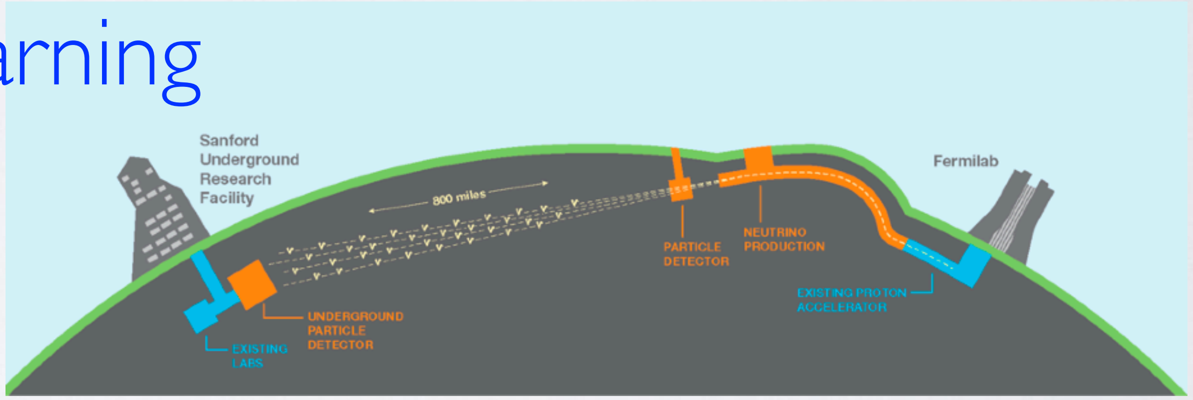
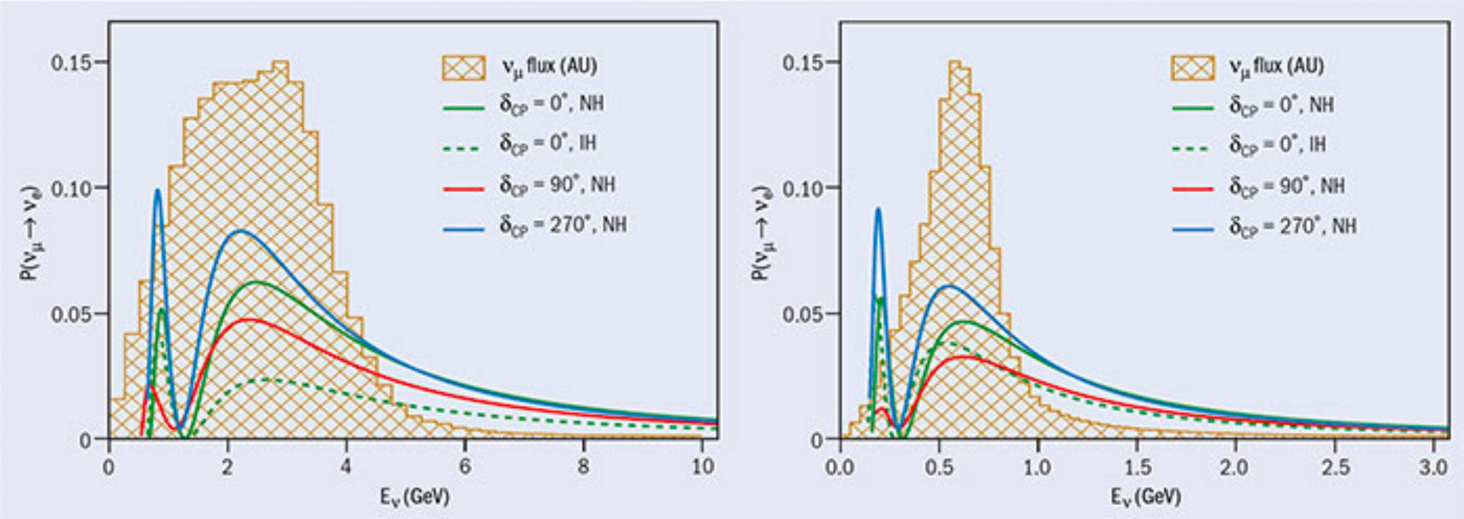
Linear Response on a Quantum Computer

A. Roggero (LANL UW),
J. Carlson (LANL),
R. Gupta (LANL)
G. Perdue (FNAL)

- HEP Quantum computing at LANL
  - Lattice QCD : QC for QFT and chiral fermions
  - Lattice QCD : machine learning
- Quantum Linear response
  - Motivation
  - Algorithm
  - Simple Example
- Outlook



DUNE T2K



Quantum Computing for QFT and Chiral Fermions
(PI: Bhattacharya, Lead Institution: LANL)

THE PROBLEM

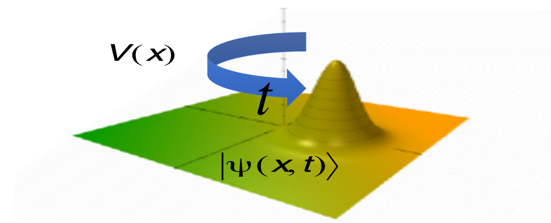
Classical simulation of the quantum hard.

- Affects fermions and gauge fields
- Affects finite density
- Affects finite time

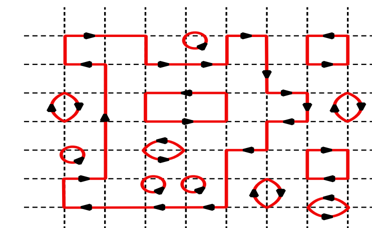
Quantum simulation of quantum system does not face this problem.

Current quantum devices do not work well with continuous variables.

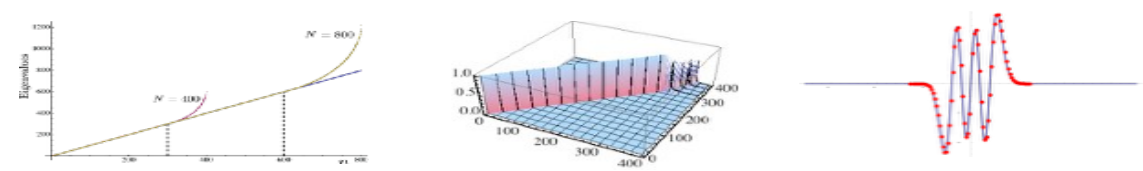
PRELIMINARY WORK



Complexity of initial state preparation and evolution



Qubit formulation mainataining O(N) symmetry



Discretization of scalar field theory

THE SOLUTION

Develop *qubit* representations of field theories that

- maintain enough symmetries
- can be simulated efficiently
- can represent chiral fermions
- can represent gauge fields

Understand the scaling behavior of these theories

Understand approximations and error bounds

Develop mappings to experimental protocols

THE IMPACT

Ability to

- calculate effects of strong interactions
- deal with chiral theories and gauge interactions
- understand phase transitions in QGP
- study strongly coupled BSM theories

Be ready to use quantum computers for HEP

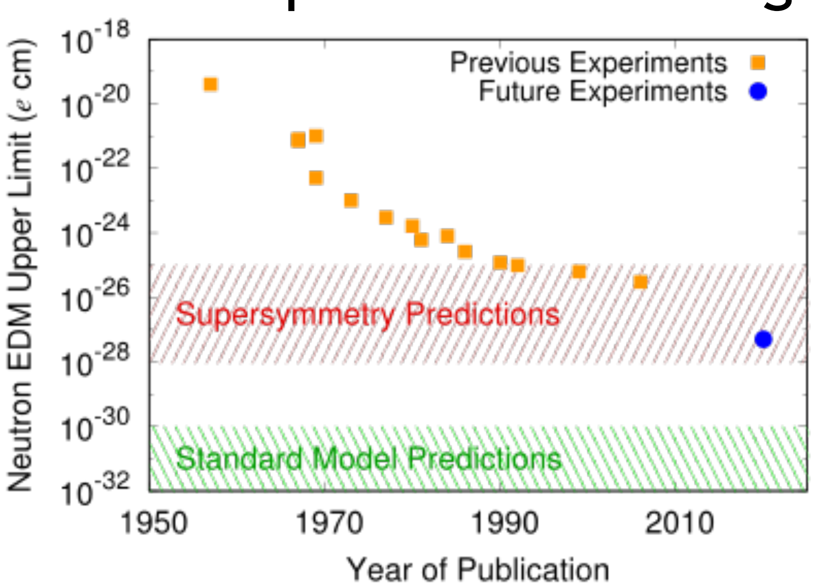
Quantum Machine Learning for Lattice QCD

- Unmeasured observables can be predicted from the measured observables using machine learning

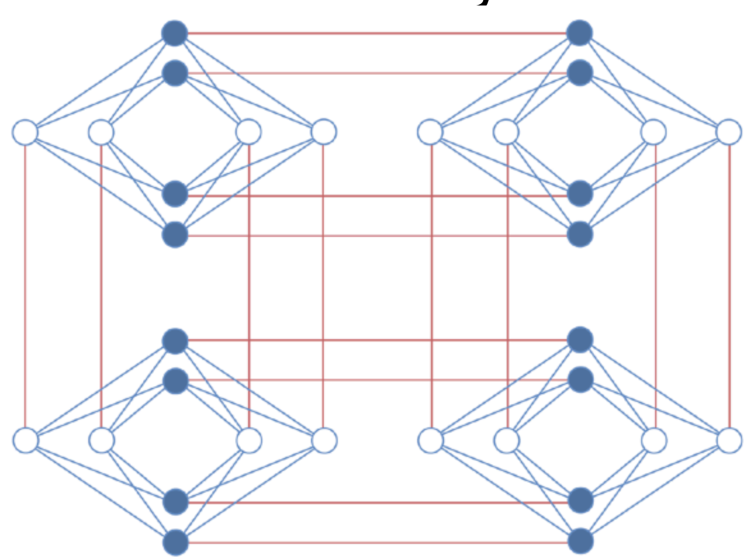
➢Decrease computing cost for **lattice QCD calculation of neutron EDM** by reducing direct measurements

- Machine learning (ML) algorithm implemented on D-Wave Quantum Annealer accelerates ML process

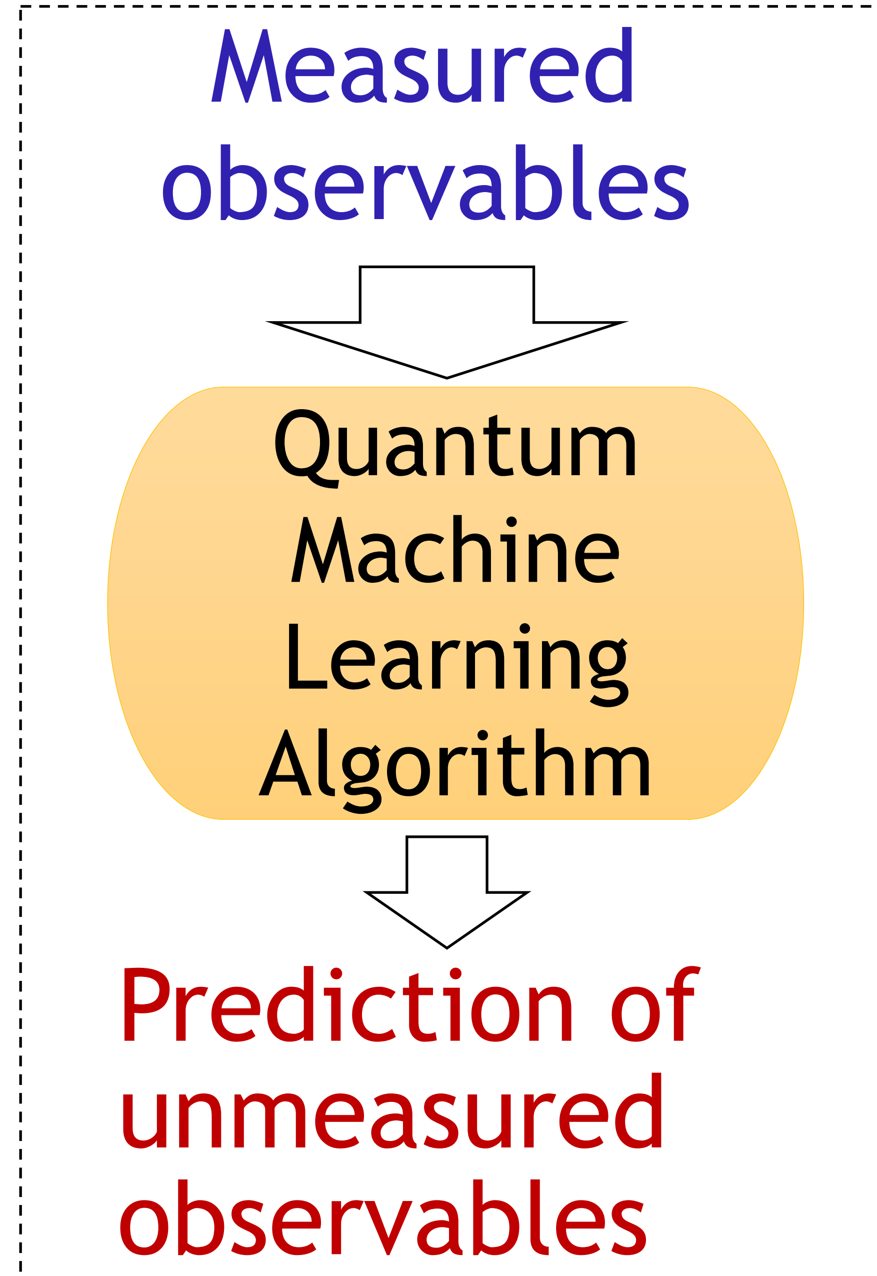
➢Develop efficient ML algorithm on D-Wave system



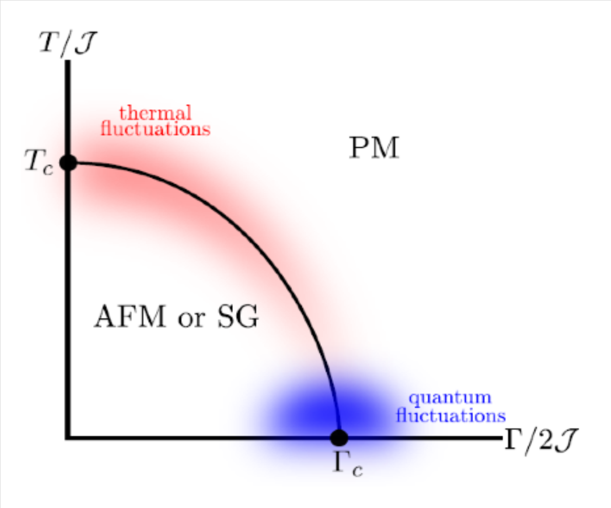
Neutron EDM experiments



D-Wave Qubit connection



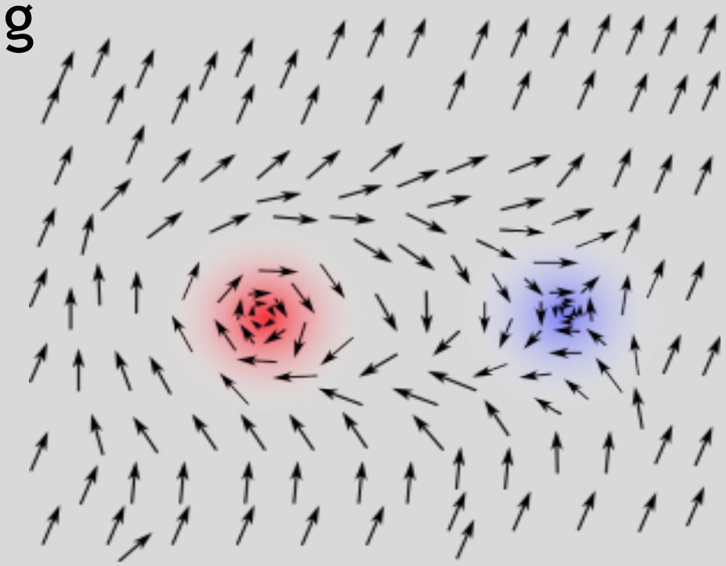
Physics / Quantum material simulation: D-wave



R. Harris

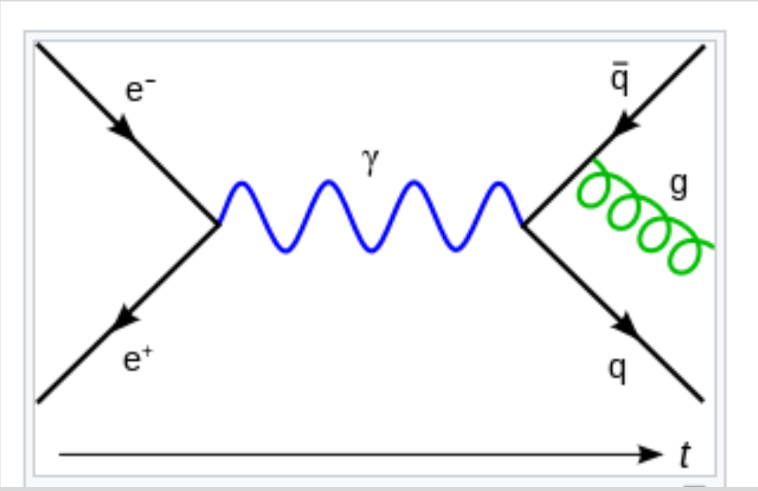
3D transverse-field Ising model

A. King



Kosterlitz-Thouless model

E. Dahl

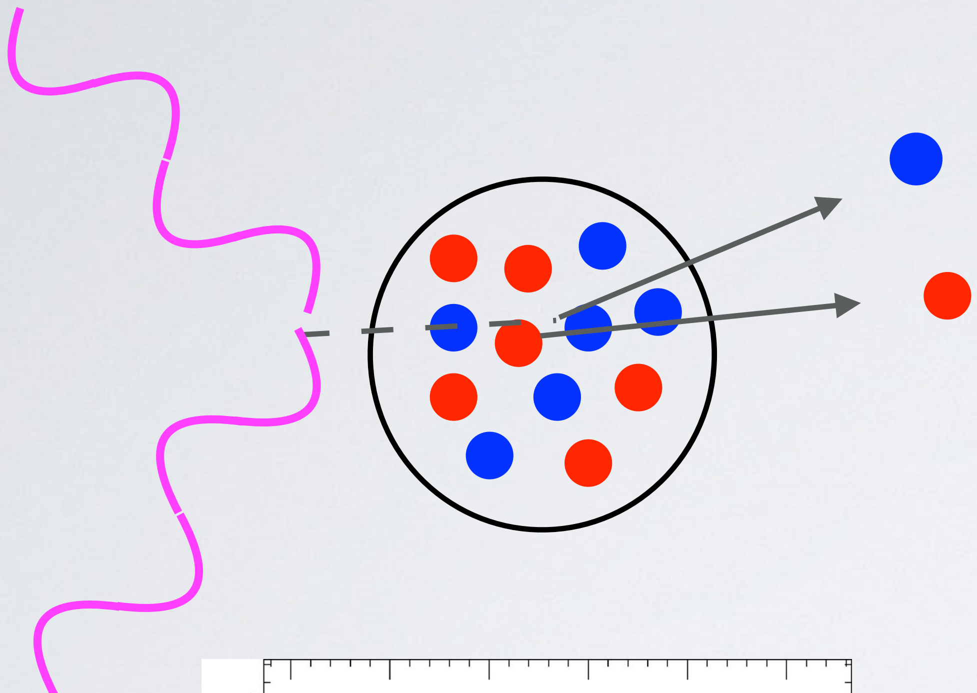


Z(2) lattice gauge theory

Linear Response on a Quantum Computer

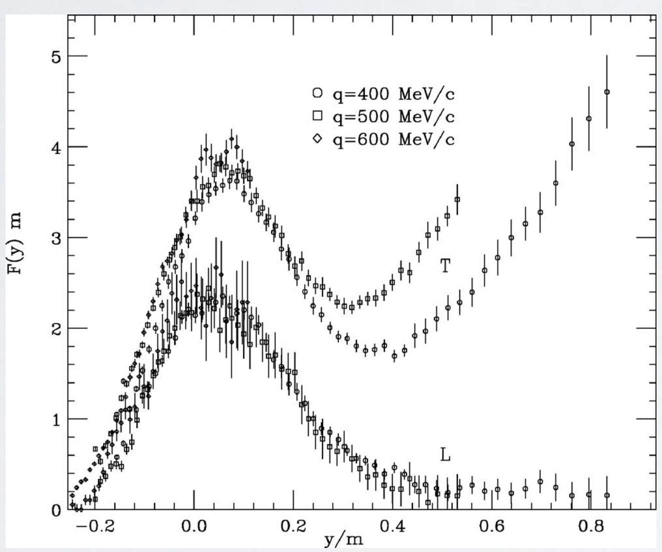
A. Roggero, J. Carlson arXiv 1804.01505

motivation: electron and neutrino scattering from nuclei



- Goal: reconstruct initial neutrino energy from observed leptons, nucleons, pions,
- Present method:
  - nuclear structure model
    - momentum distributions
    - spectral function
    - 2-particle correlations, …

generators at/after vertex to treat FSI (classical / semi-classical)



Typical rational: use simple probe to study target structure and dynamics

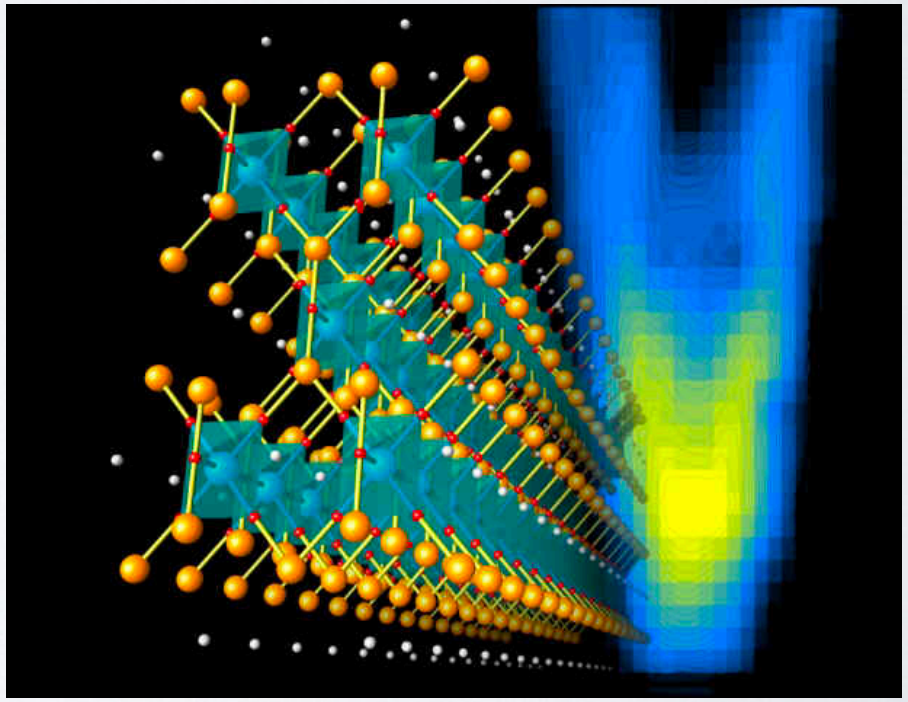
Neutrinos: determine a few parameters of the probe from interactions with (complicated) nucleus

Status for Classical Computers on Quantum Many-Body Problem

- Ground, Low-Lying Excitations : reasonably accurate for $A \gtrsim 40$
  (exact diagonalization, Coupled Cluster, Quantum Monte Carlo)
- High-energy Inclusive Scattering
  from current-current correlation functions
- Very difficult: more exclusive processes, breakup reactions, …
  number of basis states grows exponentially with N

Similar status in many areas of physics

- Electronic Structure
- Condensed Matter Physics
- Cold Atom Physics
- Lattice QCD



Linear Response on a QC: Algorithm

- natural application of a quantum computer

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

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

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

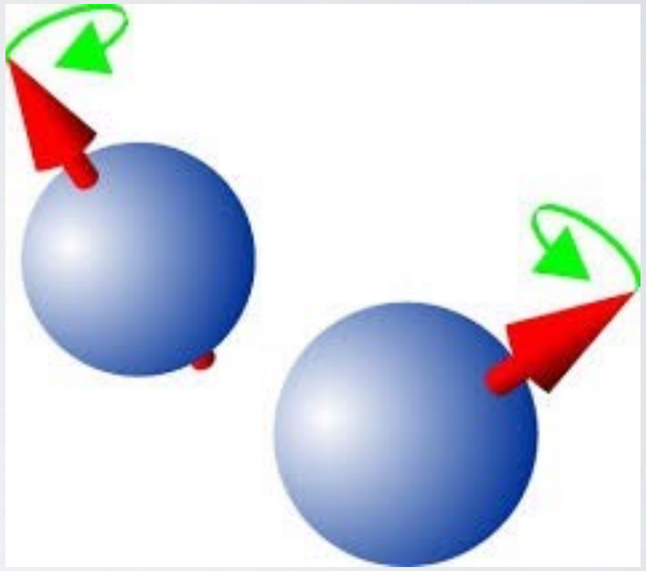
$$|\Psi(t)\rangle \;=\; [\exp[-iHt]\; \mathcal{O}\; |\Psi_0\rangle$$

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

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

Use standard phase estimation algorithm to calculate response

Kitaev (1996), Brassard et al. (2002), Score et. al (2013), …

Trotter expansion of propagation

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

- Starting vector (after vertex) with $\Psi_k = \sum_k c_k|\xi_k\rangle$
- Store time evolution of $|\Psi(t)\rangle$ in auxiliary register of M quits
- Perform Quantum Fourier transform on the auxiliary register
- Measures will return λ_n with probability $|c_n|^2$

For k = 0… 2^W-1
Depth of circuit:

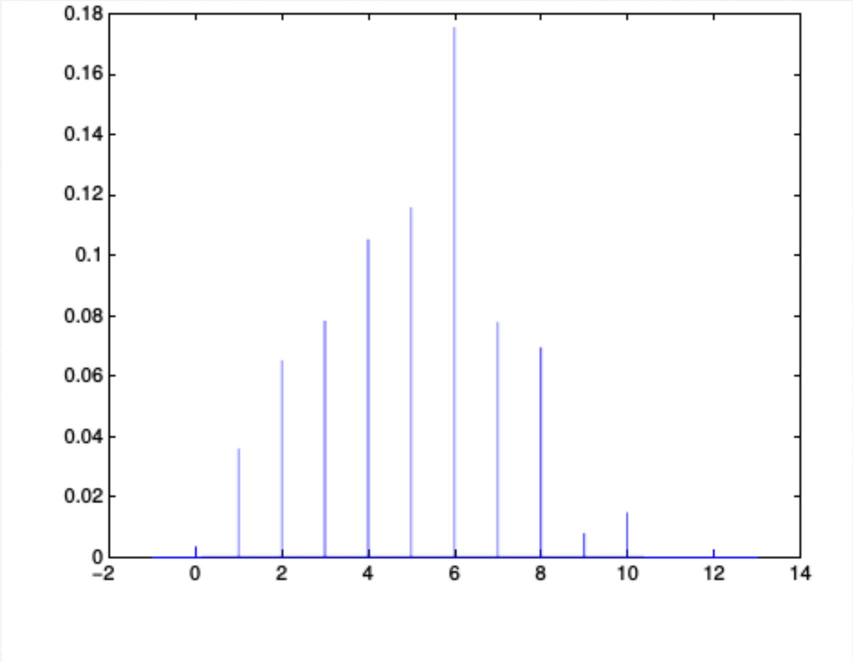
$$W\ log(W) + N_{max}$$

Probability of obtaining binary integer y is equal to

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

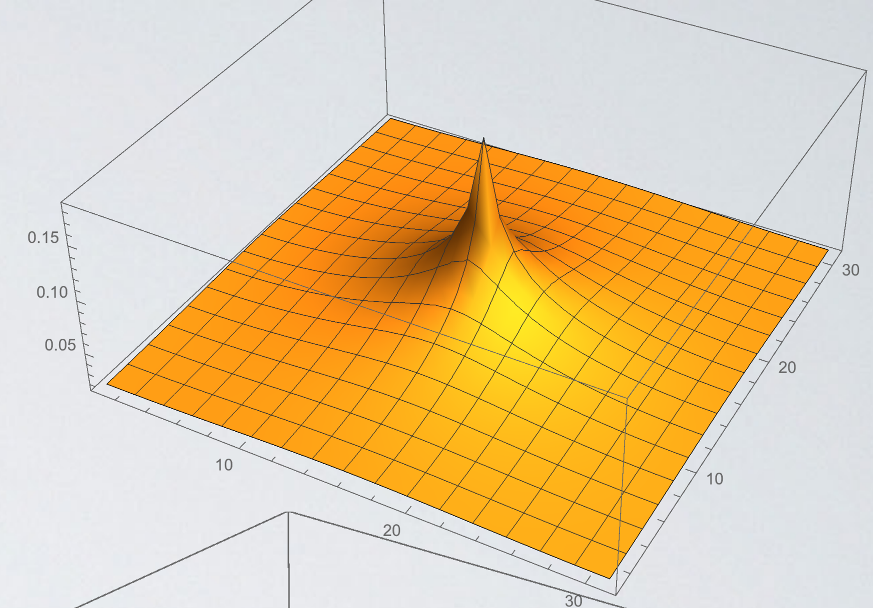
Accurate representation of the response

Example:
Ovrum & Hjorth-Jensen (2007)

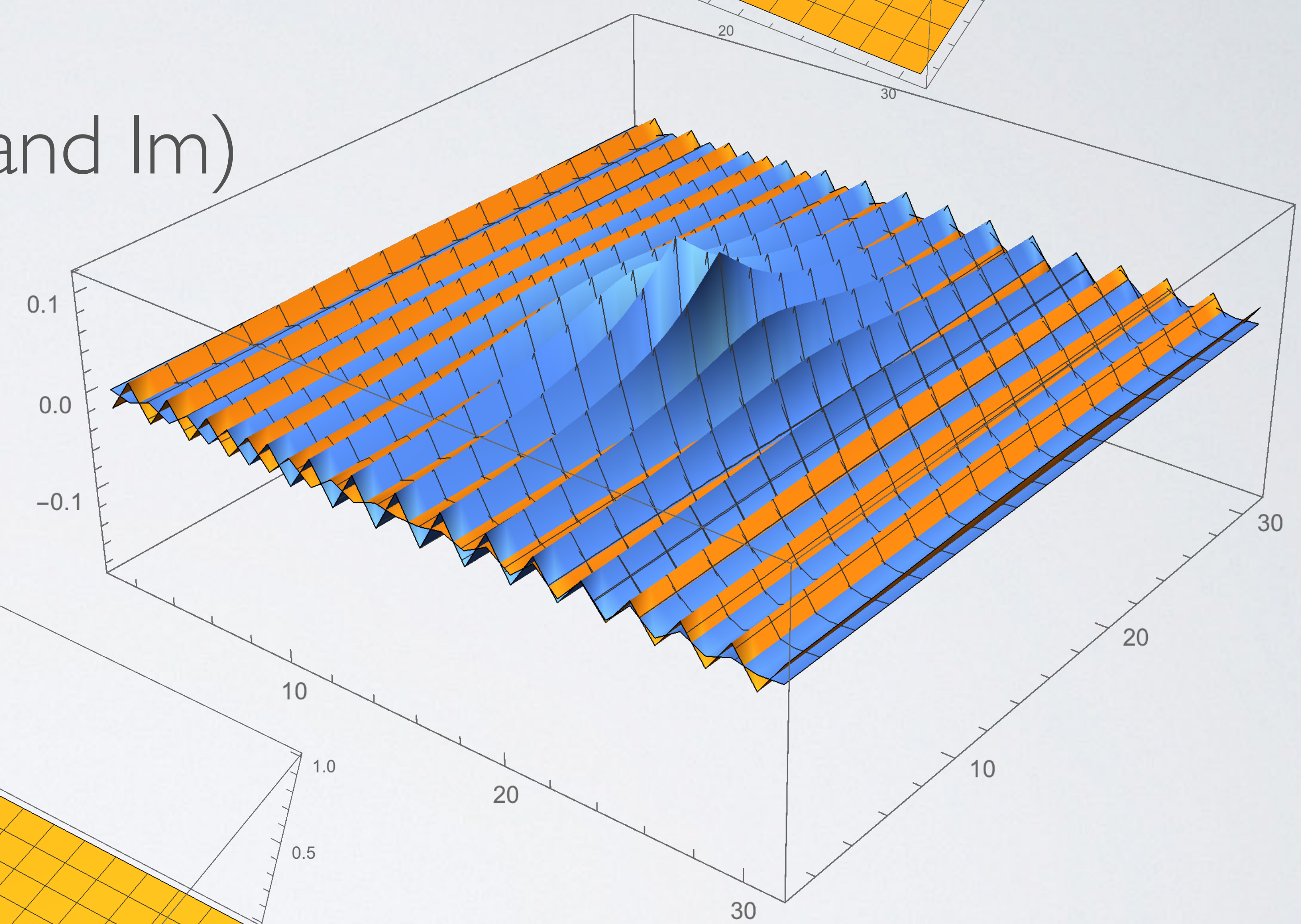


Example:
Hubbard Model
N=2, 31x31 lattice

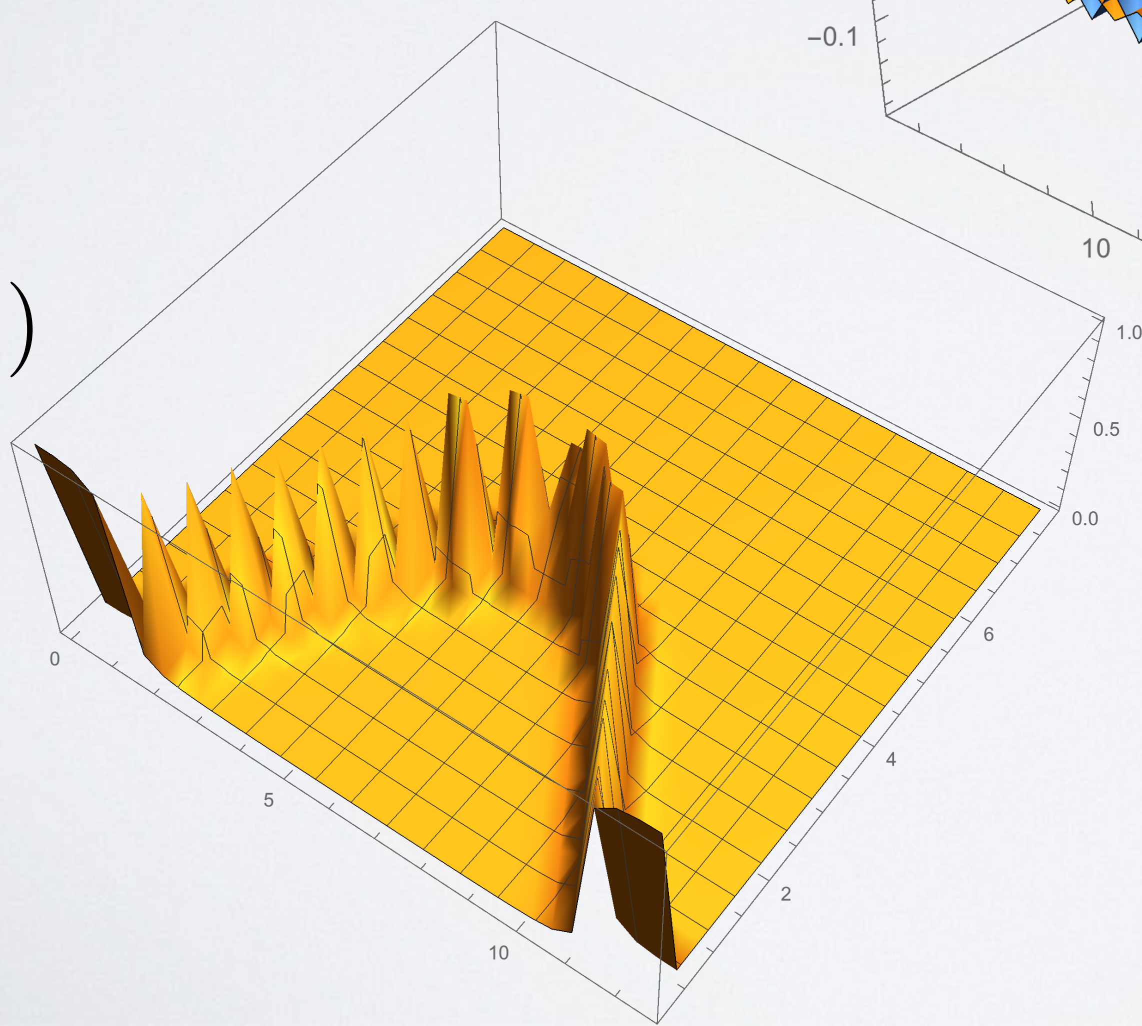
Initial State



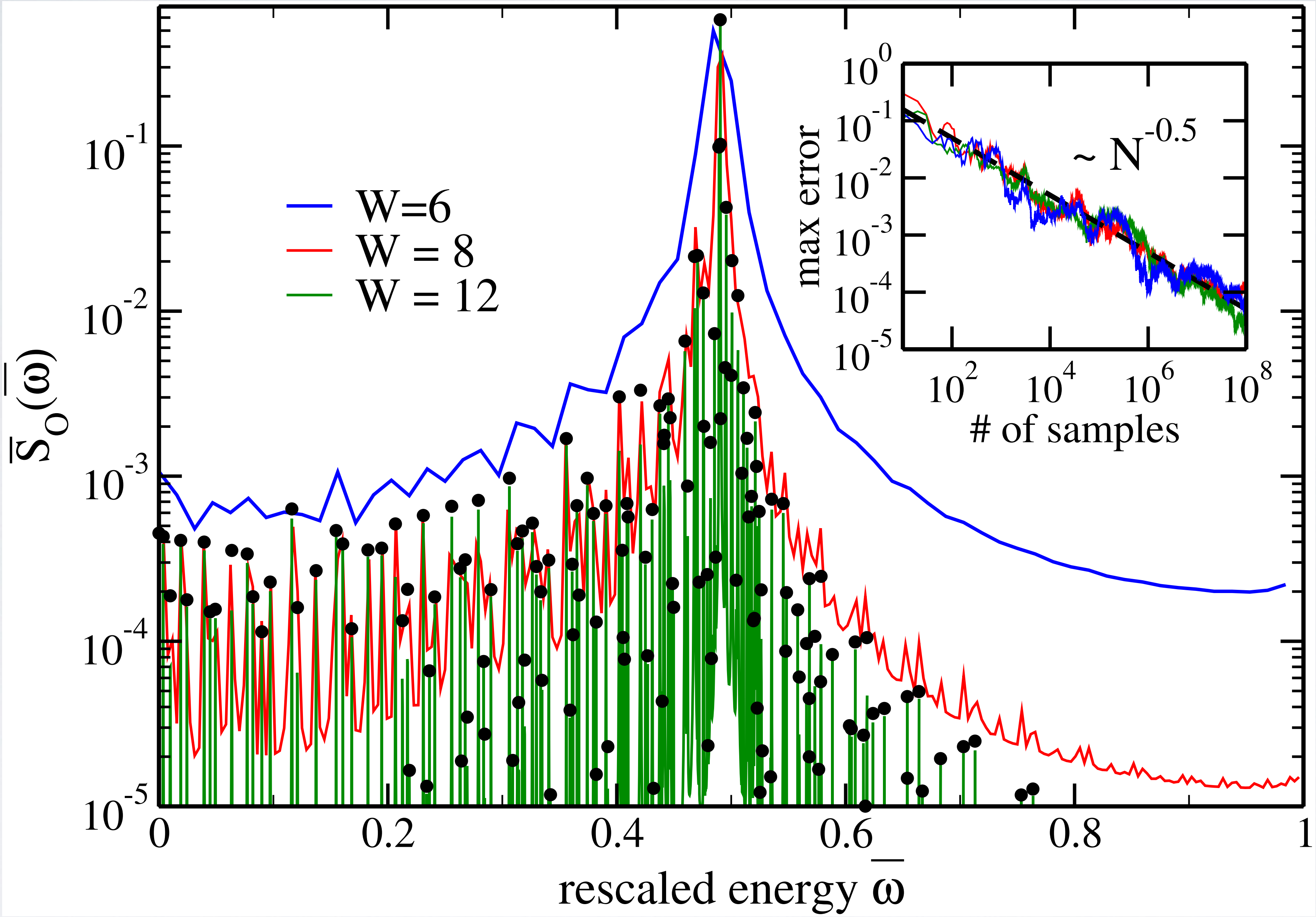
Propagated State (Re and Im)



$S\ (q,\omega)$



Simple Example: 2 body Hubbard Model: N=2, 31x31 lattice (fine-scale from particular lattice)



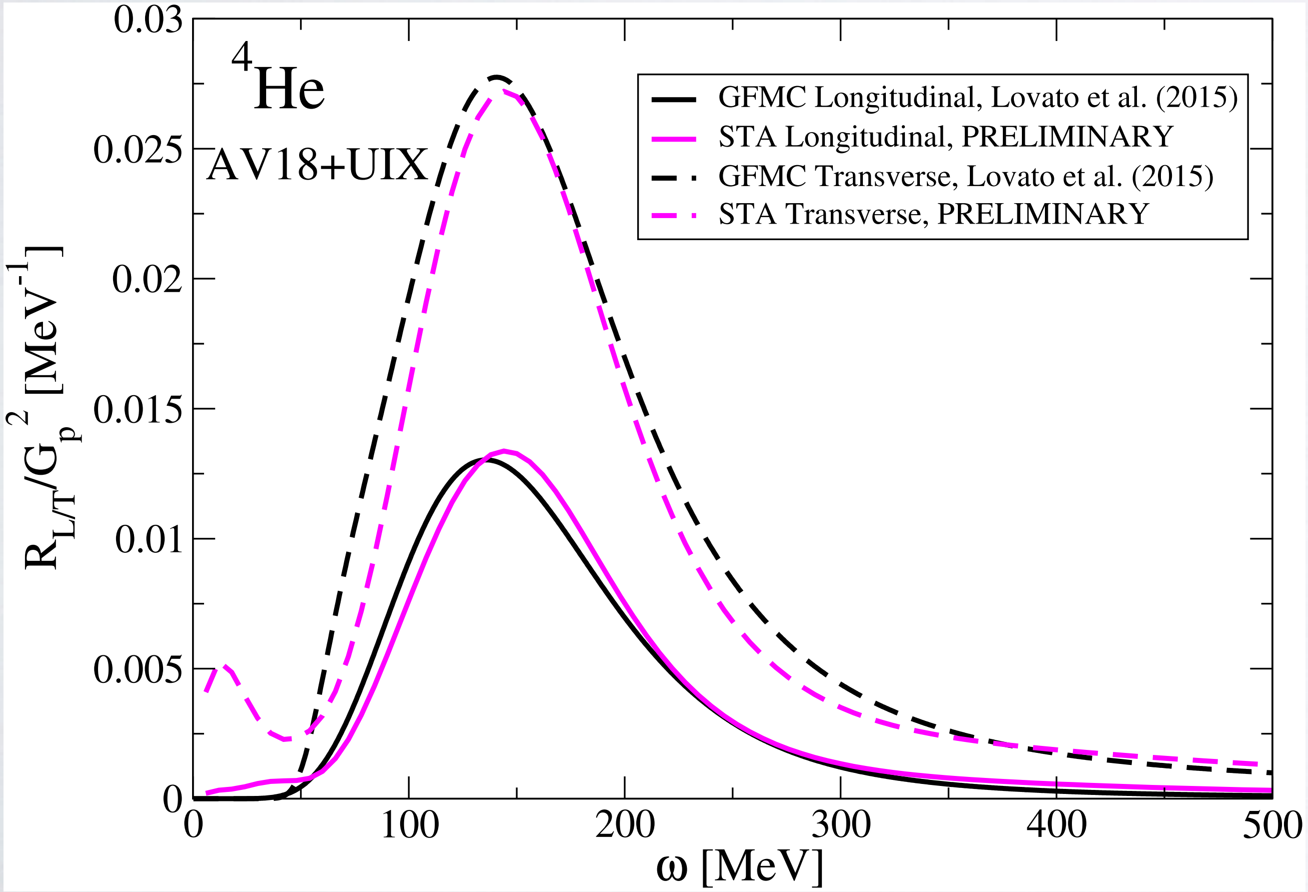
Basic features revealed with just a few steps, exact details over many order of magnitude for W=12

Why study this in the NISQ era ?

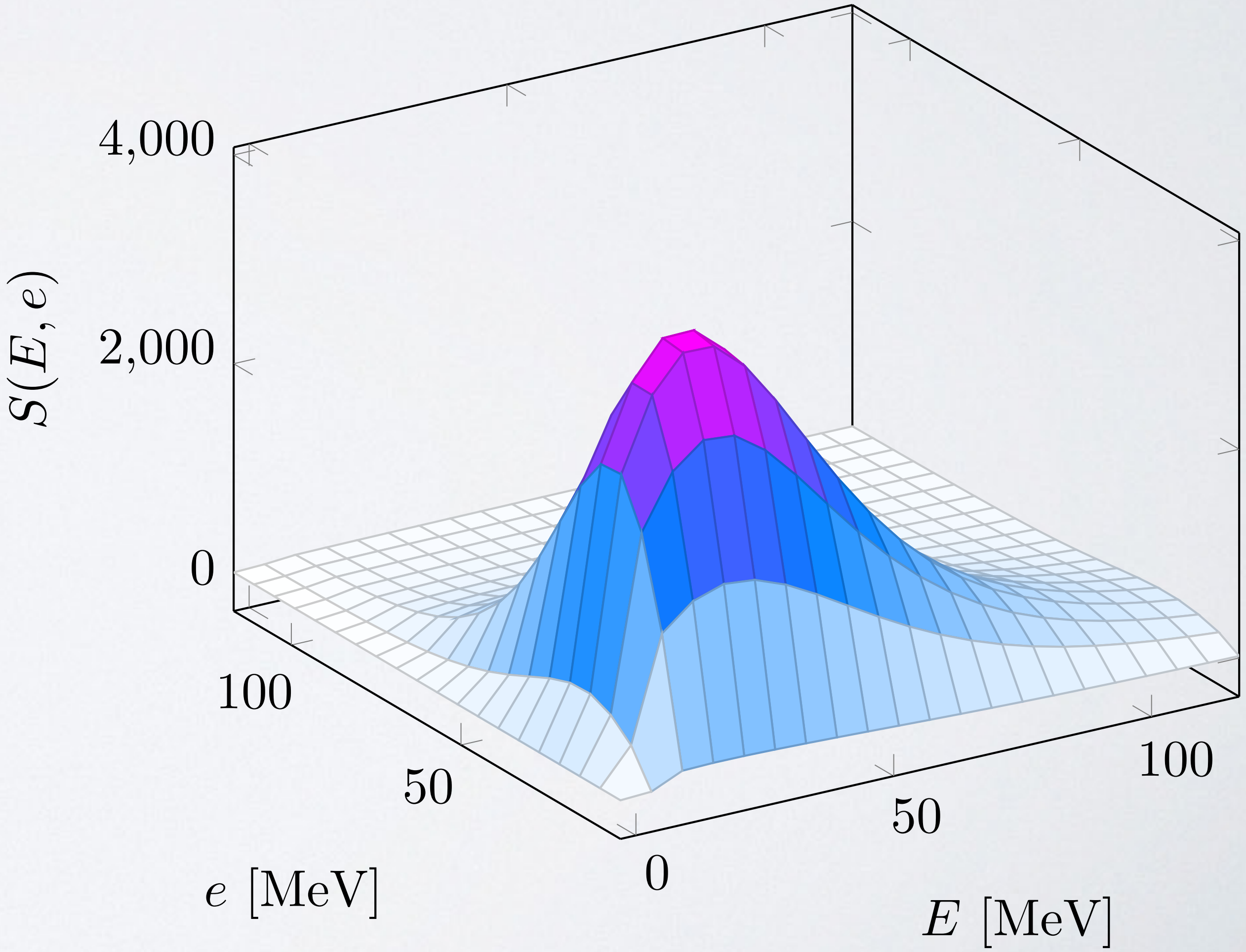
- Some information with just a few real-time steps: (sum rules, etc.)
- At high energies and momenta - few-body expansion may be feasible
- Test quantum-classical transition in quantum scattering processes
- Examine ability to 'detect' explicit final states: multi-nucleon, pion, …

Short-time (high energy) approximation at two-nucleon level (similar to OPE)

Pastore, et al (2018)



Transverse Density $q = 300$ MeV



Topics being explored now:

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

Mixture of early-stage QC and large-scale classical simulations
Present limits: 4-5 nucleons, $20^3 \times 1000$ lattice

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

- Whole new classes of experiments
  can be reliably designed, tested for
  sensitive tests of new physics