$

$$V = \left(\frac{\Delta^2}{6}\right)^{1/3}\left(A \otimes X_1 + B \otimes X_2 + C \otimes X_3\right)$$

$$H_{eff} = V_- + \frac{1}{\Delta}\sum_{k=2}^{\infty} V_{+-}\left(\frac{V_+}{\Delta}\right)^{k-2} V_{-+}$$

# Jordan-Wigner vs Bravyi-Kitaev




Babbush, R., Love, P. J. & Aspuru-Guzik, A. Adiabatic Quantum Simulation of Quantum Chemistry. 1311.3967v2 (2013).

# What couplings are needed?

$$\alpha Y_i Y_j \rightarrow \underbrace{-\alpha X_i X_j}_{A} \underbrace{Z_i Z_j}_{B}$$

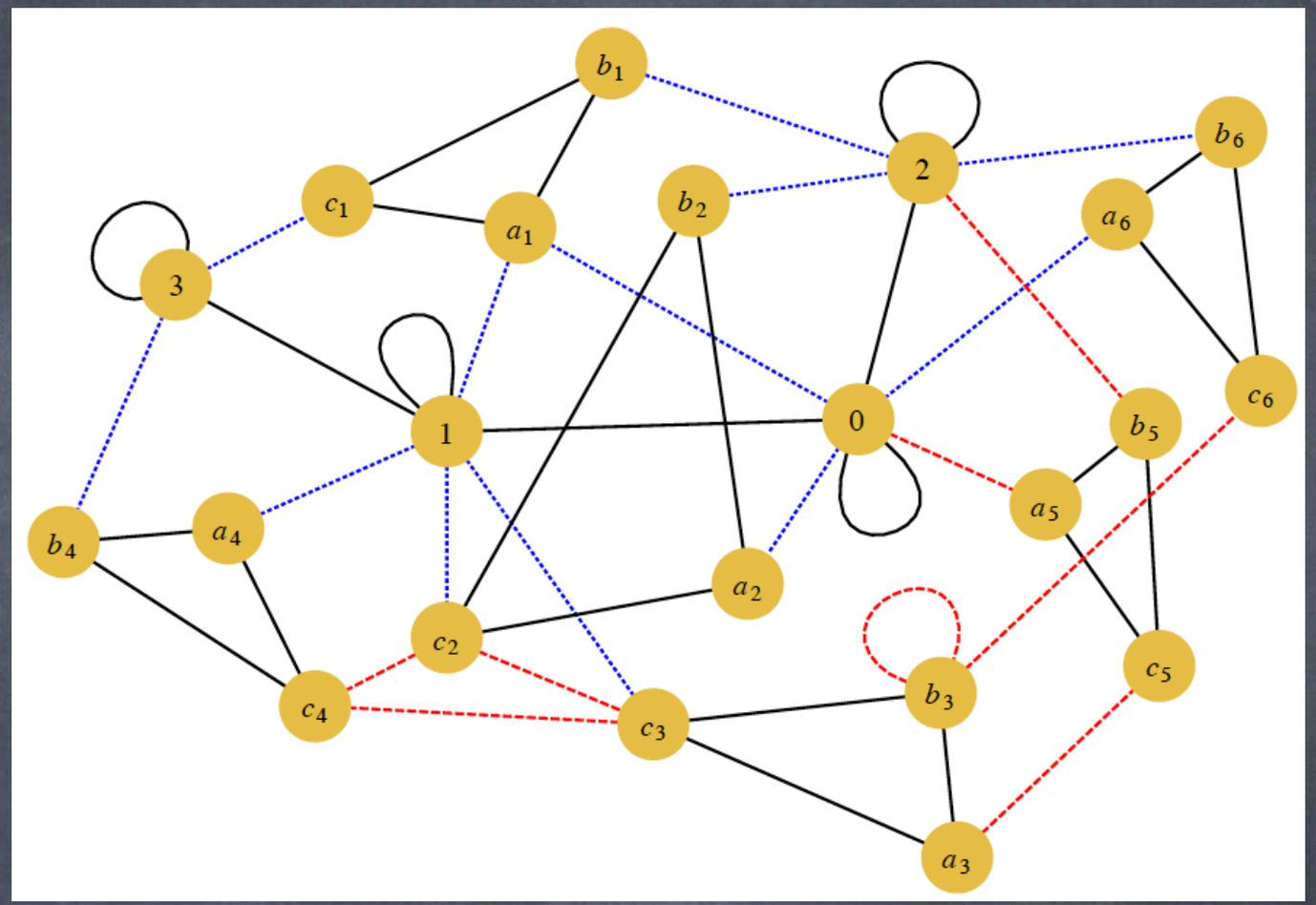
Gadgets reduce locality - they can also reduce the types of interaction to XX, ZZ and XZ

This quantum simulator has the same couplings as a Universal AQC, but not the clock

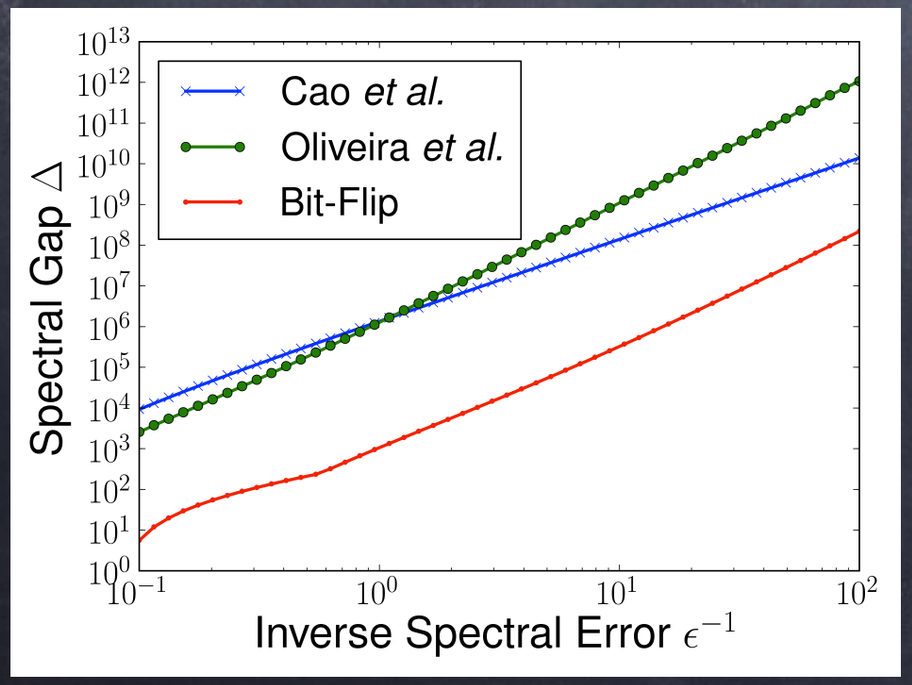
Intermediate between quantum annealing and Universal AQC

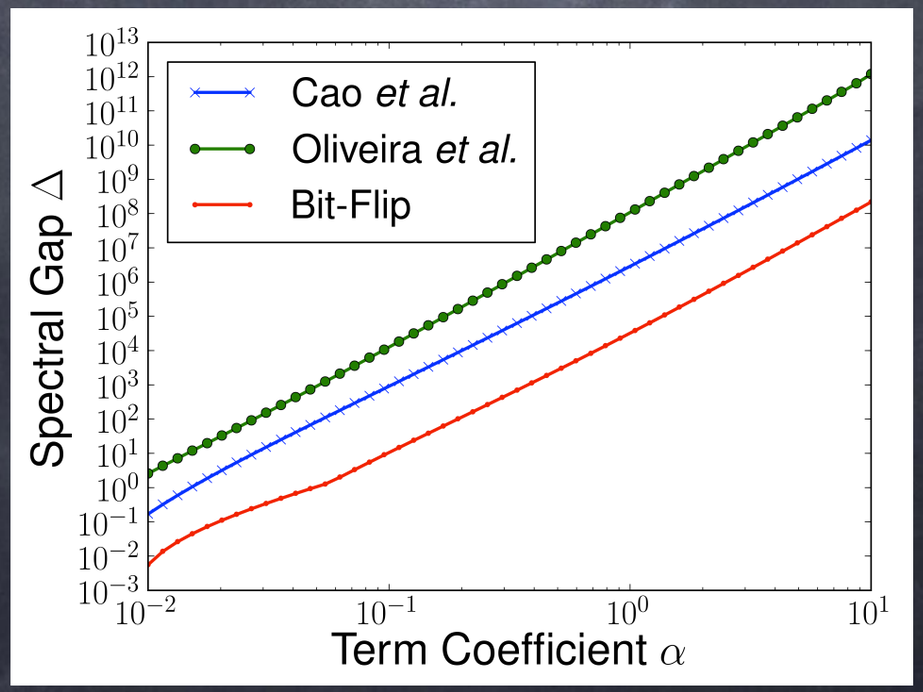
Biamonte, J. D. & Love, P. J. Realizable Hamiltonians for universal adiabatic quantum computers. Phys Rev A 78, 012352 (2008).
Babbush, R., Love, P. J. & Aspuru-Guzik, A. Adiabatic Quantum Simulation of Quantum Chemistry. 1311.3967v2 (2013).

For the example of H2 in a minimal basis




For a single gadget:



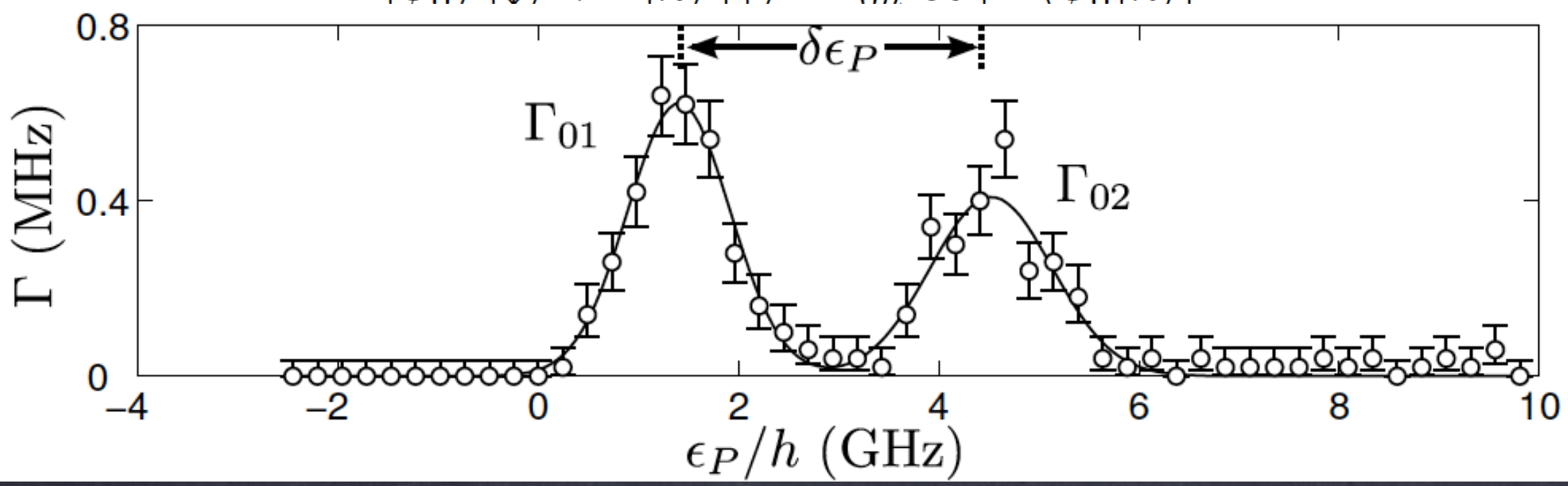
# Readout energies using the tunneling spectroscopy of a probe qubit

$$H_P = \frac{\epsilon}{2}\left(\mathbf{1}_P - Z_P\right) - \frac{\Delta}{2}X_P = \epsilon\left|\downarrow\right\rangle\left\langle\downarrow\right|_P - \frac{\Delta}{2}X_P$$

$$H_{S+P} = H_S + H_P - JZ_S \otimes \left(\mathbf{1}_P - Z_P\right) = H_S + H_P - 2JZ_S \otimes \left|\downarrow\right\rangle\left\langle\downarrow\right|_P$$

$$H_{S+P} = \underbrace{\left(\epsilon - 2JZ_S + H_S\right) \otimes \left|\downarrow\right\rangle\left\langle\downarrow\right|_P}_{\mathcal{L}_\downarrow} + \underbrace{H_S \otimes \left|\uparrow\right\rangle\left\langle\uparrow\right|_P}_{\mathcal{L}_\uparrow} - \frac{\Delta}{2}X_P$$

$$\left|\psi_0^\downarrow\right\rangle\left|\downarrow\right\rangle \overset{\Gamma_{0n}}{\rightleftharpoons} \left|n\right\rangle\left|\uparrow\right\rangle : \Gamma_{0n} \propto \left|\Delta\langle\psi_0^\downarrow|n\rangle\right|^2$$




A. J. Berkley, A. J. Przybysz, T. Lanting, R. Harris, N. Dickson, F. Altomare, M. H. Amin, P. Bunyk, C. Enderud, E. Hoskinson, M. W. Johnson, E. Ladizinsky, R. Neufeld, C. Rich, A. Yu. Smirnov, E. Tolkacheva, S. Uchaikin, and A. B. Wilson. Tunneling Spectroscopy Using a Probe Qubit. Physical Review B. **87** 020502 2013.

# Removing Phase Estimation

# Quantum Variational/RDM methods

We want to find the smallest eigenvalue of:

$$\mathcal{H} = \sum_{i\alpha} h^i_\alpha \sigma^i_\alpha + \sum_{ij\alpha\beta} h^{ij}_{\alpha\beta} \sigma^i_\alpha \sigma^j_\beta + \ldots$$

Variationally minimize:

$$\langle \mathcal{H} \rangle = \sum_{i\alpha} h^i_\alpha \langle \sigma^i_\alpha \rangle + \sum_{ij\alpha\beta} h^{ij}_{\alpha\beta} \langle \sigma^i_\alpha \sigma^j_\beta \rangle + \ldots$$

Classically separate minimization of each term fails - rdms do not correspond to global state

Quantumly one can variationally minimize a global quantum state, evaluate terms separately

A variational eigenvalue solver on a quantum processor Alberto Peruzzo, Jarrod McClean, Peter Shadbolt, Man-Hong Yung, Xiao-Qi Zhou, Peter J Love, Alán Aspuru-Guzik, and Jeremy L O'Brien http://arxiv.org/abs/1304.3061v1

# The Unitary Coupled Cluster ansatz

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

Reference state usually Hartree-Fock ground state

$$T = T_1 + T_2 + T_3 + ... + T_N$$

$$T_1 = \sum_{pr} t_p^r \hat{a}_p^\dagger \hat{a}_r \quad T_2 = \sum_{pqrs} t_{pq}^{rs} \hat{a}_p^\dagger \hat{a}_q^\dagger \hat{a}_r \hat{a}_s$$

Truncated
Cluster Operator

$$T^{(k)} = \sum_{i=1}^{k} T_i$$

Classically construction of the coupled cluster state is challenging

Quantumly it is a particular time evolution from the Hartree Fock state

# Sparse Methods

# Beyond second quantized

00001011
00001010
00001001
00001000
00000111
00000110
00000101
00000100
00000011
00000010
00000001
00000000

Second quantization maps all particle sectors to qubits. n qubits for n orbitals.

But for electronic structure Hamiltonians the number of electrons is a good quantum number.

Minimal qubit number is $n_Q = \log_2 \begin{pmatrix} n_o \\ n_e \end{pmatrix}$

For fixed electron number use first quantized basis of Slater determinants and CI matrix

# The compact mapping

| | |
|---|---|
| 00001011 | (3,1,0) |
| 00001010 | (3,1) |
| 00001001 | (3,0) |
| 00001000 | (3) |
| 00000111 | (2,1,3) |
| 00000110 | (2,1) |
| 00000101 | (2,0) |
| 00000100 | (2) |
| 00000011 | (1,0) |
| 00000010 | (1) |
| 00000001 | (0) |
| 00000000 | () |

A basis state is specified by an electron configuration

Each configuration labels a Slater determinant

$$(2,1,3) \rightarrow \begin{vmatrix} \phi_1(r_1) & \phi_2(r_1) & \phi_3(r_1) \\ \phi_1(r_2) & \phi_2(r_2) & \phi_3(r_2) \\ \phi_1(r_3) & \phi_2(r_3) & \phi_3(r_3) \end{vmatrix}$$

How is the Hamiltonian expressed in this basis?

# The CI Matrix elements

1) Diagonal element: configurations do not differ

$$\left\langle \{\phi_i\} \middle| H \middle| \{\phi_i\} \right\rangle = \sum_{i=1}^{n_e} \left\langle \phi_i \middle| h_1 \middle| \phi_i \right\rangle + \sum_{i<j} \left( \langle ij|kl\rangle - \langle ij|lk\rangle \right)$$

2) Configurations differ by one

$$\left\langle \{\phi_i, \phi_q\} \middle| H \middle| \{\phi_i, \phi_p\} \right\rangle = \left\langle \phi_p \middle| h_1 \middle| \phi_q \right\rangle + \sum_{l}^{n_e} \left( \langle pl|ql\rangle - \langle pl|lq\rangle \right)$$

3) Configurations differ by two

$$\left\langle \{\phi_i, \phi_p, \phi_q\} \middle| H \middle| \{\phi_i, \phi_r, \phi_s\} \right\rangle = \left\langle \phi_p \phi_q \middle| h_1 \middle| \phi_r \phi_s \right\rangle + \left( \langle pq|rs\rangle - \langle pq|sr\rangle \right)$$

$$\langle ij|kl\rangle = \int \phi_i^*(\mathbf{x}_1)\phi_j^*(\mathbf{x}_2)\frac{1}{\mathbf{r}_{12}}\phi_k(\mathbf{x}_1)\phi_l(\mathbf{x}_2)d\mathbf{x}_1 d\mathbf{x}_2$$

# The CI Matrix is Sparse

$$d = \frac{1}{4} n_e (n_e - 1)(n_o - n_e)(n_o - n_e - 1) + n_e (n_o - n_e) + 1$$

Can apply sparse matrix techniques to this which require a number of calls polynomial in d, e.g.

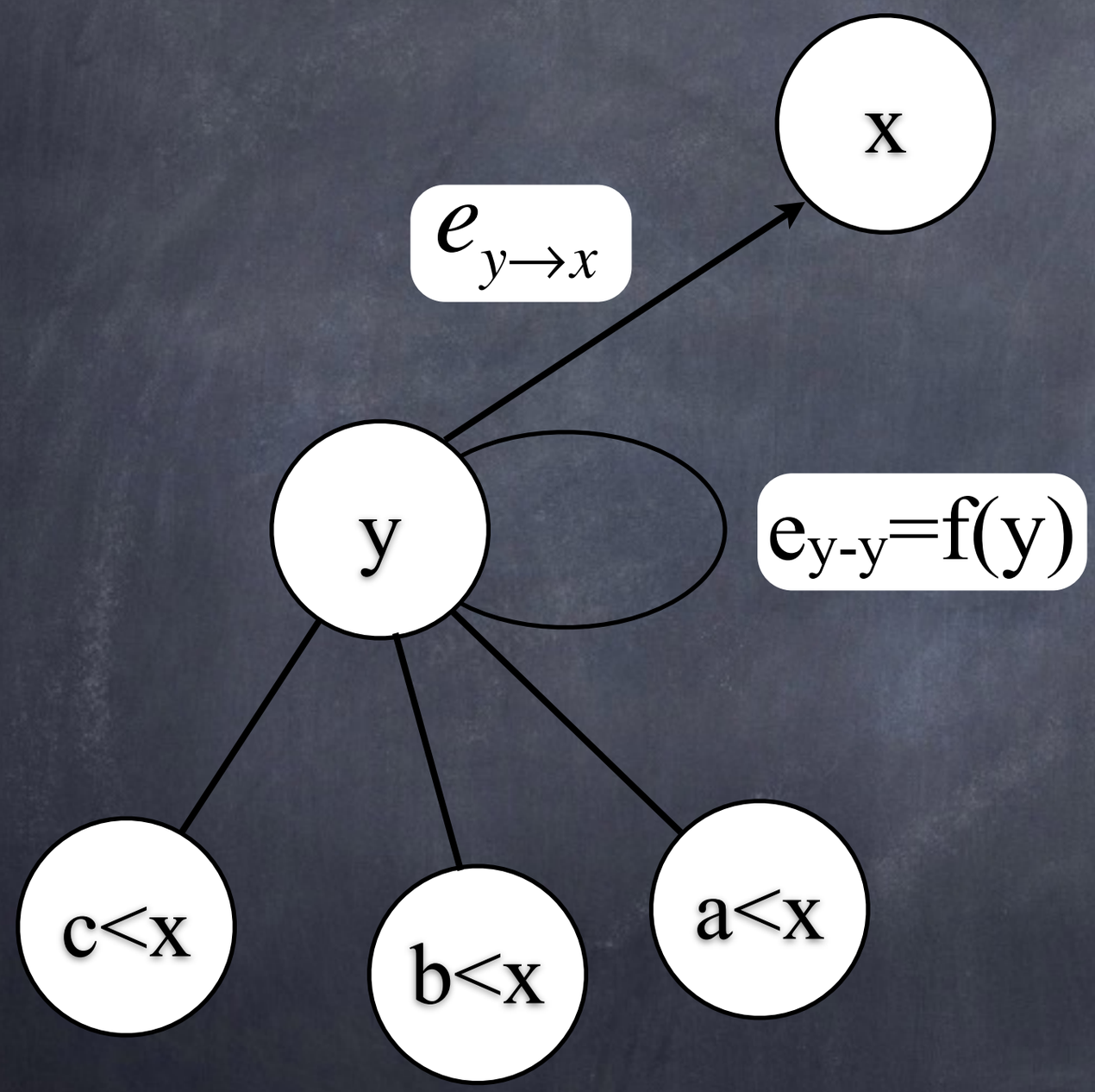
D. W. Berry and A. M. Childs, "Black-box Hamiltonian simulation and unitary implementation," Quantum Information and Computation, vol. 12, no. 1-2, pp. 29-62, 2012.

| | |
|---|---|
| For $\Lambda > ||H||$, $\Lambda_{\max} > ||H||_{\max}$ | $O(\Lambda t \frac{1}{\epsilon^{1/2}} + d||\Lambda_{\max}||t)$ |
| If $\epsilon d > ||H||t > \sqrt{\epsilon}$ | $O(d^{2/3}[\log\log d||H||t]^{4/3}\frac{1}{\epsilon})$ |
| If all terms have comparable norms | $O((\Lambda t)^{3/2}\sqrt{d}(\log d)^{7/4})\frac{1}{\sqrt{\epsilon}}$ |

Hence simulation of the CI matrix using these methods is efficient, and qubit optimal.

# Graph coloring for the CI matrix

A scheme using at most $d^2$ colors:




$e_{y\to x}$ # of nodes $x' \leq x$ to which y is connected. It is the number of nodes connected to y that come before x

This gives a pair of labels for each undirected edge

Can prove for CI matrix this gives a 1-sparse decomposition

Quantum Algorithms for Quantum Chemistry based on the sparsity of the CI-matrix, Borzu Toloui, Peter J. Love, arXiv:1312.2579

Using the definition of the CI matrix.

1) Diagonal element: configurations do not differ

$$\left\langle \{\phi_i\} \middle| H \middle| \{\phi_i\} \right\rangle$$ Label 0

2) Configurations differ by one

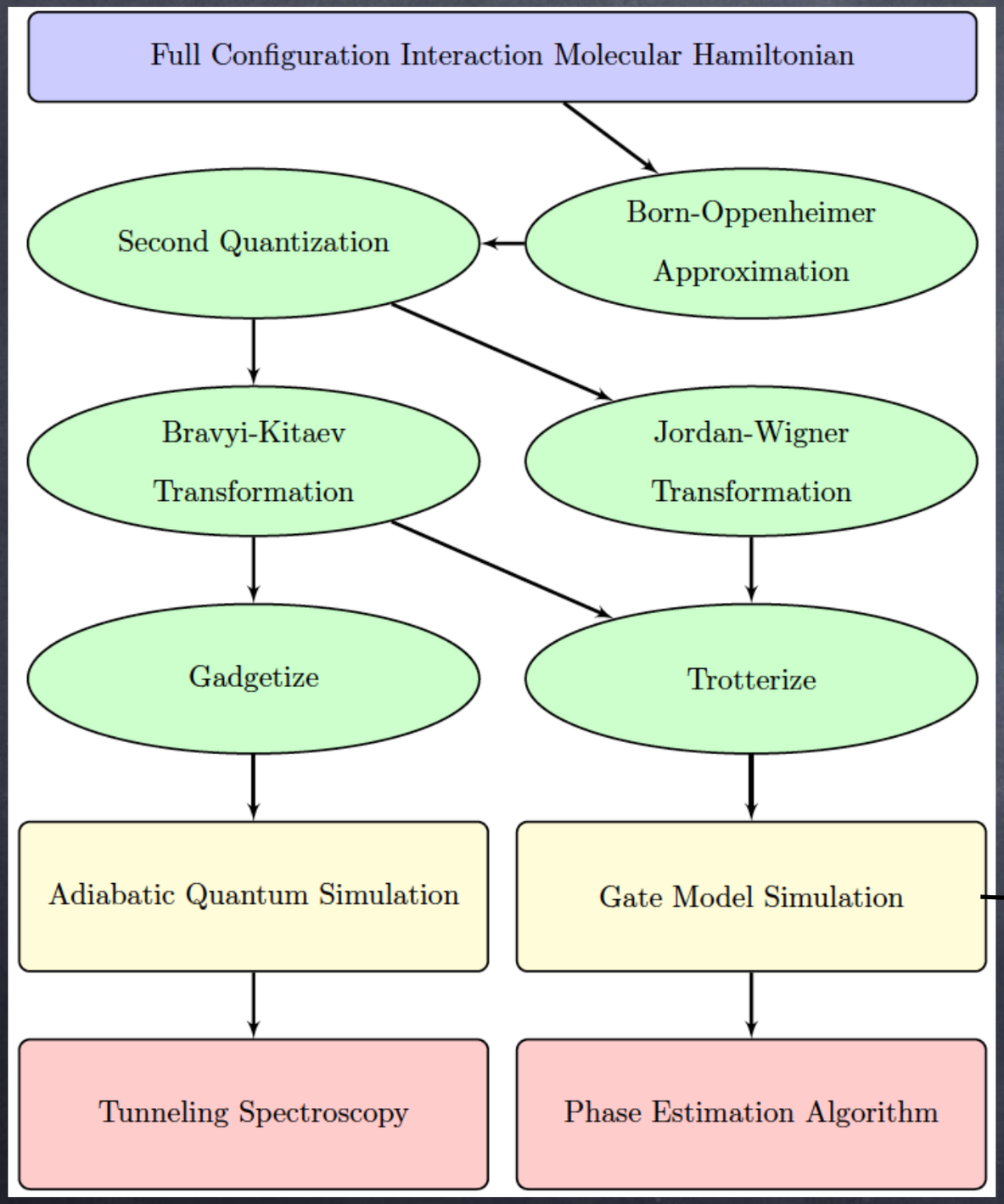
$$\left\langle \{\phi_i, \phi_q\} \middle| H \middle| \{\phi_i, \phi_p\} \right\rangle$$ Label (p,q)

3) Configurations differ by two

$$\left\langle \{\phi_i, \phi_p, \phi_q\} \middle| H \middle| \{\phi_i, \phi_r, \phi_s\} \right\rangle$$ Label (p,q,r,s)

This gives exactly d colors

# Conclusions




Many algorithmic improvements

None exploit structure of problem beyond the definition of the electronic structure problem

Further simulation studies and experiments needed to assess new methods

Connection to CI matrix may enable theoretical progress in bounding cost of state preparation

Variational Methods

Recent dramatic progress in sparse methods yet to be considered

Exponential improvement in precision for simulating sparse Hamiltonians, Dominic W. Berry, Andrew M. Childs, Richard Cleve, Robin Kothari, Rolando D. Somma arxiv:1312.1414

# Thanks!

NSF

QIQC

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BE THE FUTURE

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HHMI
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