

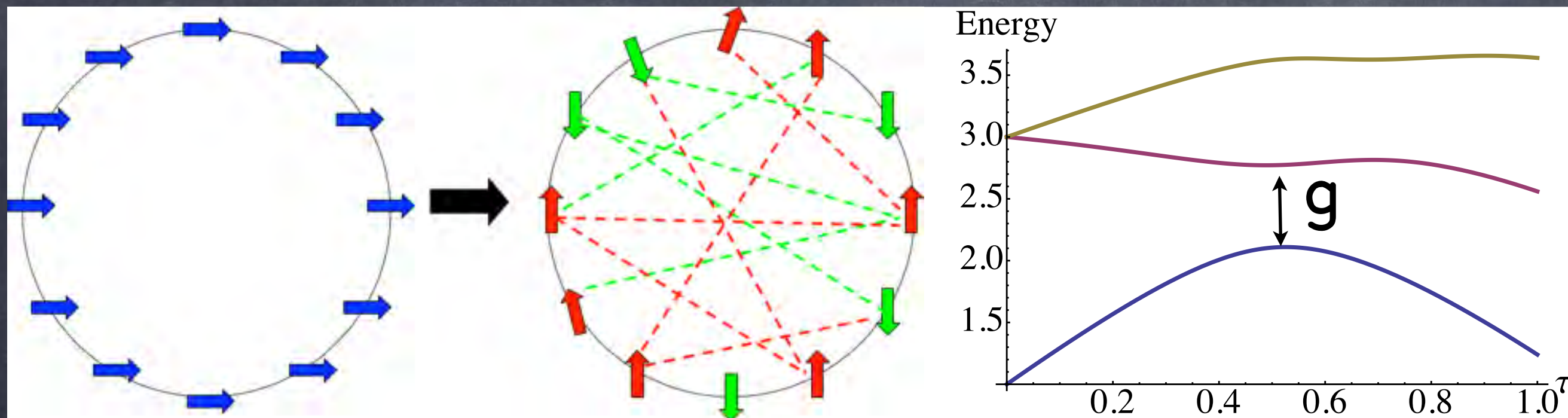
# Testing Adiabatic Quantum Computers Using Simple Quantum Simulation

Peter Love  
Tufts University





# The Adiabatic Model



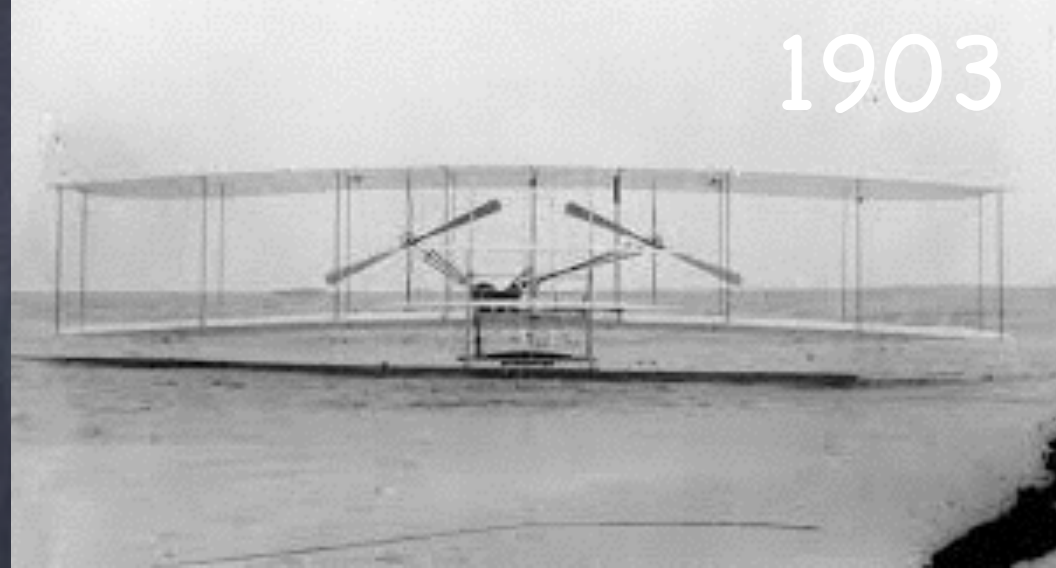
$$H_i = g \sum_i X_i \rightarrow (1-s)H_i + sH_f \rightarrow H_f = \sum_{\langle i,j \rangle} J_{ij} Z_i Z_j + \sum_i h_i Z_i$$

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





1903



1964

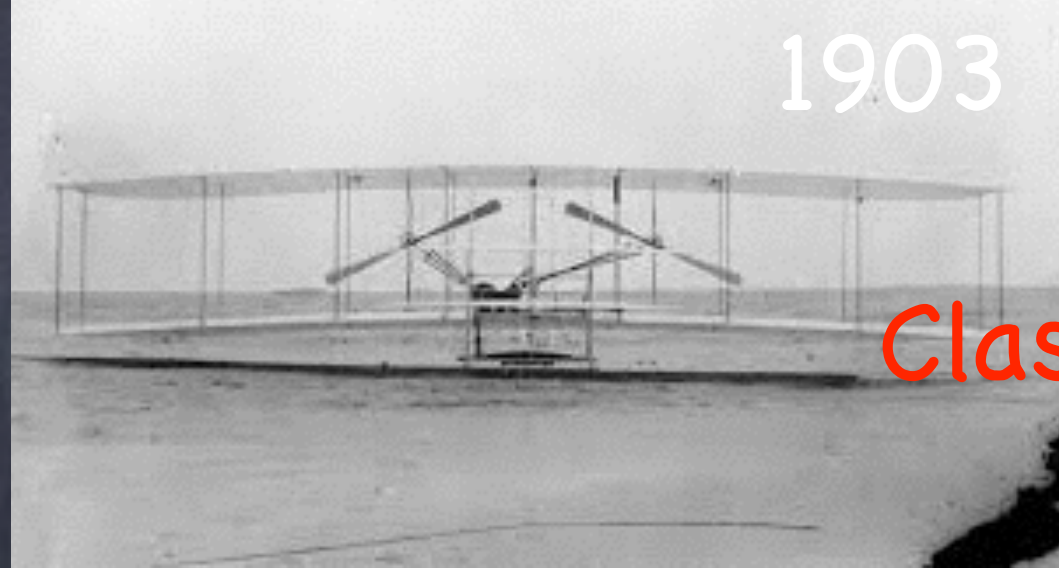


2016





1903



1964



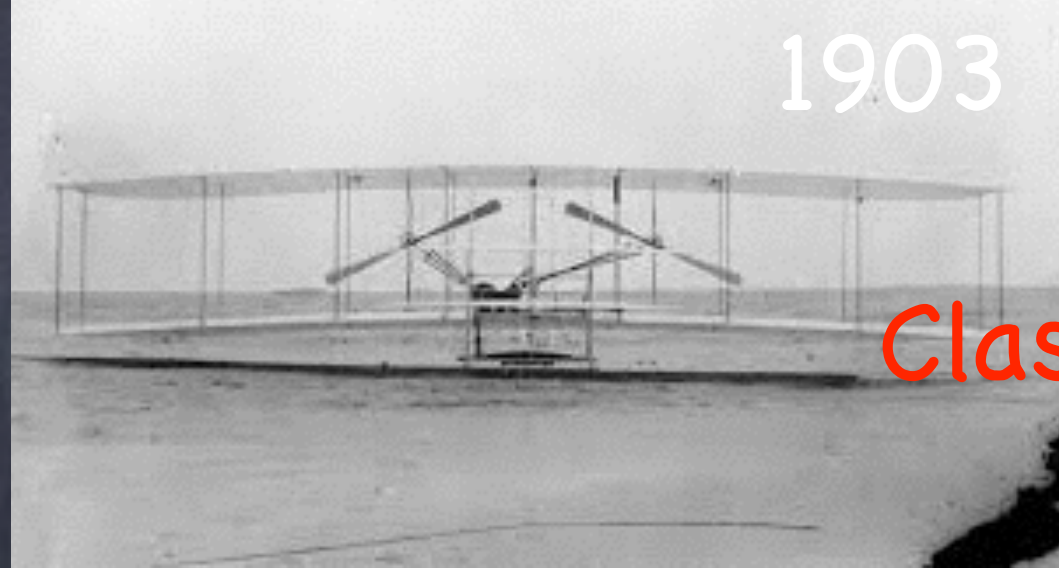
2016



Classical Computing



1903



1964



2016



Classical Computing

1926



1945

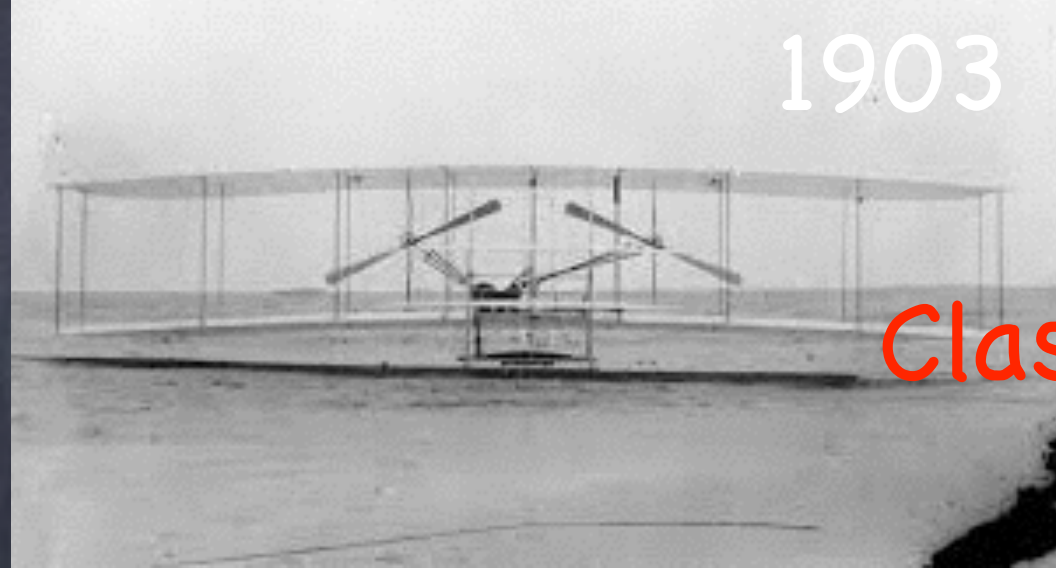


20??





1903



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Classical Computing

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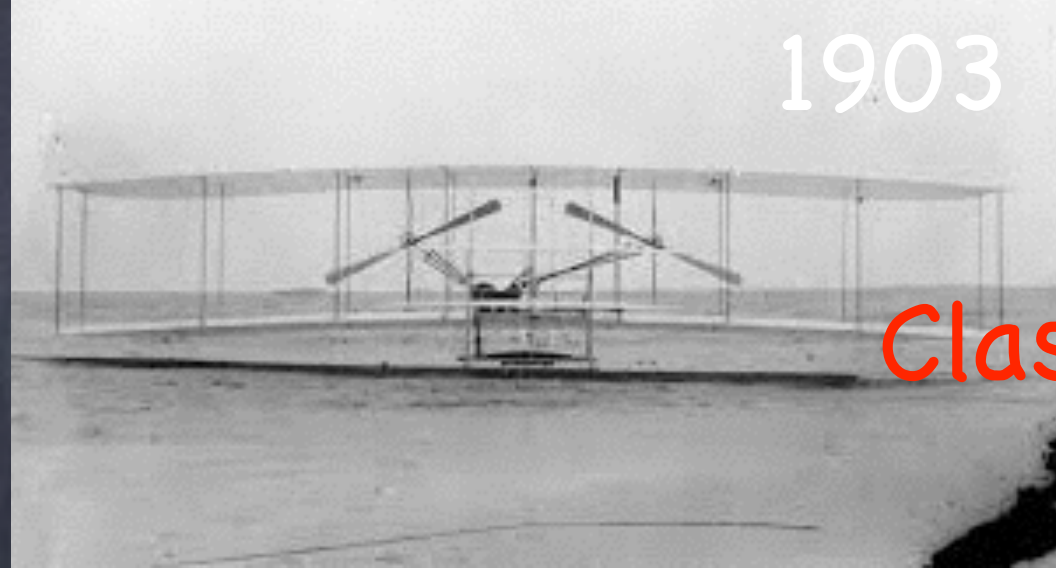
Quantum Computing

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Quantum Computing

1783



1929

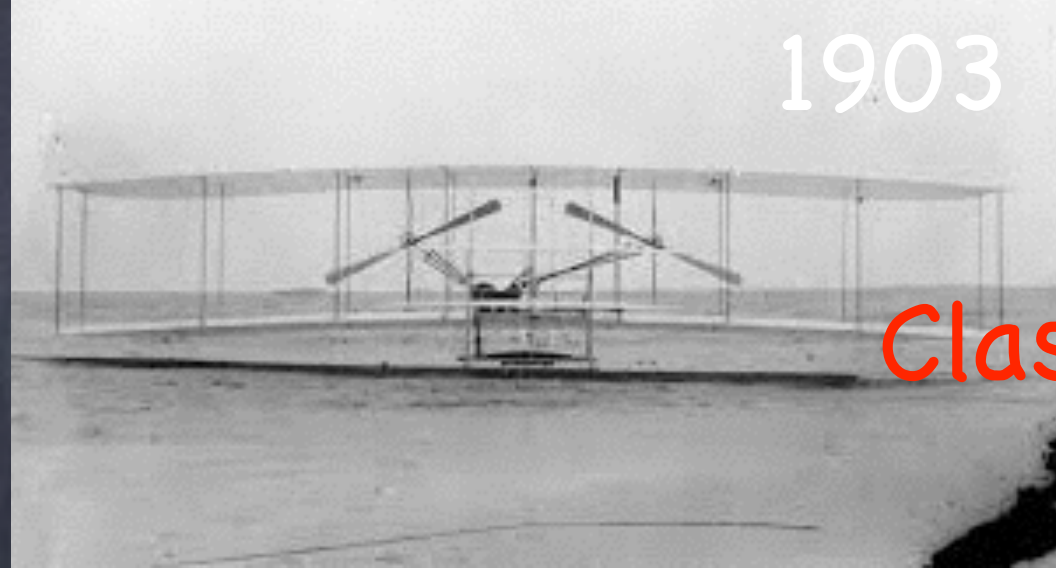


2012





1903



1964



2016



Classical Computing

1926



1945



20??



Quantum Computing

1783



1929



Quantum Annealing

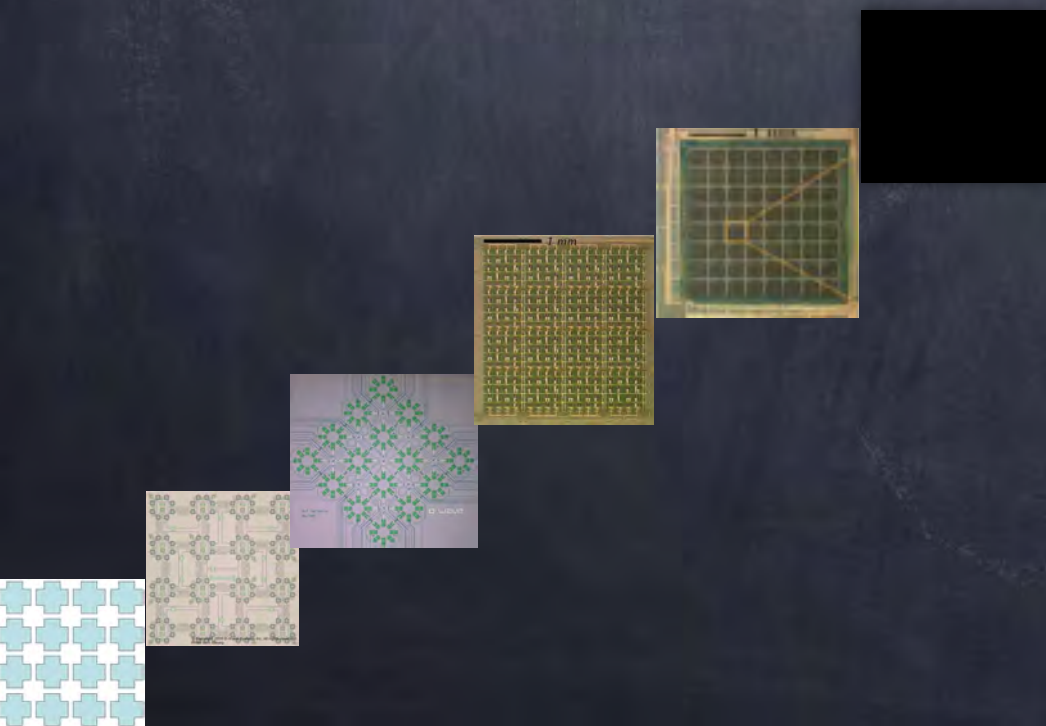
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2012





Is there a distant future  
for quantum annealers?  
What's the first step?





Full QC



Is there a distant future  
for quantum annealers?  
What's the first step?



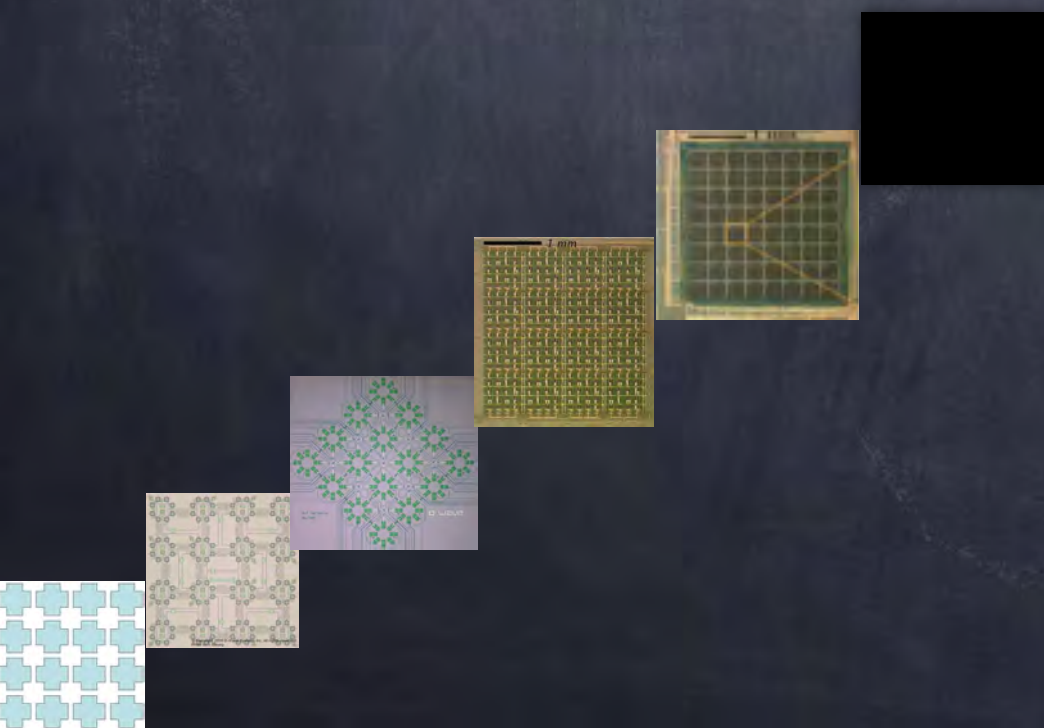
Full QC

NorthLock  
Goog  
IntelBM  
SoftWave

Universal AQC

Post-Annealing  
Modifications

Is there a distant future  
for quantum annealers?  
What's the first step?





# Universal AQC

How do we simulate time evolution in a ground state?



# Universal AQC

How do we simulate time evolution in a ground state?

$$|0\rangle|0\rangle \rightarrow |\psi_{t=1}\rangle|\psi_{t=2}\rangle$$



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Forbidden by no-cloning



# Universal AQC

How do we simulate time evolution in a ground state?

$$\cancel{|0\rangle|0\rangle \rightarrow |\psi_{t=1}\rangle|\psi_{t=2}\rangle}$$

Forbidden by no-cloning

Ground state is History state

$$|\psi_{hist}\rangle = \frac{1}{\sqrt{T+1}} \sum_{t=0}^T \left( \prod_{i=0}^t U_i \right) |\psi_{init}\rangle = \frac{1}{\sqrt{T+1}} \sum_{t=0}^T |\psi(t)\rangle \otimes |t\rangle$$



# Universal AQC

How do we simulate time evolution in a ground state?

Ground state is History state

$$|\psi_{hist}\rangle = \frac{1}{\sqrt{T+1}} \sum_{t=0}^T |\psi(t)\rangle \otimes |t\rangle$$

System state

Two white arrows originate from the text labels below. One arrow points from 'System state' to the  $|\psi(t)\rangle$  term in the equation above. The other arrow points from 'Clock state' to the  $|t\rangle$  term in the equation above.

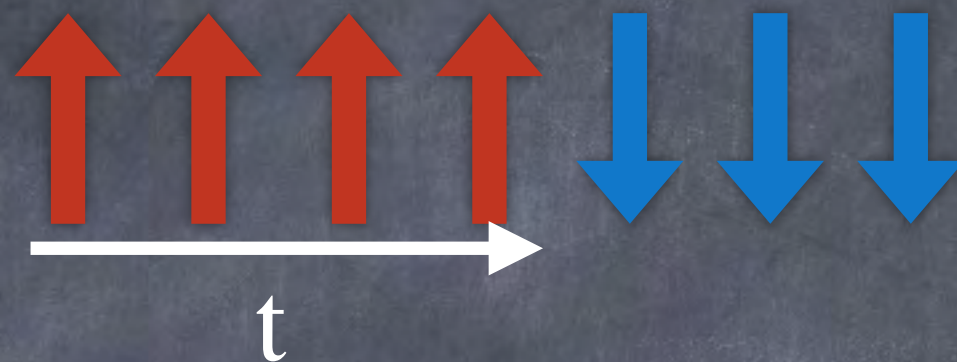
Clock state

Probability to observe  $|\psi_T\rangle \otimes |T\rangle$  is  $\frac{1}{T+1}$



# Universal AQC – the clock construction

Clock Register



Logical register



$$H = H_{clock} + H_{init} + \sum_{t=0}^T (1 - U_t) \otimes |t+1\rangle\langle t| + (1 - U_t)^\dagger \otimes |t\rangle\langle t+1|$$

Clock  
Hamiltonian

Initialization  
Hamiltonian

Propagation  
Hamiltonian



# Universal AQC - gap

$$H = H_{clock} + H_{init} + \sum_{t=0}^T (1 - U_t) \otimes |t+1\rangle\langle t| + (1 - U_t)^\dagger \otimes |t\rangle\langle t+1|$$

Apply change of basis:

$$W = \sum_{j=0}^T U_j \dots U_0 \otimes |j\rangle\langle j|$$

Hamiltonian becomes independent of circuit:

$$H = -\frac{1}{2} \begin{pmatrix} -1 & 1 & 0 & 0 & 0 & \dots \\ 1 & -2 & 1 & 0 & 0 & \dots \\ 0 & 1 & -2 & 1 & 0 & \dots \\ \vdots & 0 & \ddots & \ddots & \ddots & \vdots \\ \vdots & \vdots & 0 & \ddots & \ddots & \ddots \\ \vdots & \vdots & \vdots & \vdots & \ddots & \ddots \end{pmatrix} = D \left[ -\frac{1}{2} \frac{d^2}{dx^2} \right]$$

Gap goes like  $1/T^2$



# Desiderata

Gap scaling –  $1/T^2$  implies many repetitions, or requires a quadratic Moore's Law for refrigerators, or quadratically increasing connectivity. Need gadgets to increase norm

Types of Coupling – build XZ or XX and ZZ, or build multiple types of coupling. With fixed coupling types need gadgets.

Locality: clock constructions vary from 5-local to 2-local

Complexity proofs: polynomial scaling of Hamiltonian norm is OK  
Buildable devices: fixed coupling strength and connectivity.

Biamonte, J. D. & Love, P. J. Realizable Hamiltonians for universal adiabatic quantum computers. Phys Rev A 78, 012352 (2008).



# Universal Quantum Computation with a Time-Independent Hamiltonian

New J. Phys. 18 (2016) 023042

doi:10.1088/1367-2630/18/2/023042

## New Journal of Physics

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IOP Institute of Physics

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Gesellschaft and the Institute  
of Physics

### PAPER

## Adiabatic and Hamiltonian computing on a 2D lattice with simple two-qubit interactions

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<sup>2</sup> JARA Institute for Quantum Information, RWTH Aachen University, D-52056 Aachen, Germany

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**Keywords:** quantum computing, Hamiltonian quantum computing, superconducting quantum computing

### Abstract

We show how to perform universal Hamiltonian and adiabatic computing using a time-independent Hamiltonian on a 2D grid describing a system of hopping particles which string together and interact to perform the computation. In this construction, the movement of one particle is controlled by the presence or absence of other particles, an effective quantum field effect transistor that allows the construction of controlled-NOT and controlled-rotation gates. The construction translates into a model for universal quantum computation with time-independent two-qubit ZZ and XX+YY interactions on an (almost) planar grid. The effective Hamiltonian is arrived at by a single use of first-order perturbation theory avoiding the use of perturbation gadgets. The dynamics and spectral properties of the effective Hamiltonian can be fully determined as it corresponds to a particular realization of a mapping between a quantum circuit and a Hamiltonian called the space-time circuit-to-Hamiltonian construction. Because of the simple interactions required, and because no higher-order perturbation gadgets are employed, our construction is potentially realizable using superconducting or other solid-state qubits.

Two local Adiabatic QC!

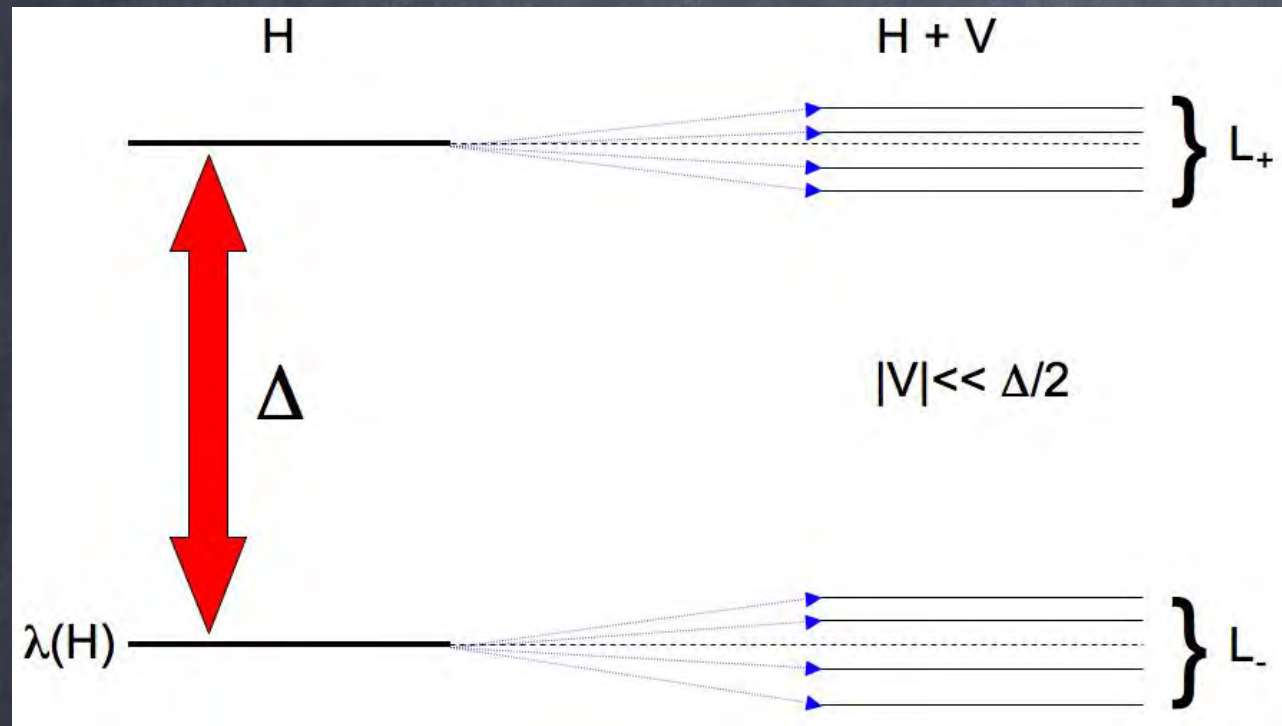
Gap scales as  $1/n^3$

Also consider ballistic  
implementation – no problem  
with gap



# Gadgets

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



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

$\Pi_-$  = projector of  $V$  onto low energy subspace

$\Pi_+ = I - \Pi_-$  = projector of  $V$  onto low energy subspace

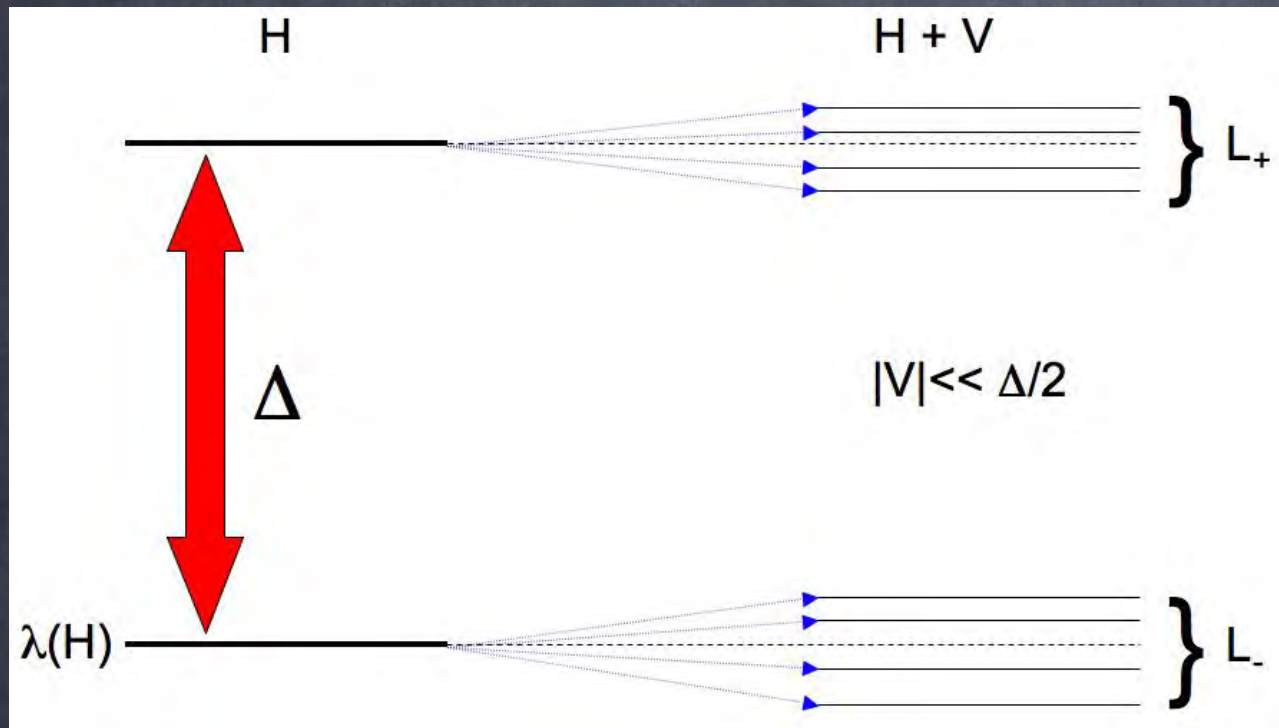
$V_{\pm\mp} = \Pi_{\pm} V \Pi_{\mp}$  = generators of virtual excitations

$V_{\pm\pm} = \Pi_{\pm} V \Pi_{\pm}$  = projections of  $V$

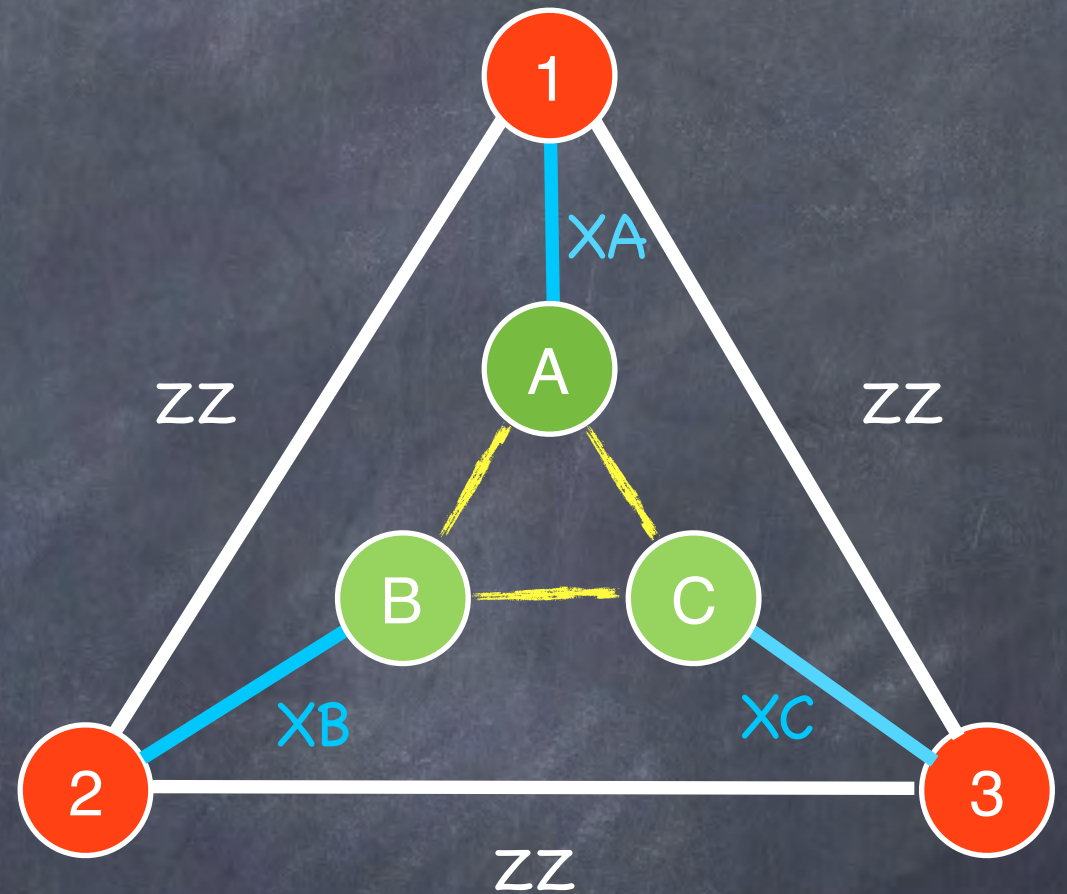


# Gadgets

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



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



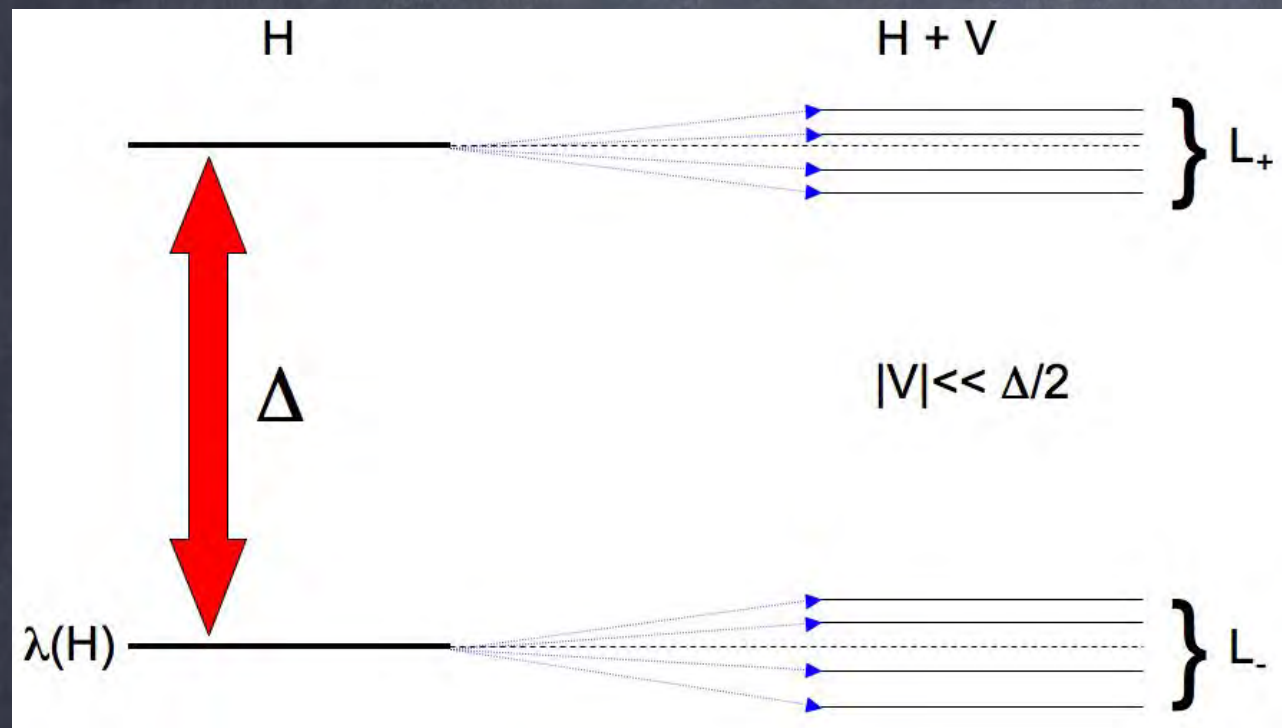
$$H_{anc} = -\Delta (Z_1 \otimes Z_2 + Z_1 \otimes Z_3 + Z_2 \otimes Z_3)$$

$$H_T = A \cdot B \cdot C$$



# Gadgets

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



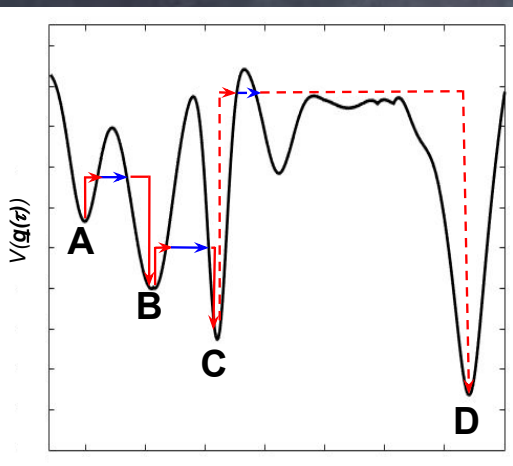
$$H_{\text{eff}} = \text{Old terms} + \text{New terms}$$

Flow of parameters

Terms not  
Physically realizable



# Quantum Annealing

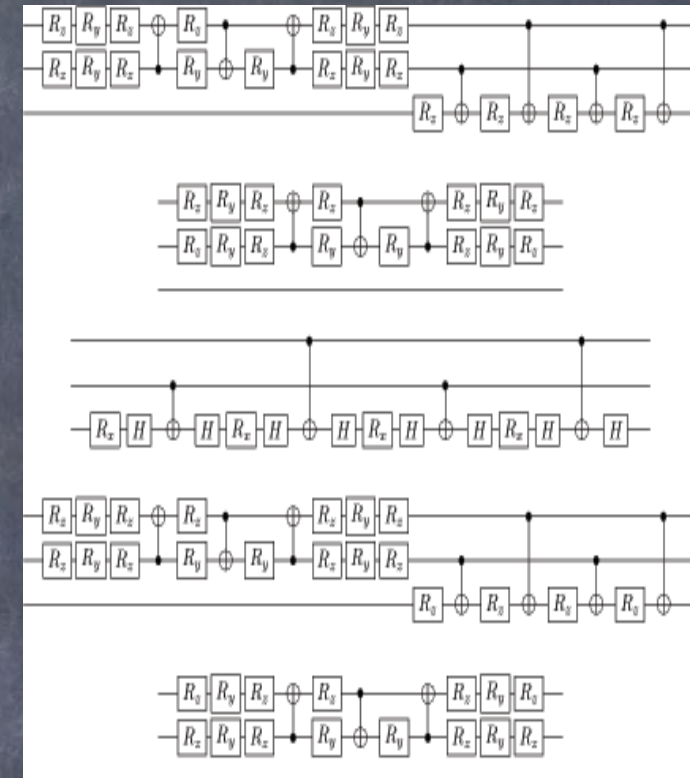


## Universal AQC



Add XX,  
Gadgets  
and clock

## Gate Model





# Post-Annealing modifications

- Non-stochastic
- Gadgets (k-local terms)
- Complex interactions (XX)





# Post-Annealing modifications

- Non-stochastic
- Gadgets (k-local terms)
- Complex interactions (XX)

Justification for XX





# Post-Annealing modifications

- Non-stoquastic
- Gadgets (k-local terms)
- Complex interactions (XX)

## Justification for XX

- Simplest Non-stoquastic term





# Post-Annealing modifications

- Non-stoquastic
- Gadgets (k-local terms)
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## Justification for XX

- Simplest Non-stoquastic term
- Powers gadgets, simulation, universal AQC





# Post-Annealing modifications

- Non-stoquastic
- Gadgets (k-local terms)
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## Justification for XX

- Simplest Non-stoquastic term
- Powers gadgets, simulation, universal AQC
- Useful for annealing? See Hormozi, Nishimori, Farhi





# Post-Annealing modifications

- Non-stoquastic
- Gadgets (k-local terms)
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## Justification for XX

- Simplest Non-stoquastic term
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- Removes QMC talks from agenda





# Post-Annealing modifications

- Non-stoquastic
- Gadgets (k-local terms)
- Complex interactions (XX)

## Justification for XX

- Simplest Non-stoquastic term
- Powers gadgets, simulation, universal AQC
- Useful for annealing? See Hormozi, Nishimori, Farhi
- Removes QMC talks from agenda
- It's what's next!





# Stoquastic

- All off-diagonal elements are negative or zero
- (up to simple transformations)

$$H = \sum_{\langle ij \rangle} J_{ij} Z_i Z_j + \sum_i h_i Z_i + \Gamma \sum_i X_i$$



# Stoquastic

- All off-diagonal elements are negative or zero
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$$H = \sum_{\langle ij \rangle} J_{ij} Z_i Z_j + \sum_i h_i Z_i + \Gamma \sum_i X_i$$

$$Z_k H Z_k = \sum_{\langle ij \rangle} J_{ij} Z_i Z_j + \sum_i h_i Z_i + \Gamma \sum_{i \neq k} X_i - \Gamma X_k$$



# Stoquastic

- All off-diagonal elements are negative or zero
- (up to simple transformations)

$$H = \sum_{\langle ij \rangle} J_{ij} Z_i Z_j + \sum_i h_i Z_i + \Gamma \sum_i X_i$$

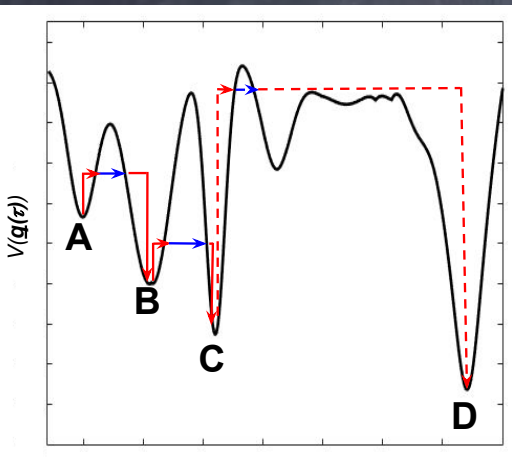
$$Z_k H Z_k = \sum_{\langle ij \rangle} J_{ij} Z_i Z_j + \sum_i h_i Z_i + \Gamma \sum_{i \neq k} X_i - \Gamma X_k$$

- Simplest non-stoquastic:

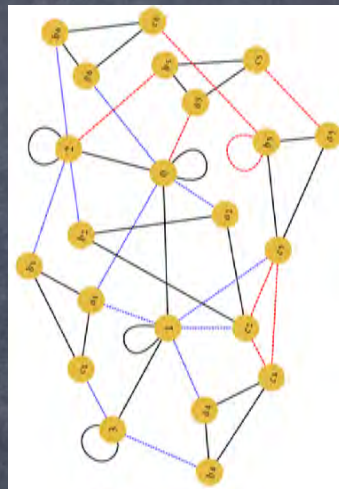
$$H = \sum_{\langle ij \rangle} J_{ij} Z_i Z_j + \sum_{\langle ij \rangle} K_{ij} X_i X_j + \sum_i h_i Z_i + \Gamma \sum_i X_i$$



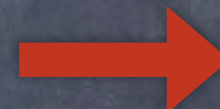
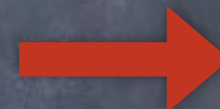
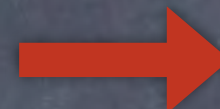
## Quantum Annealing



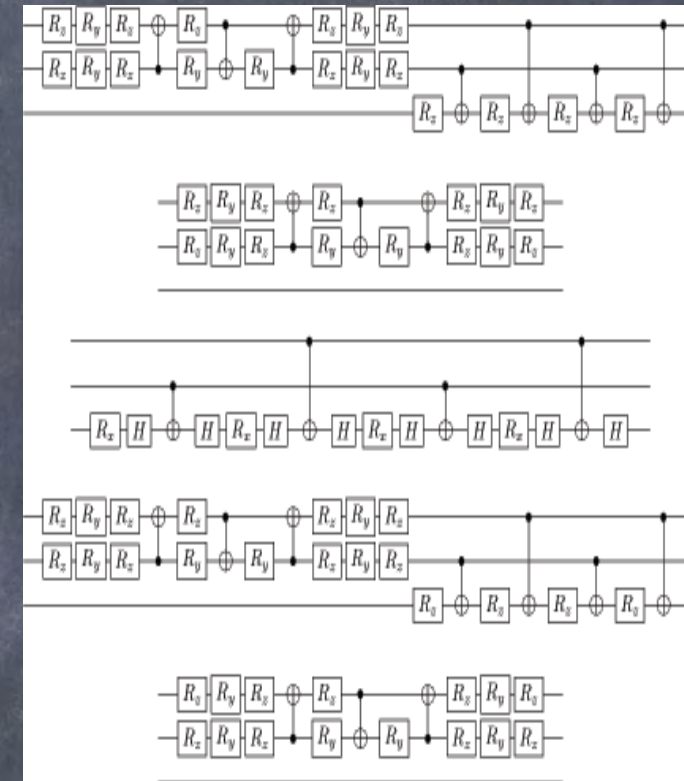
## Adiabatic Simulation



## Universal AQC



## Gate Model

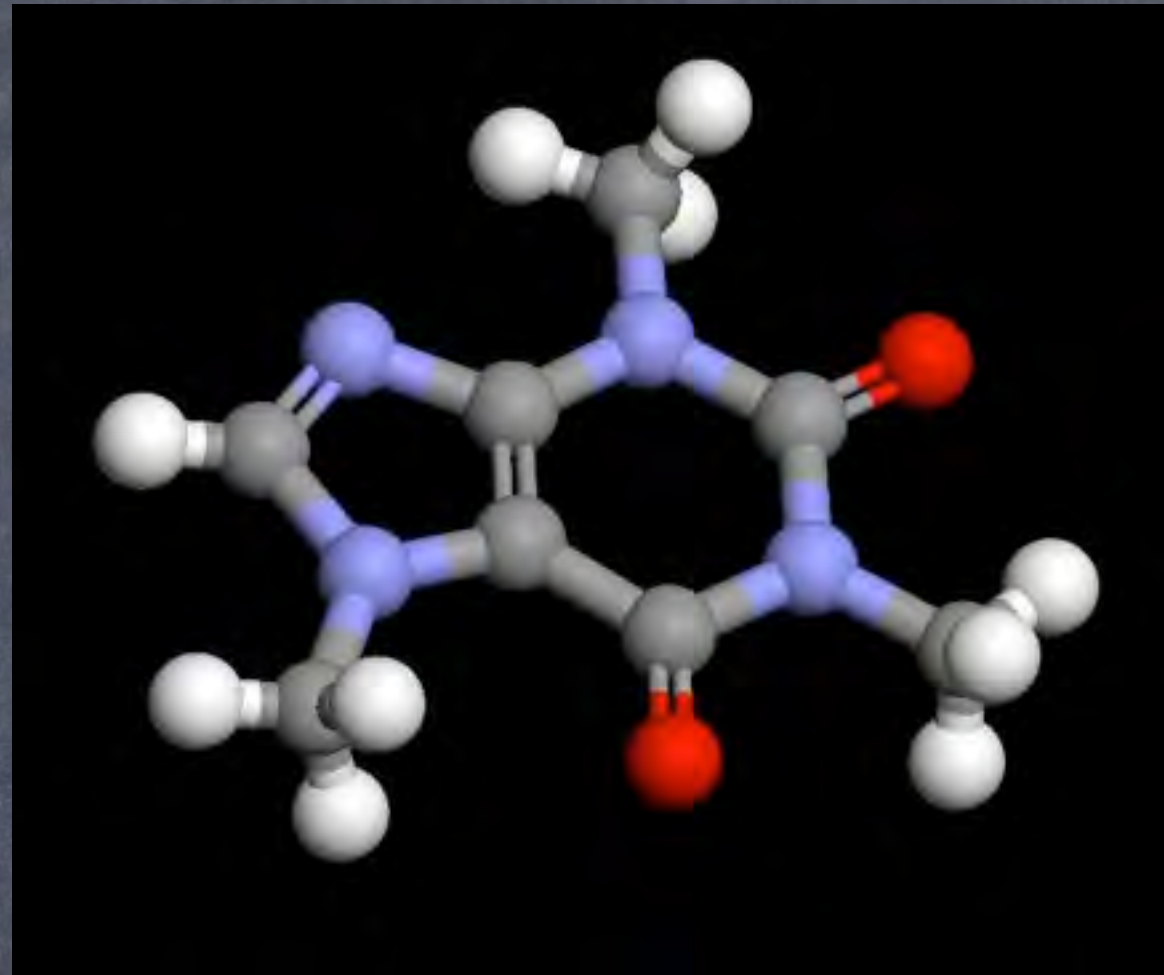


Add XX  
and  
Gadgets

Add  
Clock



# Molecular electronic Hamiltonian

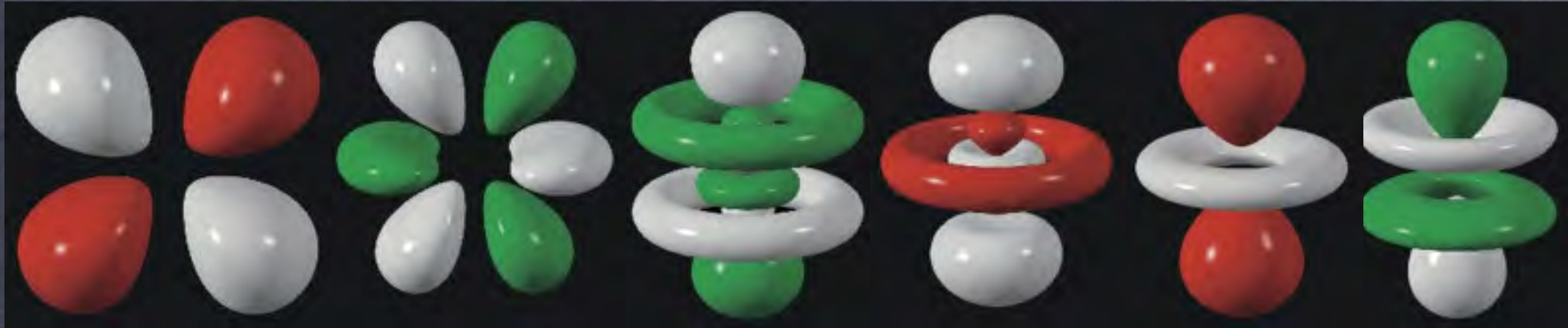


$$H = \sum_{i=1}^{n_e} \left( -\frac{\hbar^2}{2m_e} \nabla_i^2 - \sum_A \frac{Z_A}{4\pi\epsilon_0 |\vec{r}_i - \vec{R}_A|} \right) + \sum_{i<j}^{n_e} \frac{e^2}{4\pi\epsilon_0 |\vec{r}_i - \vec{r}_j|}$$

To represent as a qubit problem we must discretize



# Discretize in a basis of Molecular orbitals



For each orbital define  $a_k$  and  $a_k^\dagger$  satisfying:

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



# Discretize in a basis of Molecular orbitals



For each orbital define  $a_k$  and  $a_k^\dagger$  satisfying:

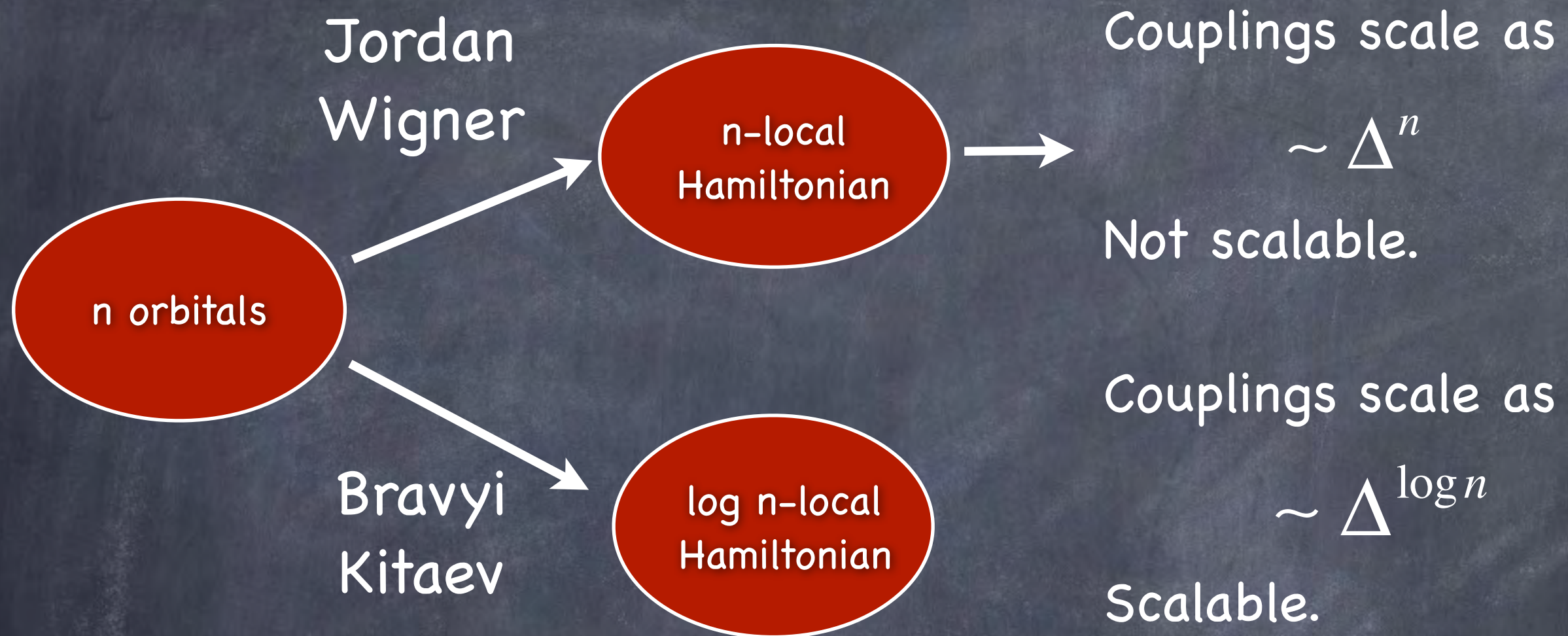
$$\{a_j, a_k\} = 0 \quad \{a_j^\dagger, a_k^\dagger\} = 0 \quad \{a_j, a_k^\dagger\} = \delta_{jk} 1$$

Write the second-quantized Hamiltonian:

$$H = \sum_{ij} h_{ij} a_i^\dagger a_j + \sum_{ijkl} h_{ijkl} a_i^\dagger a_j^\dagger a_k a_l$$



# Fermionic analog simulator



S. Bravyi and A. Yu. Kitaev, *Annals of Physics*, **298** 210–226 (2002)  
J. T. Seeley, M. Richard, P. J. Love *J. Chem. Phys.* **137**, 224109 (2012),  
*Adiabatic Quantum Simulation of Quantum Chemistry*, Ryan Babbush, Peter J. Love Alan  
Aspuru-Guzik arXiv:1311.3967, *Scientific Reports*, **4**, 6603, (2014)





# 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).



# Validation by inefficient simulation of elementary quantum systems

- If we think we will need gadgets and clocks in the future, what could we be doing now to make sure they work?
- Can we display properties of simple single particle QM – superposition, dispersion, energy quantization in an AQC?
- Can we show evidence that superposition states exist in an AQC between logical basis states with widely different hamming weights?



In gate model requirements for validation (tomography) are the same as the requirements for computation

In restricted models of QC validation is a separate problem

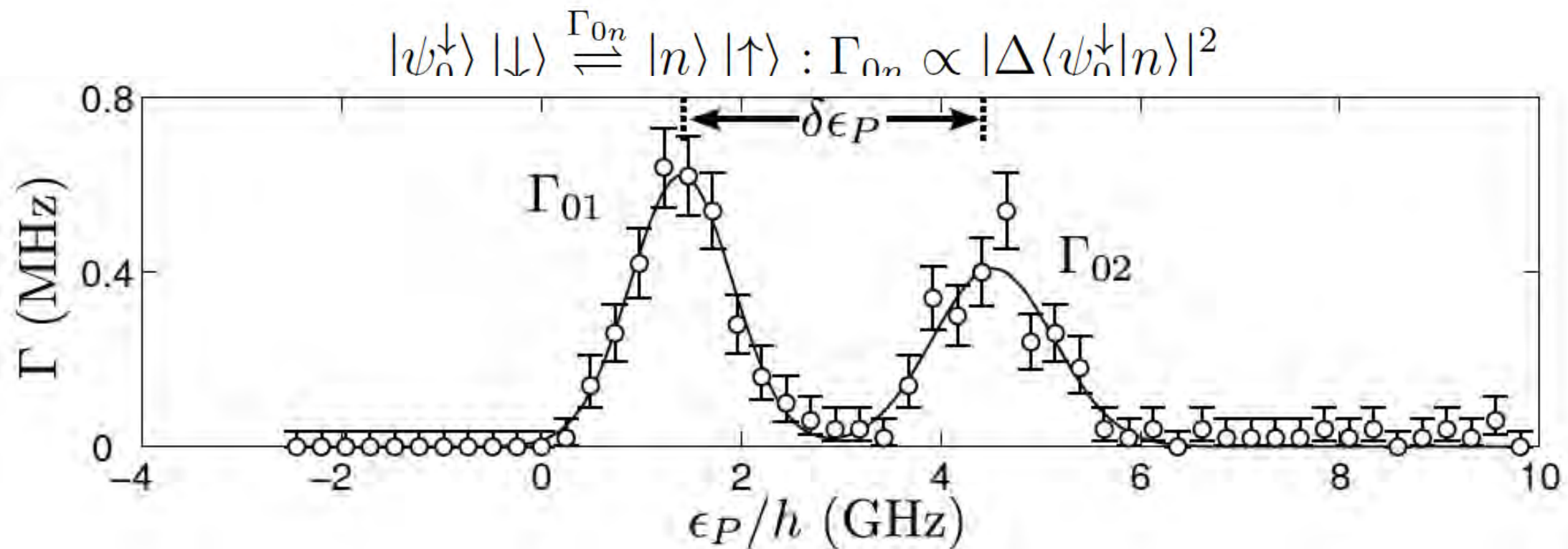


With a hammer, everything looks like....

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

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

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



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.

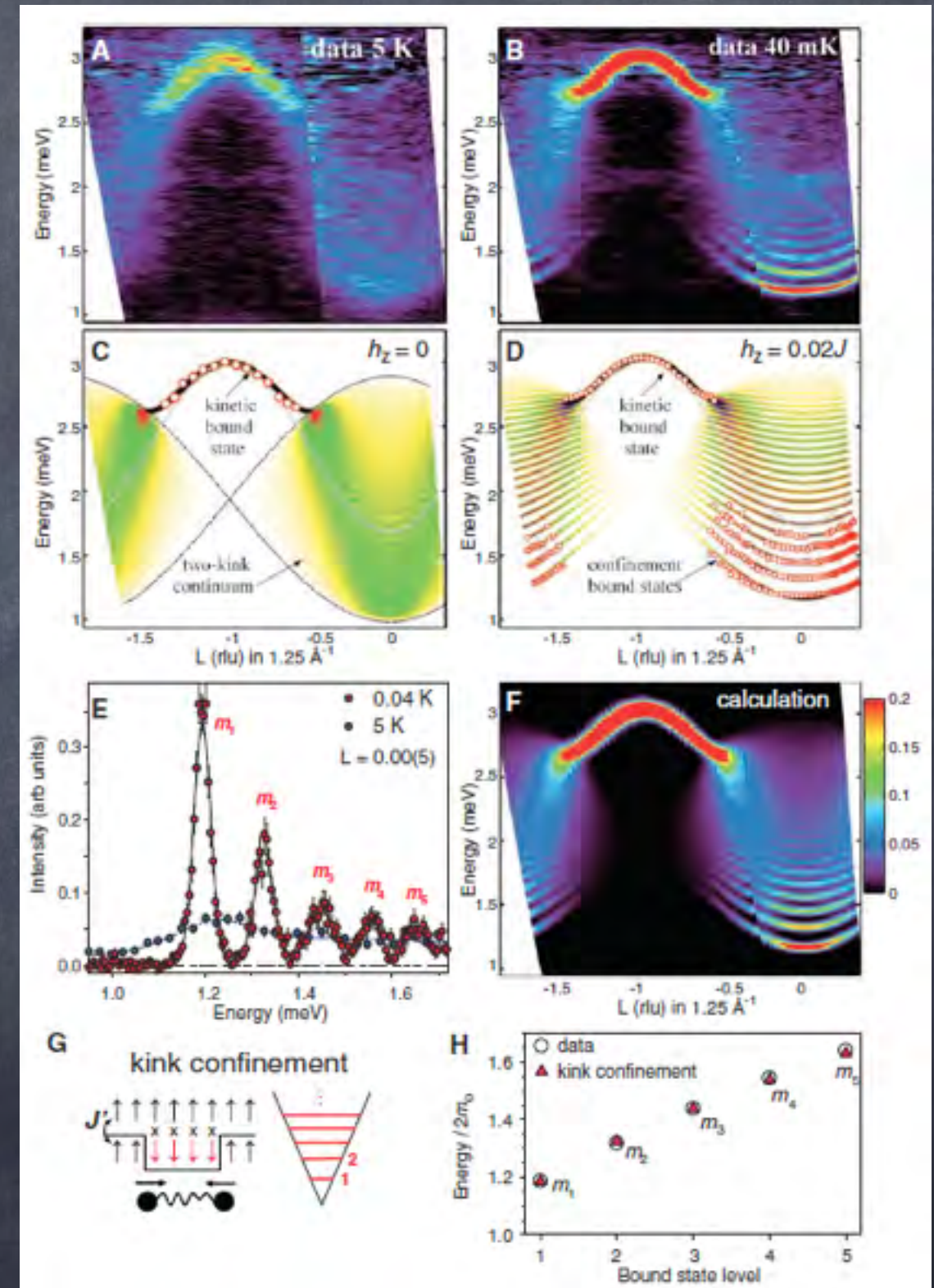
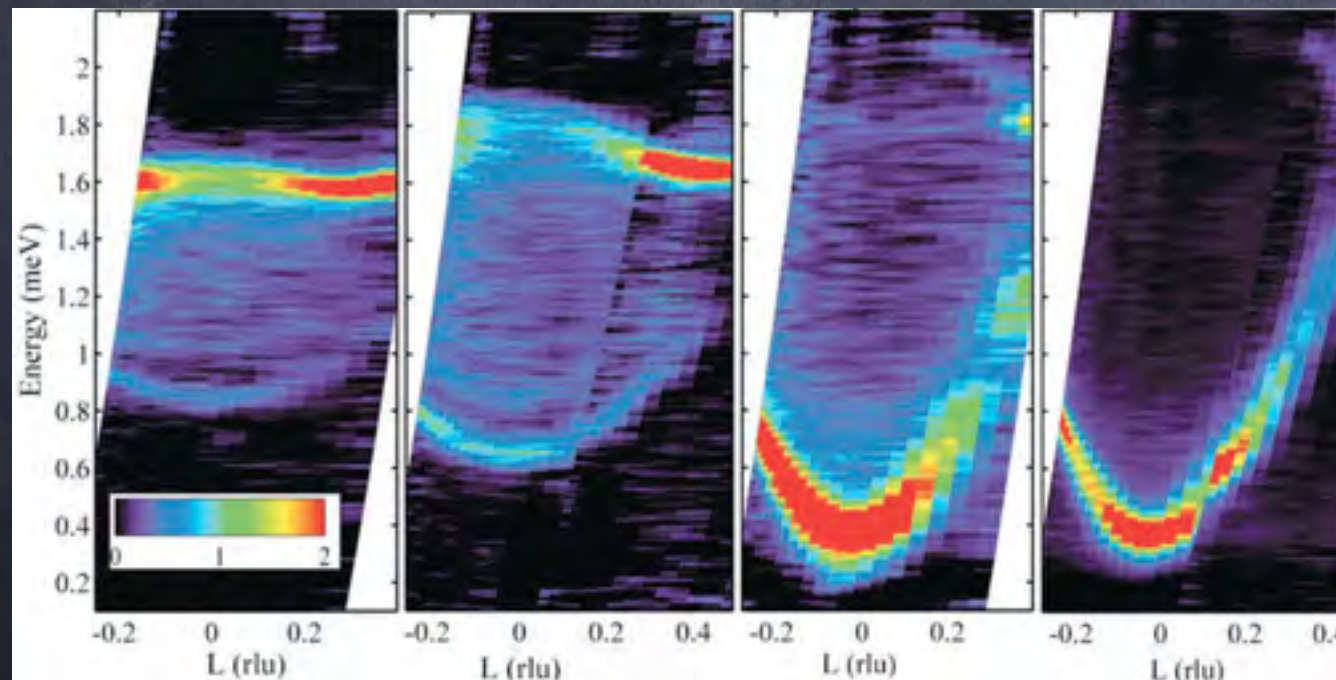


# Quantum Criticality in an Ising Chain: Experimental Evidence for Emergent $E_8$ Symmetry

R. Coldea,<sup>1\*</sup> D. A. Tennant,<sup>2</sup> E. M. Wheeler,<sup>1†</sup> E. Wawrzynska,<sup>3</sup> D. Prabhakaran,<sup>1</sup>  
M. Telling,<sup>4</sup> K. Habicht,<sup>2</sup> P. Smeibidl,<sup>2</sup> K. Kiefer<sup>2</sup>

Quantum phase transitions take place between distinct phases of matter at zero temperature. Near the transition point, exotic quantum symmetries can emerge that govern the excitation spectrum of the system. A symmetry described by the  $E_8$  Lie group with a spectrum of eight particles was long predicted to appear near the critical point of an Ising chain. We realize this system experimentally by using strong transverse magnetic fields to tune the quasi-one-dimensional Ising ferromagnet  $\text{CoNb}_2\text{O}_6$  (cobalt niobate) through its critical point. Spin excitations are observed to change character from pairs of kinks in the ordered phase to spin-flips in the paramagnetic phase. Just below the critical field, the spin dynamics shows a fine structure with two sharp modes at low energies, in a ratio that approaches the golden mean predicted for the first two meson particles of the  $E_8$  spectrum. Our results demonstrate the power of symmetry to describe complex quantum behaviors.

SCIENCE VOL 327 (2010) P177





# The kink basis – clock states

$$E = P$$



$|6\rangle$



Ferromagnetic  
penalty on adjacent  
pairs

$$H_F = J(1 - ZZ)/2$$

$|5\rangle$



$|4\rangle$



Boundary  
penalty

$$H_P = P(1 - Z_1)/2 + P(1 - Z_N)/2$$

$|3\rangle$



$|2\rangle$



$|1\rangle$



$$E = 0$$



# The transverse field in the kink basis

$$\sum_{i=1} X_i |k\rangle = \text{uniform superposition of all states} \\ \text{Hamming distance one from } |k\rangle$$

Projecting back onto the kink basis:

$$\sum_{i=1} X_i \uparrow\uparrow\uparrow\uparrow\downarrow\downarrow\downarrow = \uparrow\uparrow\uparrow\uparrow\uparrow\downarrow\downarrow + \uparrow\uparrow\uparrow\downarrow\downarrow\downarrow\downarrow$$

Or:

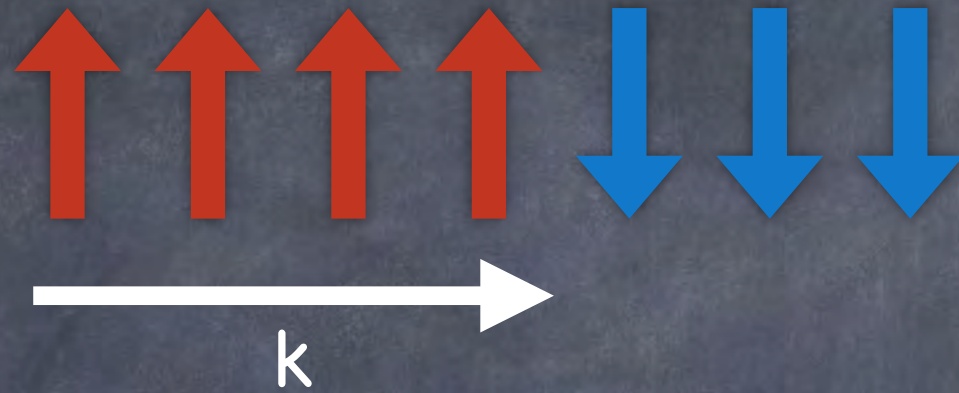
$$P\left(\sum_{i=1} X_i |k\rangle\right) = |k+1\rangle + |k-1\rangle$$

Can build a 1-D kinetic energy from this:

$$P\left(\frac{1}{L^2} \sum_{i=1} X_i |k\rangle - \frac{1}{L^2} |k\rangle\right) = \frac{|k+1\rangle - 2|k\rangle + |k-1\rangle}{L^2} = D\left[\frac{d^2}{dx^2}\right]$$



# The local field in the kink basis



$$\sum_{i=1}^L h_i Z_i |k\rangle = \left( \sum_{i=k+1}^L h_i - \sum_{i=1}^k h_i \right) |k\rangle = \left( \sum_{i=1}^L h_i - 2 \sum_{i=1}^k h_i \right) |k\rangle$$

Can interpret this as a potential, where up to a constant:

$$V(k) = -2 \sum_{i=1}^k h_i$$

Obvious case: linear potential, constant field, kink confinement.



# Polynomial potentials

Find  $h_i$  such that

$$V(k) = -2 \sum_{i=1}^k h_i = k^p$$

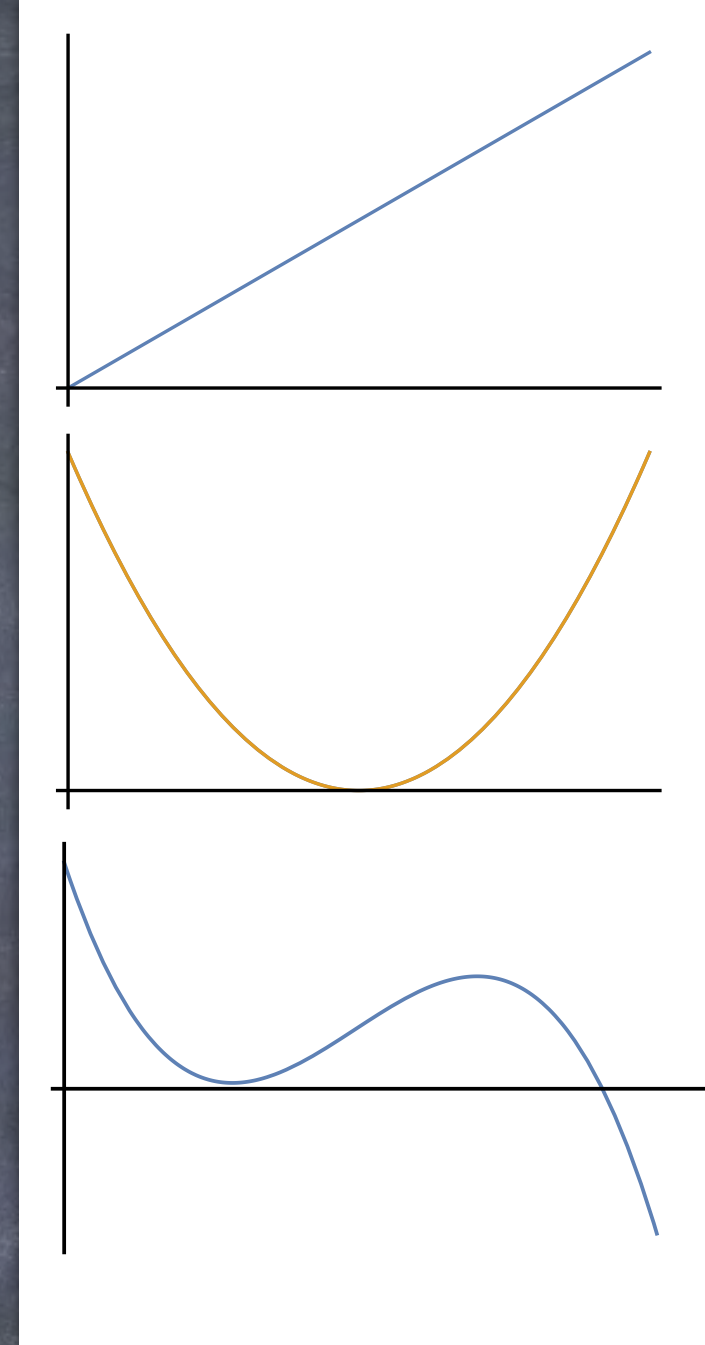
Straightforward: use Pascal's Identity:

$$(k+1)^p = 1 + \sum_{l=0}^{p-1} \binom{p}{l} \sum_{i=1}^k i^l$$

Up to a constant:

$$h_i = -\frac{1}{2} \sum_{l=0}^{p-1} \binom{p}{l} i^l = \frac{i^p - (1+i)^p}{2}$$

Maximum required local field grows exponentially with polynomial degree – recall the goal here is validation not simulation.





# Errors

Discretization error:

$$\lim_{n \rightarrow \infty} P(H) = H_{cont}$$

Standard numerical analysis

Leakage error:

$$\lim_{J \rightarrow \infty} H = P(H)$$

Gadget analysis tells you corrections to  $P(H)$ .

These corrections tell you about virtual excitations in your system.



Inefficient elementary simulations are probes of requirements for post-annealing AQC

If simple kink basis simulations work at all then you can make clock states.

Leakage Errors in simple simulations tell you whether Gadgets will work in your system.

First error can be used to detect XX



# Gadgets

$$H_{eff} = P(H) + \sum_{k=2}^{\infty} V_{-+} G_+ (V_+ G_+)^{k-2} V_{+-}$$

3J Eight Kinks

$$G_+ = - \sum_{E>0} \sum_{r=1}^{d_E} \frac{|E, r\rangle \langle E, r|}{E}$$

$\Pi_-$  projector onto two kink space

$$\Pi_+ = I - \Pi_-$$

2J Six Kinks

$$V_{\pm\mp} = \Pi_{\pm} V \Pi_{\mp} \quad V_{\pm\pm} = \Pi_{\pm} V \Pi_{\pm}$$

p Zero Kinks

J Four Kinks

Potential is diagonal – doesn't couple states with different numbers of kinks.

0 Two Kinks

Error analysis is same for all potentials.



3J Eight Kinks

2J Six Kinks

P Zero Kinks

J Four Kinks

0 Two Kinks

Two kinds of term:

Terms that are already present – flow of coefficients.

Terms that are new. Errors.

$$H_{eff} = P(H) - \frac{\lambda^2(L-3)}{2J} I - \frac{3\lambda^2}{4J} [ |1\rangle\langle 1| + |L\rangle\langle L| ] - \frac{\lambda^2}{2J} P \left( \sum_{i=1}^{L-1} X_i X_{i+1} \right)$$



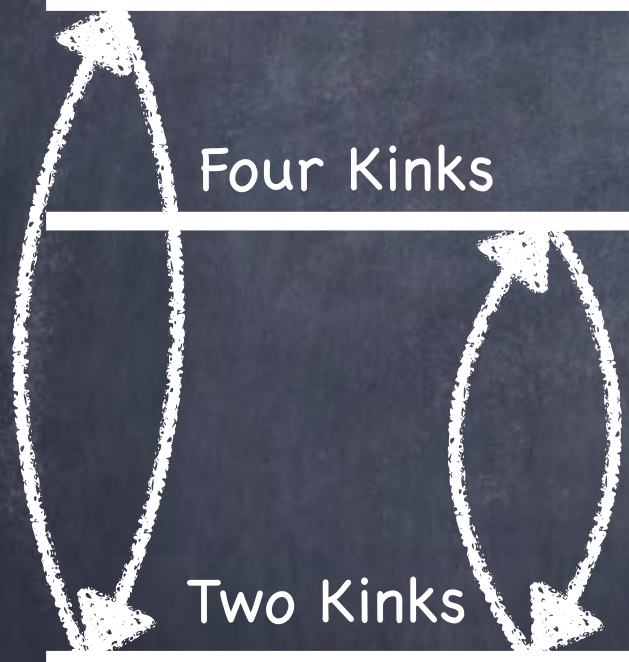
3J Eight Kinks

2J Six Kinks

P Zero Kinks

J Four Kinks

0 Two Kinks



Two kinds of term:

Terms that are already present – flow of coefficients.

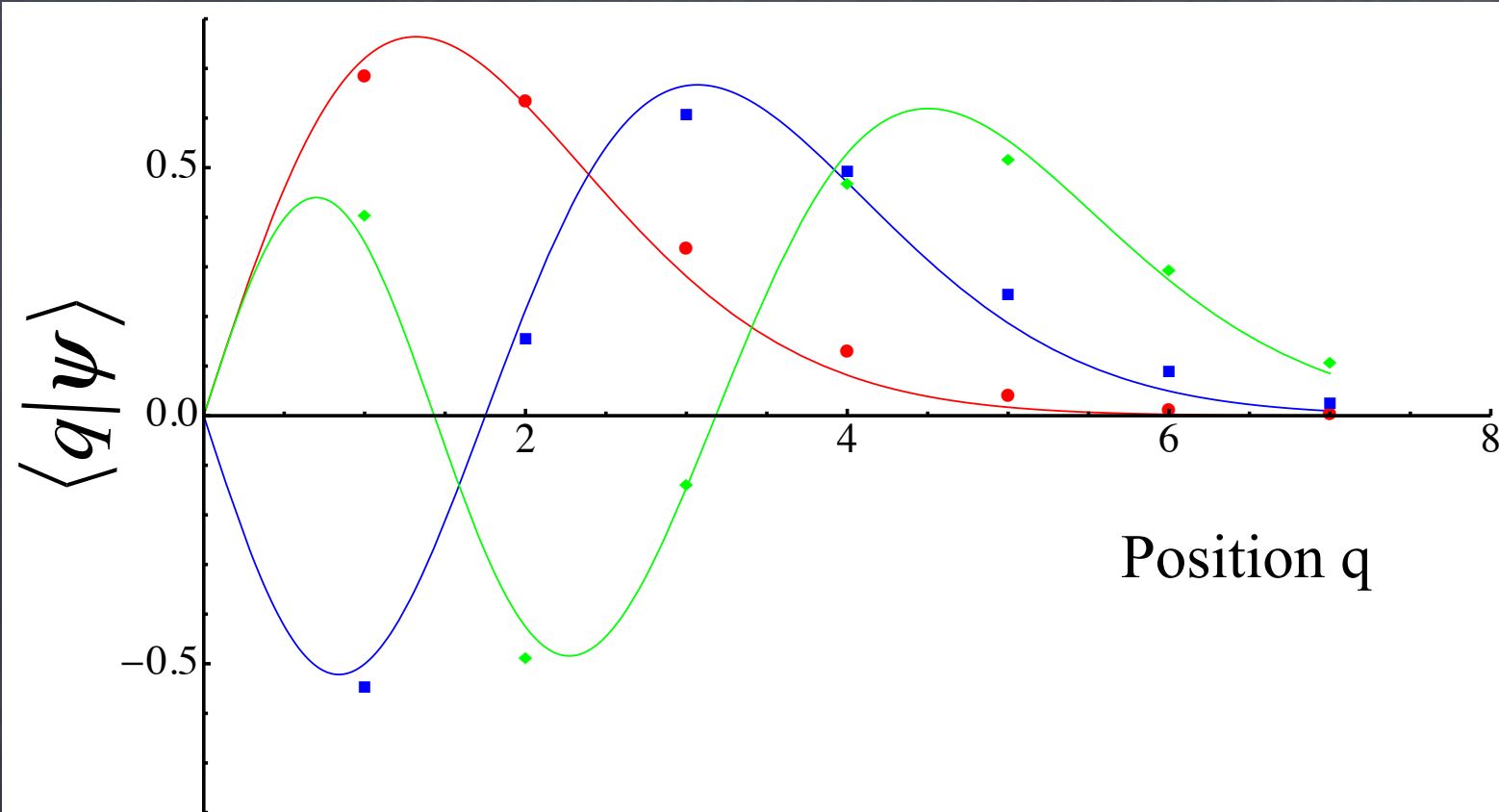
Terms that are new. Errors.

Stoquastic XX

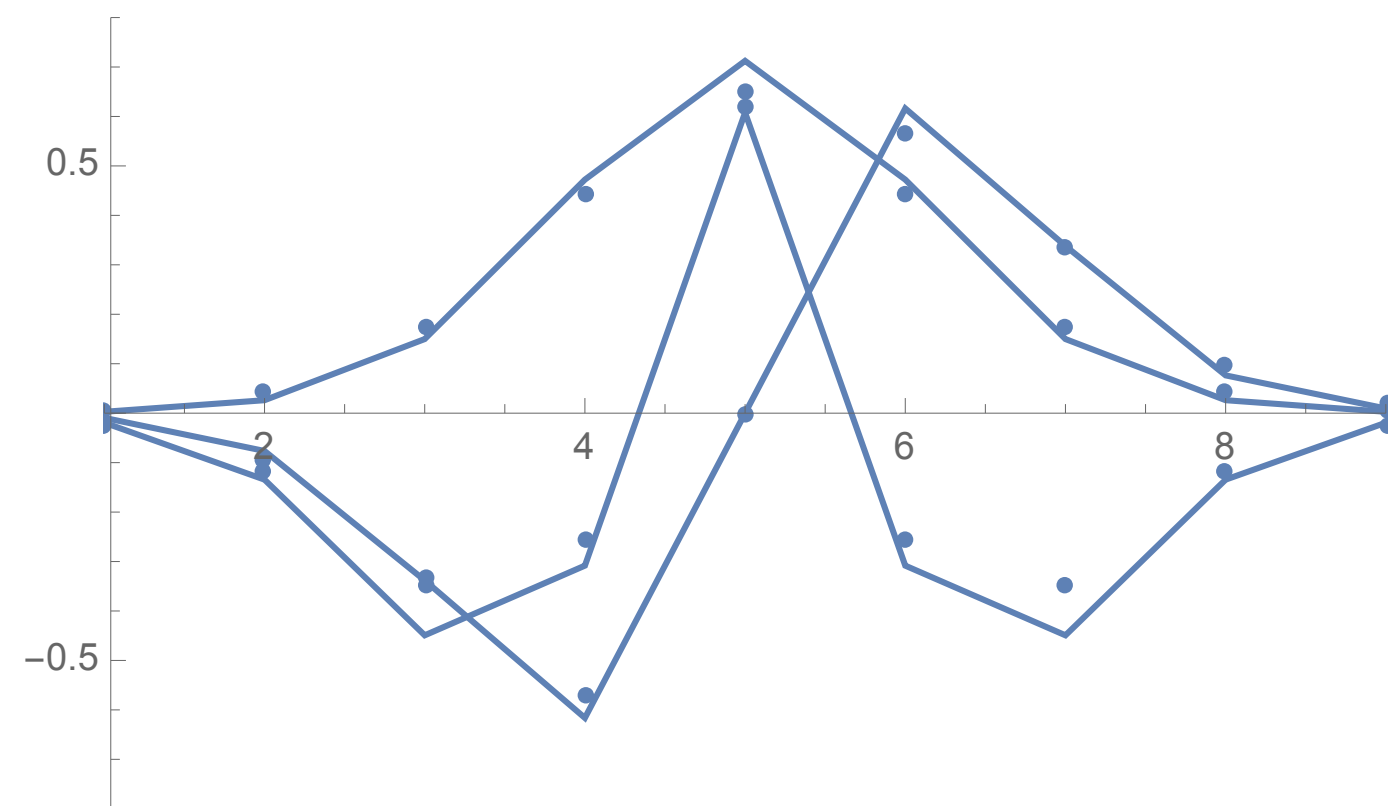


$$H_{eff} = P(H) - \frac{\lambda^2(L-3)}{2J} I - \frac{3\lambda^2}{4J} [|1\rangle\langle 1| + |L\rangle\langle L|] - \frac{\lambda^2}{2J} P \left( \sum_{i=1}^{L-1} X_i X_{i+1} \right)$$





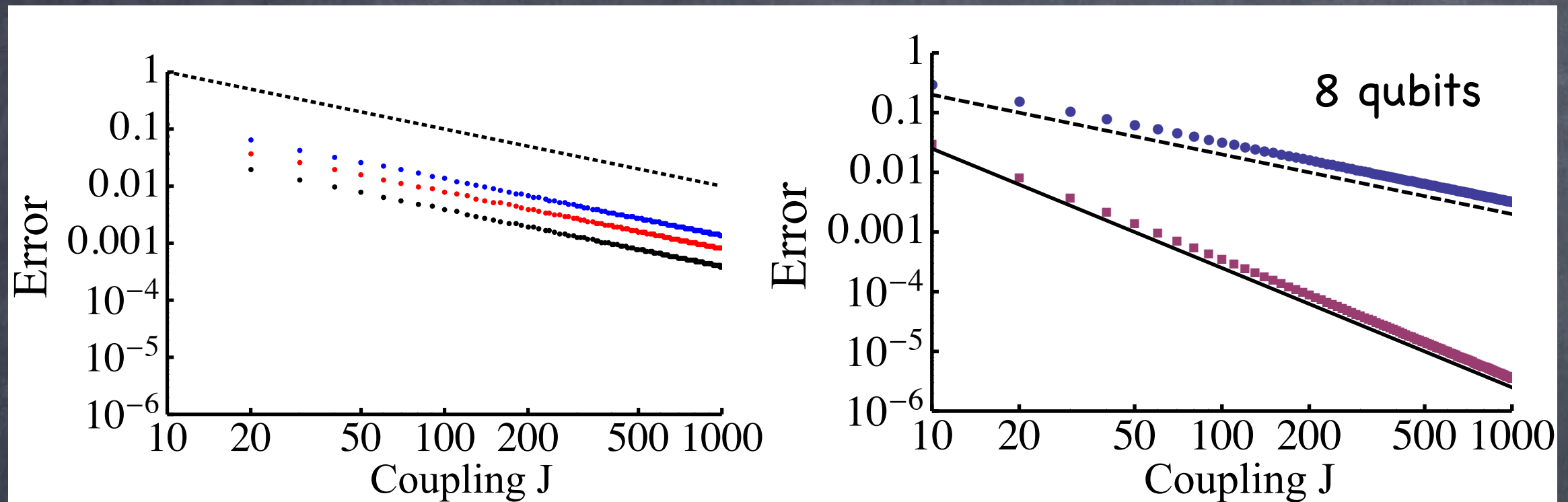
Linear  
Potential



SHO



# Linear Potential



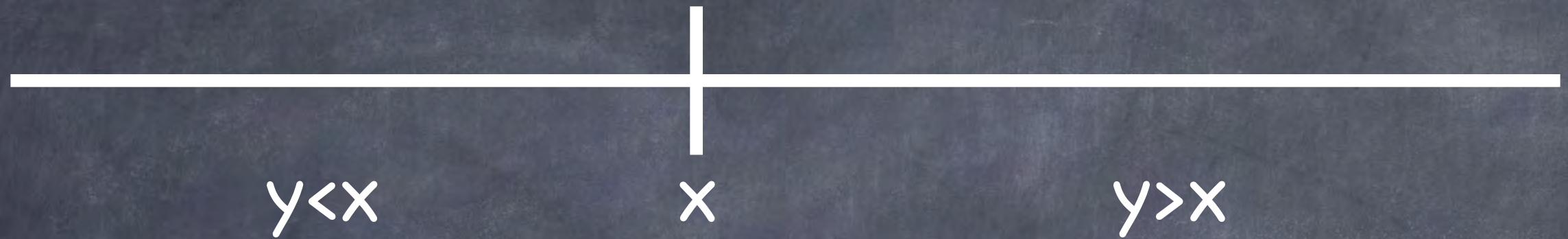
8, 10, 12 qubits should be sufficient to detect the scaling of the eigenvalues with penalty strength. Renormalizing coefficients should improve accuracy.

If you can engineer further terms (specifically XX) you should be able to see the scaling change.

Experiments observing these effects would fail to invalidate the presence of effects necessary for gadgets to work



# Entanglement and delocalization



What is the entanglement of  $y < x$  with  $y > x$ ?

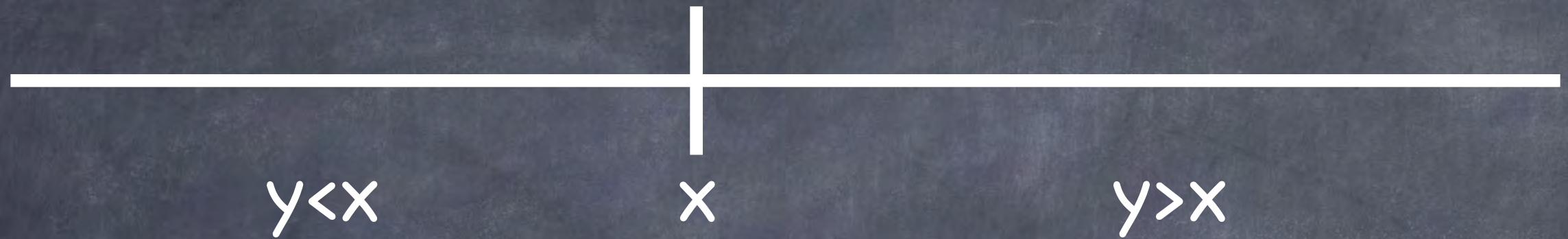
Define reduced state:  $\rho_x = \text{Tr}_{y>x} \rho$

And linear entropy (also Meyer-Wallach measure):

$$\rho_x = \frac{2^L}{2^L - 1} \left[ 1 - \text{Tr}(\rho_x^2) \right]$$



# Entanglement and delocalization



$$\rho_x = \frac{2^L}{2^L - 1} \left[ 1 - \text{Tr}(\rho_x^2) \right]$$

For kink states entanglement is really a measure of delocalization.

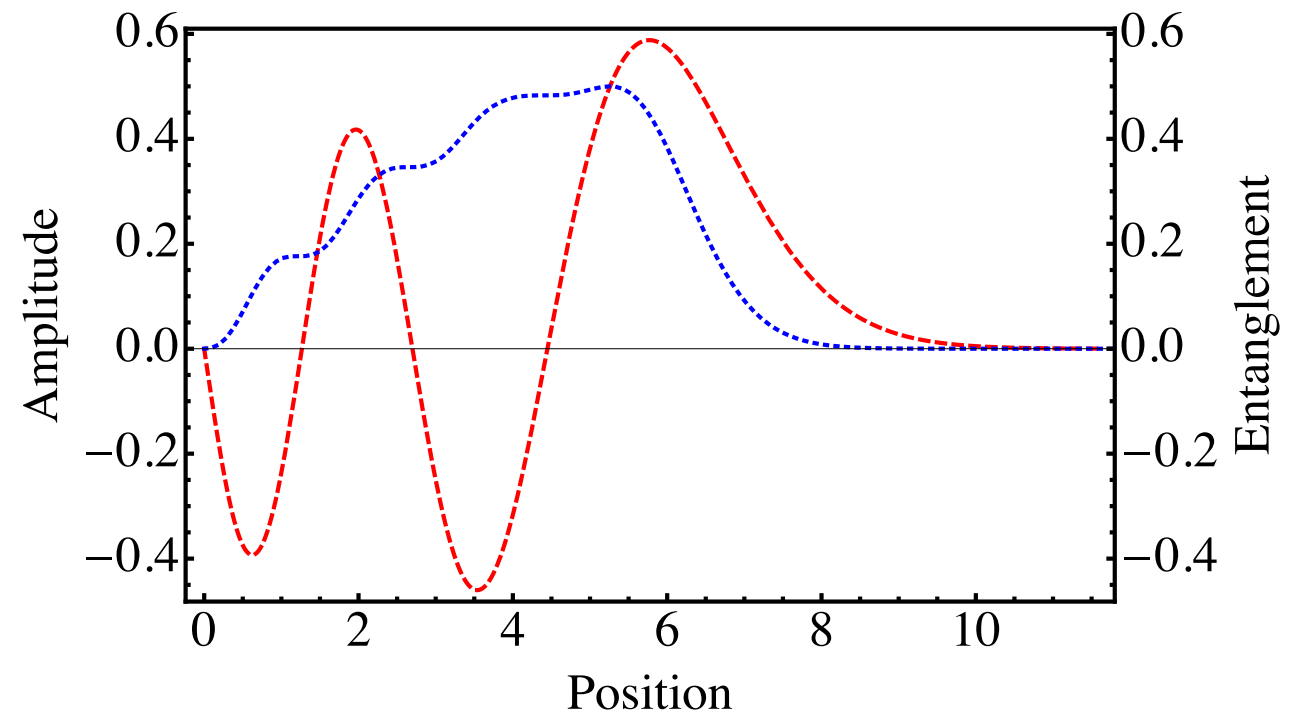
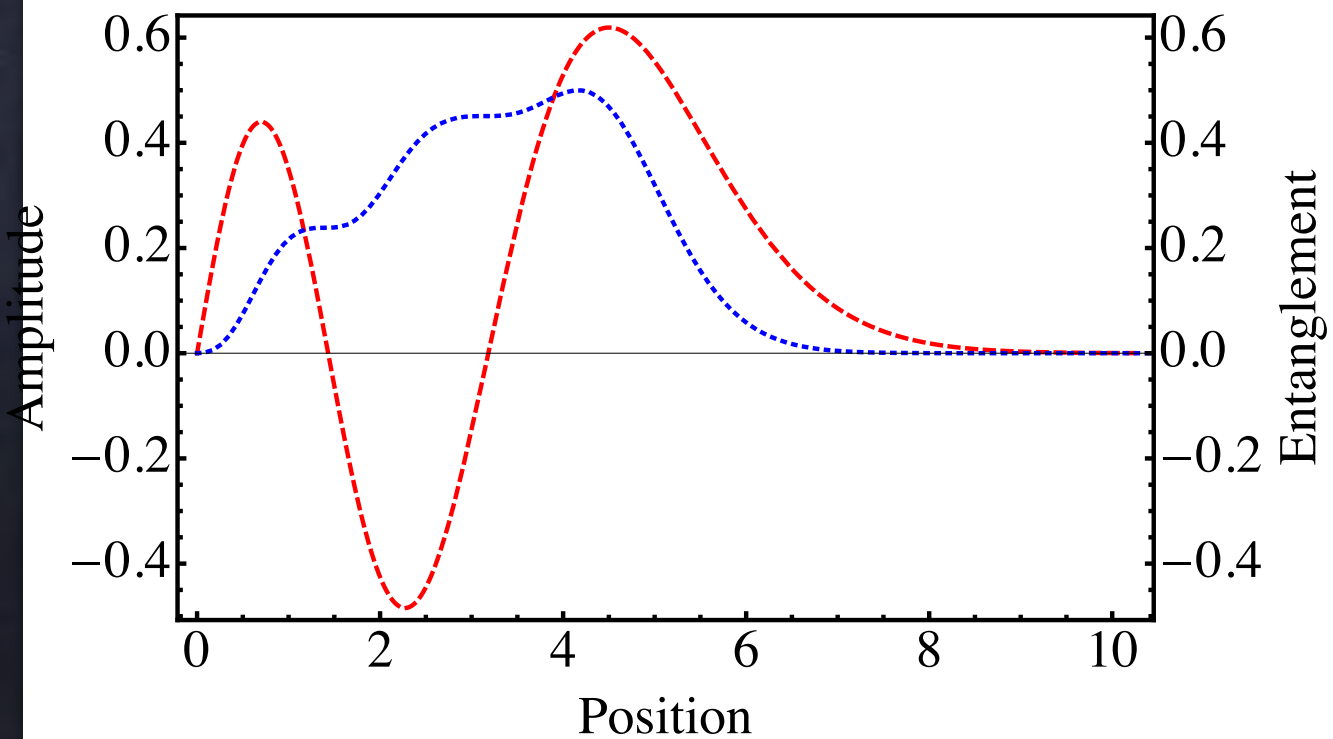
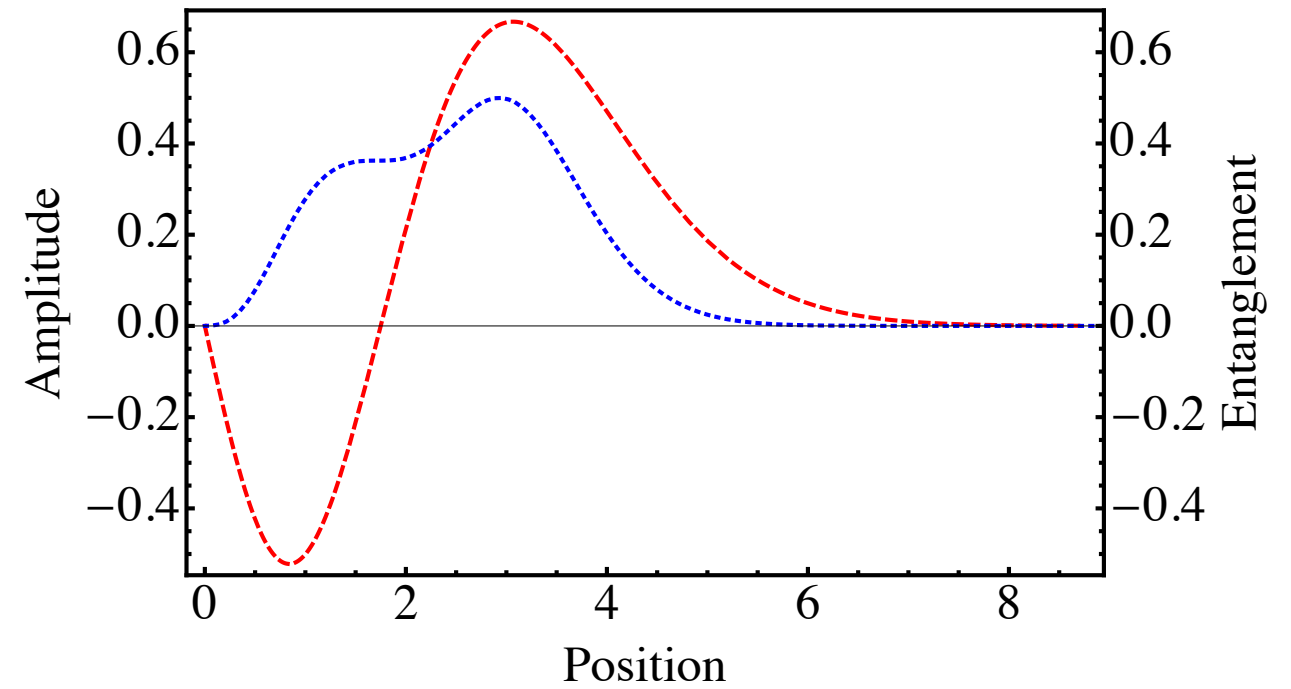
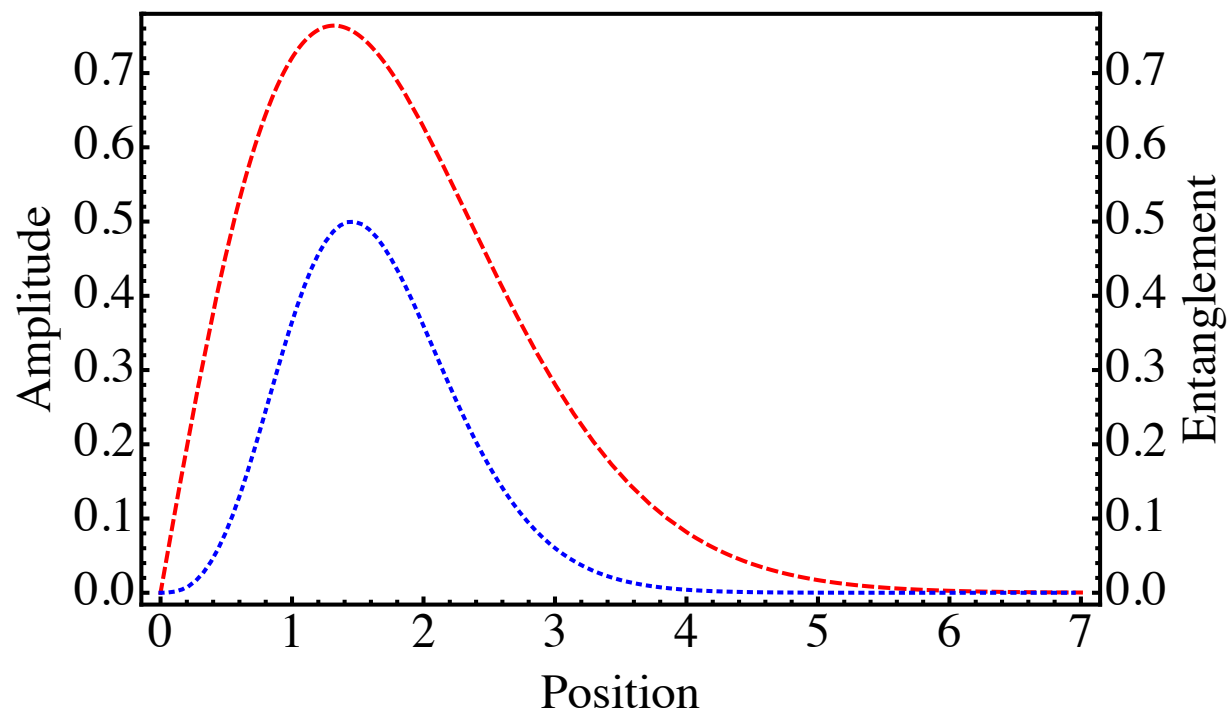
$$\text{Tr}(\rho_x^2) = \sum_{q=1}^N |\langle q | \psi \rangle|^4 + 2 \sum_{q=1}^x \sum_{l=1}^{q-1} |\langle q | \psi \rangle|^2 |\langle l | \psi \rangle|^2 + 2 \sum_{q=x+1}^x \sum_{l=x+1}^{q-1} |\langle q | \psi \rangle|^2 |\langle l | \psi \rangle|^2$$



Participation ratio



# Entanglement and delocalization





# Summary

- Non-scalable simulation is a good probe of properties relevant to post-quantum annealing AQC.
- Lets do some XX experiments!
- We will always ~~be at war with eurasia~~ need better locality reduction techniques
- Case for quantumness in AQC will likely rely on many forms of indirect evidence.
- Worry: can techniques from fermion QMC be adapted to non-stoquastic XX?



Thanks!