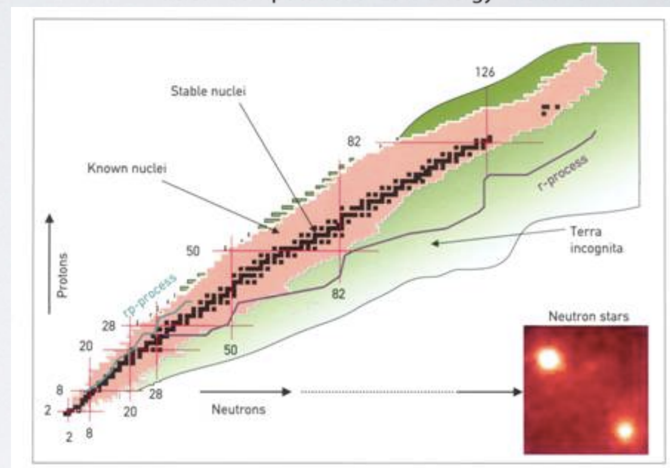
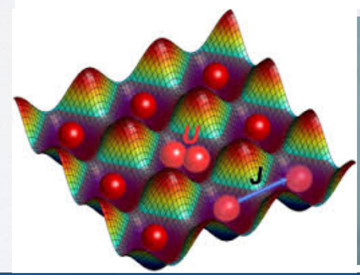
Linear Response on a Quantum Computer

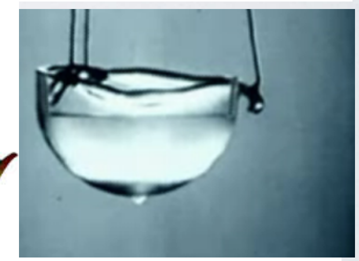
A. Roggero, J. Carlson
- LANL

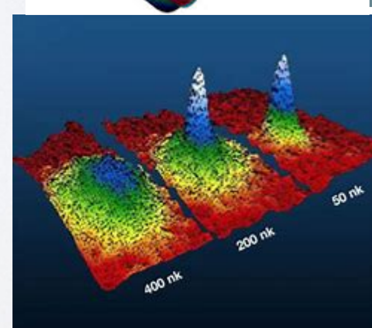
- Quantum computing at LANL
- Quantum Linear response
  - Motivation
  - Algorithm
  - Simple Example
- Outlook

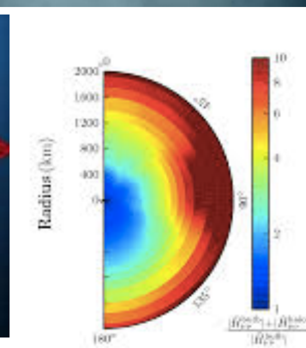
NUCLEI
Nuclear Computational Low-Energy Initiative











- Quantum computing at LANL

Long history and new efforts staff:

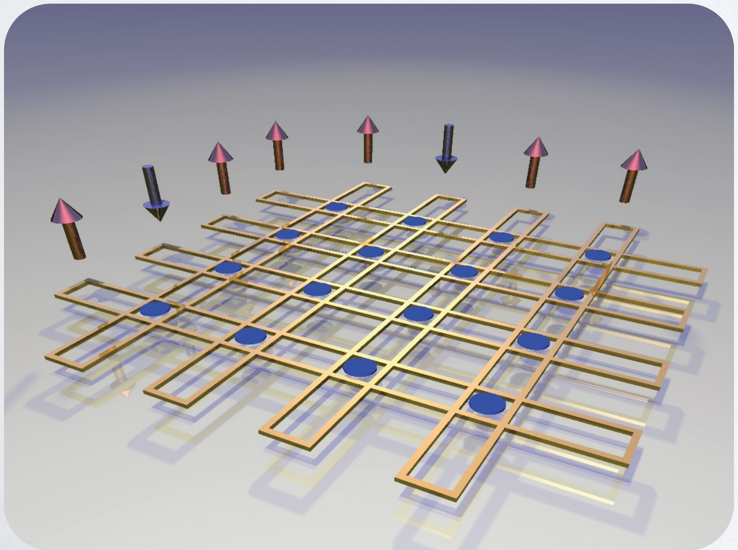
Zurek, Somma, Coles (condensed matter)

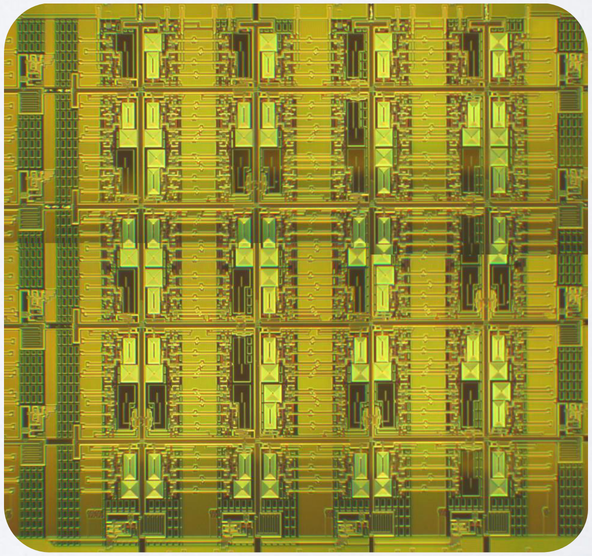
Increased interest across fields, particularly in

the Theoretical Division

Math/CS, Particle physics, Nuclear physics

- Hardware
- D-wave machine locally
- Use of other external machines: IBM, Rigetti, …





D-Wave "Rapid Response" Projects (Stephan Eidenbenz, ISTI)

Round 1 (June 2016)

1. Accelerating Deep Learning with Quantum Annealing
2. Constrained Shortest Path Estimation
3. D−Wave Quantum Computer as an Efficient Classical Sampler
4. Efficient Combinatorial Optimization using Quantum Computing
5. Functional Topological Particle Padding
6. gms2q—Translation of B-QCQP to D−Wave
7. Graph Partitioning using the D−Wave for Electronic Structure Problems
8. Ising Simulations on the D−Wave QPU
9. Inferring Sparse Representations for Object Classification using the Quantum D−Wave 2X machine
10. Quantum Uncertainty Quantification for Physical Models using ToQ.jl
11. Phylogenetics calculations

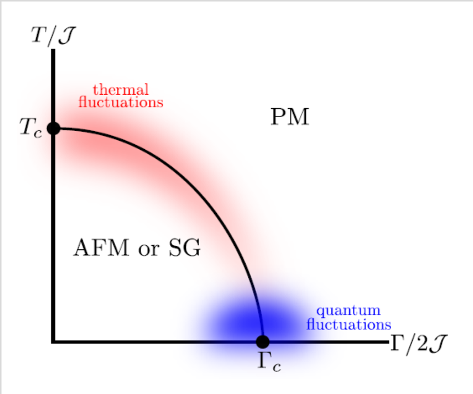
Round 2 (December 2016)

1. Preprocessing Methods for Scalable Quantum Annealing
2. QA Approaches to Graph Partitioning for Electronic Structure Problems
3. Combinatorial Blind Source Separation Using "Ising"
4. Rigorous Comparison of "Ising" to Established B-QP Solution Methods

Round 3 (January 2017)

1. The Cost of Embedding
2. Beyond Pairwise Ising Models in D-Wave: Searching for Hidden Multi-Body Interactions
3. Leveraging "Ising" for Random Number Generation
4. Quantum Interaction of Few Particle Systems Mediated by Photons
5. Simulations of Non-local-Spin Interaction in Atomic Magnetometers on "Ising"
6. Connecting "Ising" to Bayesian Inference Image Analysis
7. Characterizing Structural Uncertainty in Models of Complex Systems
8. Using "Ising" to Explore the Formation of Global Terrorist Networks

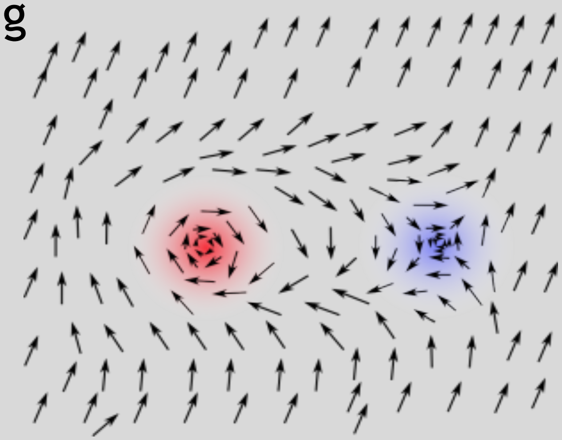
Physics / Quantum material simulation: D-wave



R. Harris

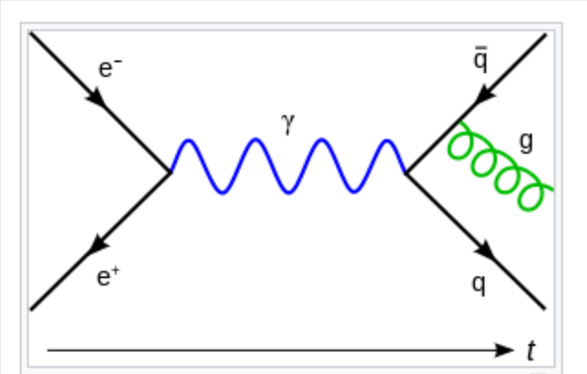
3D transverse-field Ising model

A. King



Kosterlitz-Thouless model

E. Dahl

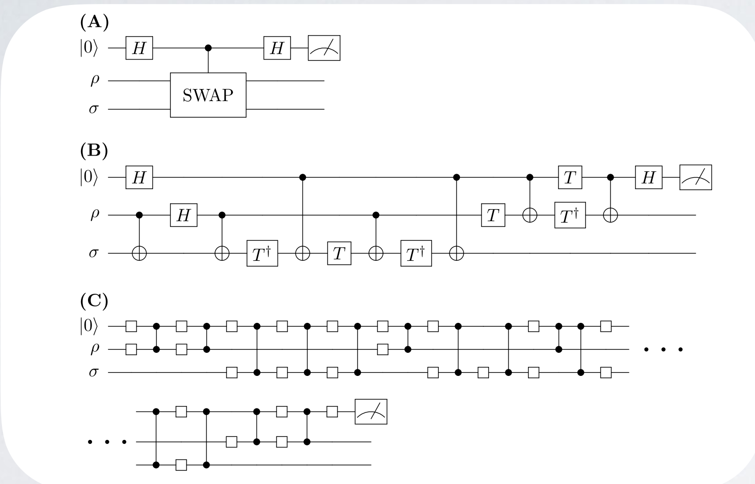


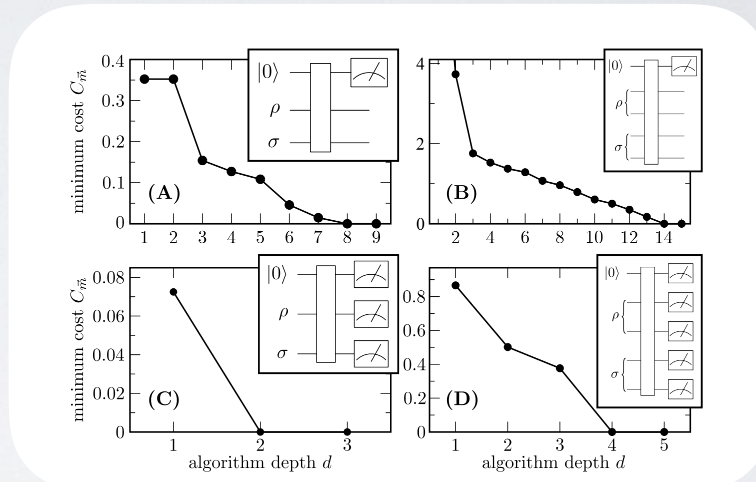
Z(2) lattice gauge theory

Other recent examples:

P. Coles

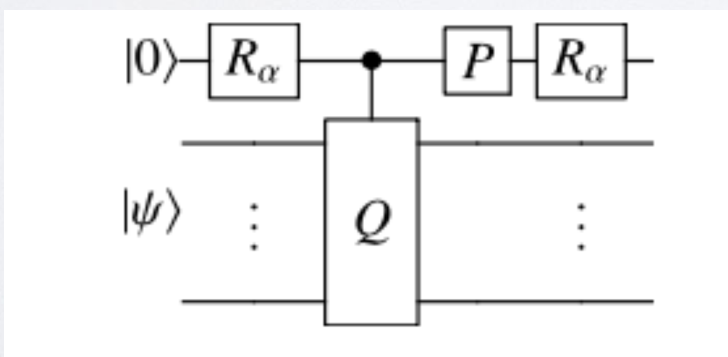
Learning the quantum algorithm for state overlap
L Cincio, Y Subaşı, AT Sornborger, PJ Coles
arXiv preprint arXiv:1803.04114





R. Somma

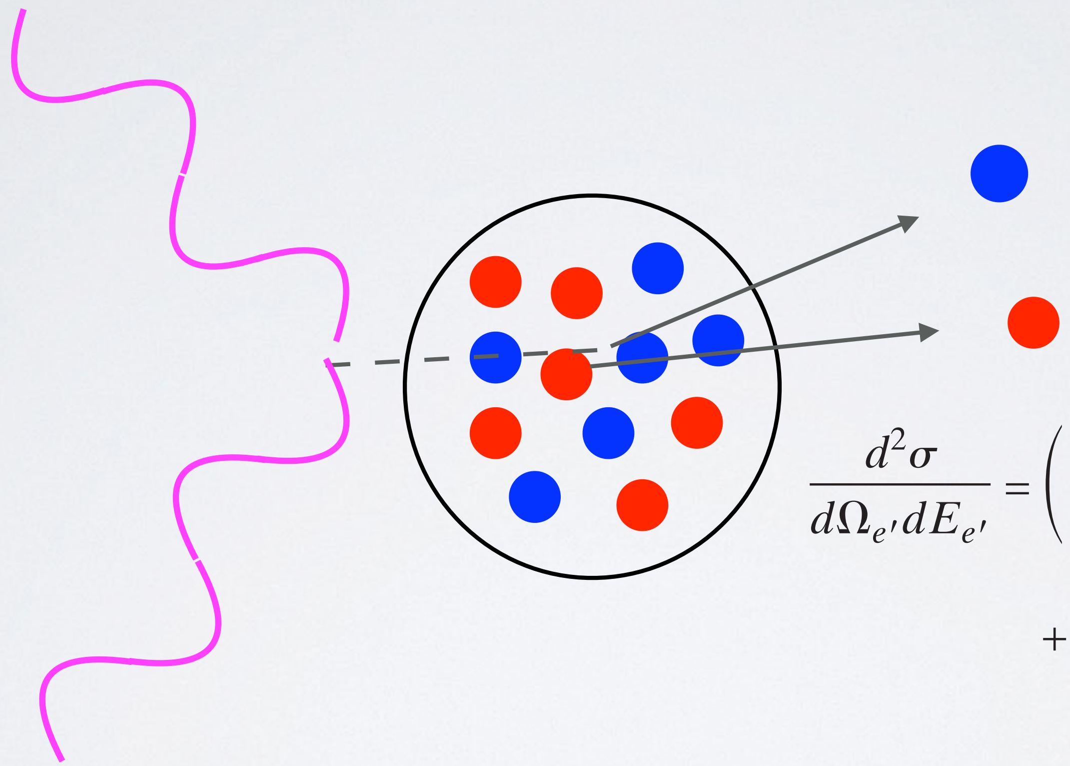
Exponential improvement in precision for simulating sparse Hamiltonians
DW Berry, AM Childs, R Cleve, R Kothari, RD Somma
Forum of Mathematics, Sigma 5 (2017)



Linear Response on a Quantum Computer

A. Roggero, J. Carlson arXiv 1804.01505

motivation: Electron and neutrino scattering from nuclei



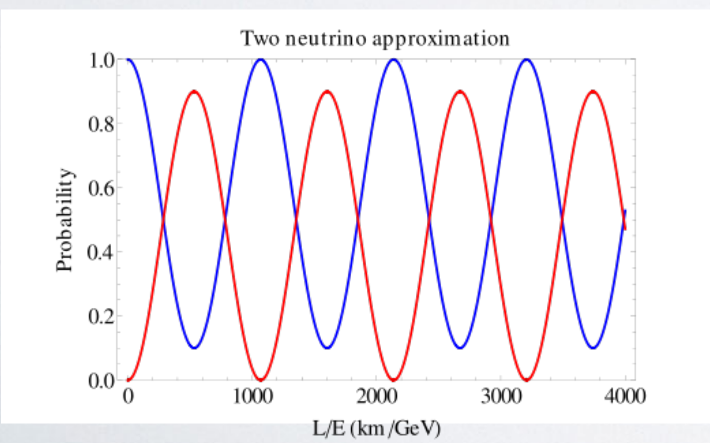
$$\frac{d^2\sigma}{d\Omega_{e'}dE_{e'}} = \left(\frac{d\sigma}{d\Omega_{e'}}\right)_M \left[\frac{Q^4}{|\mathbf{q}|^4} R_L(|\mathbf{q}|,\omega) + \left(\frac{1}{2}\frac{Q^2}{|\mathbf{q}|^2} + \tan^2\frac{\theta}{2}\right) R_T(|\mathbf{q}|,\omega)\right]$$

Typical rational: use simple probe to study target structure and dynamics
Neutrinos: determine a few parameters of the probe from interactions with (complicated) nucleus

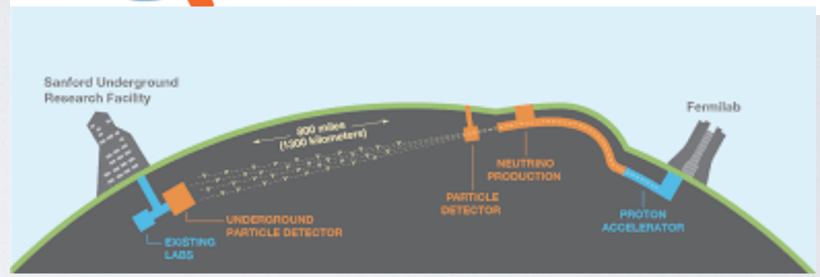
Electron and Neutrino Scattering from Nuclei

Jefferson Lab

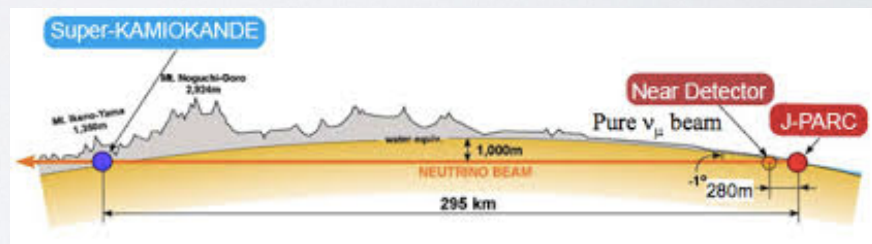
mass differences,
mixings from oscillations

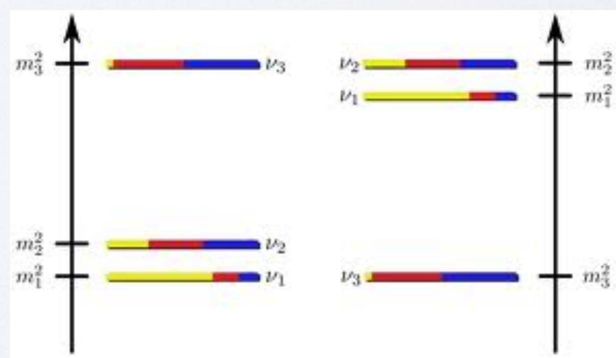


DUNE DEEP UNDERGROUND NEUTRINO EXPERIMENT



T2K





Linear Response on a QC: Algorithm

Linear Response: $$S_O(\omega) = \sum_\nu |\langle\psi_\nu|\hat{O}|\psi_0\rangle|^2 \delta(E_\nu - E_0 - \omega)$$

Rescaled version: $$S_O^r(\omega) = \sum_\nu \frac{|\langle\psi_\nu|\hat{O}|\psi_0\rangle|^2}{\langle\hat{O}^2\rangle_0} \delta(E_\nu - E_0 - \omega)\ .$$

3 ingredients to algorithm:

- State preparation: Ground state (or finite T) $|\Psi_0\rangle$
- Unitary Operator which implements linear coupling O(q) $\mathcal{O}|\Psi_0\rangle$
- Unitary Operator which implements time evolution

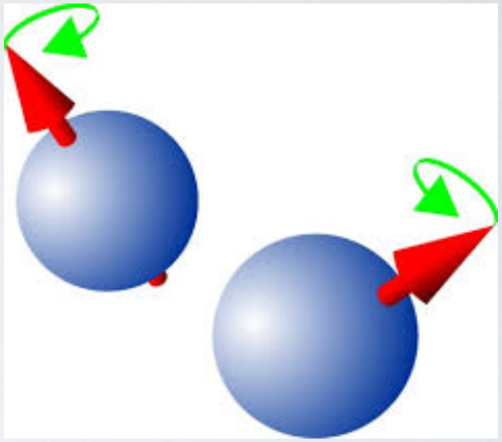
$$|\Psi(t)\rangle \ = \ [\exp[-iHt]\ \mathcal{O}\ |\Psi_0\rangle$$

Algorithm (continued)

To produce a state: $\Psi_{\mathcal{O}} = \mathcal{O}\,|\Psi_0\rangle$

Define an ancillary q-bit and a unitary oeprator:

$$\hat{U}_S^{\gamma} = e^{-i\gamma\hat{O}\otimes\sigma_y} = \begin{pmatrix} cos(\gamma\hat{O}) & -sin(\gamma\hat{O}) \\ sin(\gamma\hat{O}) & cos(\gamma\hat{O}) \end{pmatrix}$$



Initialize this bit to |1> and apply this operator

$$(\mathbb{1}\otimes|0\rangle\langle 0|)\,\hat{U}_S^{\gamma}|\psi_0\rangle\otimes|1\rangle = \frac{|\Phi_O\rangle}{\sqrt{\langle\Phi_O|\Phi_O\rangle}} + \mathcal{O}\left(\gamma^2\|\hat{O}\|^2\right)$$

Probability for success for creating the state

$$\begin{aligned} P_{success} = P(|0\rangle) &= \langle\psi_0|sin(\gamma\hat{O})^2|\psi_0\rangle \\ &= \gamma^2\langle\hat{O}^2\rangle_0 + \mathcal{O}\left(\gamma^4\right) \end{aligned}$$

Use standard phase estimation algorithm to calculate response

$$U^k = e^{i2k\pi\widetilde{H}} \;\Rightarrow\; U^k|\psi_\nu\rangle = e^{i2k\pi\lambda_\nu}|\psi_\nu\rangle$$

For k = 0… 2^W-1

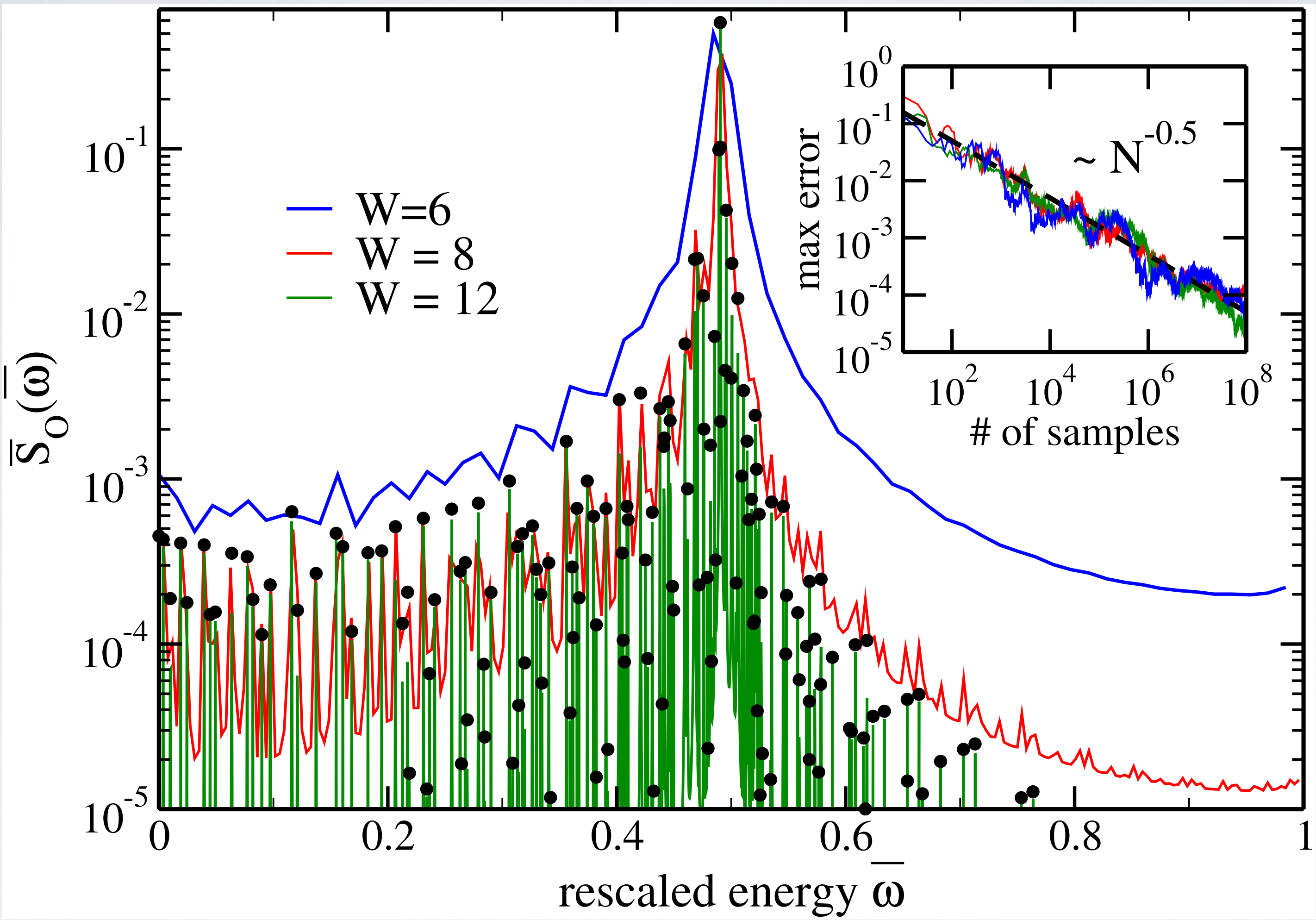
Depth of circuit: $W\ log(W) + N_{max}$

Probability of obtaining binary integer y is equal to

$$\begin{aligned} P(y) &= \frac{1}{2^{2W}}\sum_\nu |\langle\psi_\nu|\Phi_O\rangle|^2 \frac{sin^2\left(2^W\pi\left(\lambda_\nu - \frac{y}{2^W}\right)\right)}{sin^2\left(\pi\left(\lambda_\nu - \frac{y}{2^W}\right)\right)} \\ &\equiv \frac{1}{2^W}\sum_\nu |\langle\psi_\nu|\Phi_O\rangle|^2 F_{2^W}\left(2\pi\left(\lambda_\nu - \frac{y}{2^W}\right)\right) \end{aligned}$$

Accurate representation of the response

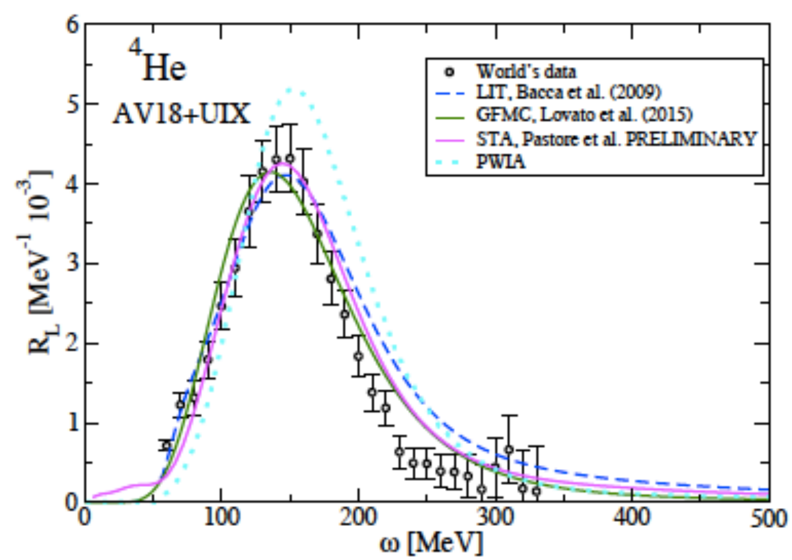
Simple Example: 2 body Hubbard Model: N=2, 31x31 lattice



Basic features revealed with just a few steps, exact details over many order of magnitude for W=12

Topics being explored now:

- Access to explicit final states:
  Energy and momenta of outgoing particles
- Reducing circuit depth for high energy scattering
- Actual implementation of simple problem on QC
- Related problems in NP and other fields



Longitudinal Response function at $q = 500$ MeV

* Preliminary results *

Thanks for support from LANL LDRD: ISTI

Longer Term

Whole new fields of both theory and experiment
with full treatment quantum dynamics:

- More sophisticated theories of quantum structure and dynamics
- Much wider range of direct confrontation between
  theory and experiment
- Enables much more reliable extrapolations to regimes
  not experimentally accessible