Neutrino nucleus response functions on a quantum computer

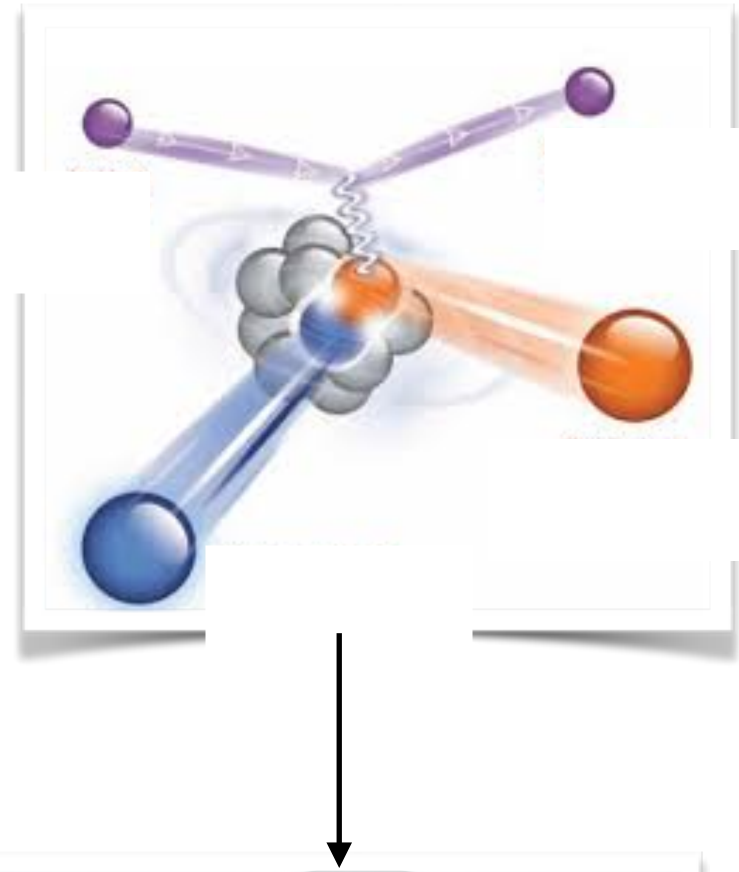
Alessandro Baroni

In collaboration with:

A. Roggero (UW, USA), J. Carlson, R. Gupta (LANL, USA), A. Li, G. Perdue (FermiLab, USA)

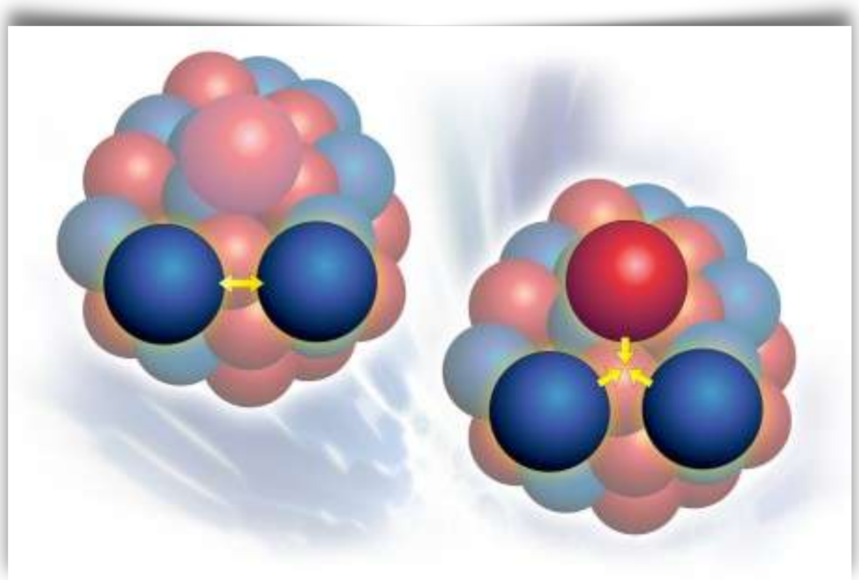
Outline

- Nuclear interactions
- Response functions
- Quantum simulation
- Results



Basic model

Nucleons interact between each others through many-body forces



Nuclear strong hamiltonian

$$H = \sum_{i=1}^{N} \frac{p_i^2}{2m} + V_{2N} + V_{3N} + \cdots$$

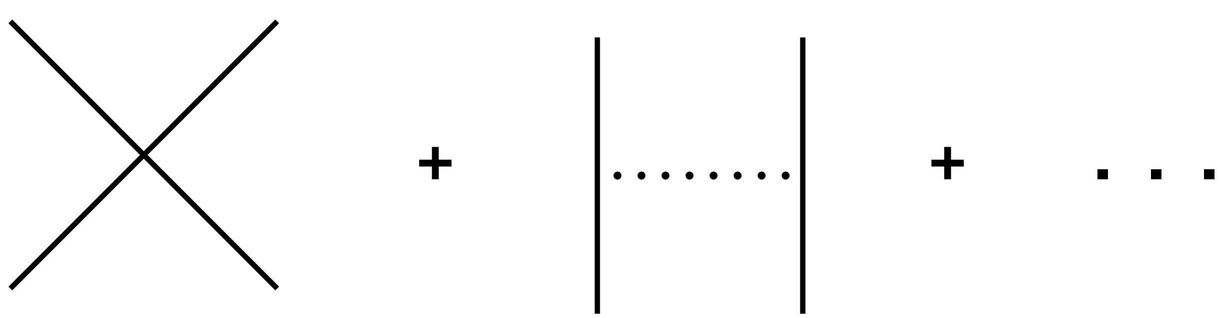
Non-relativistic Kinetic term

Two and three body forces

Negligible >3 -body forces

Potentials derived in chiral EFT

$V_{2N} =$



Scaling of classical resources

- Each nucleon has quantum numbers

Number of nucleons

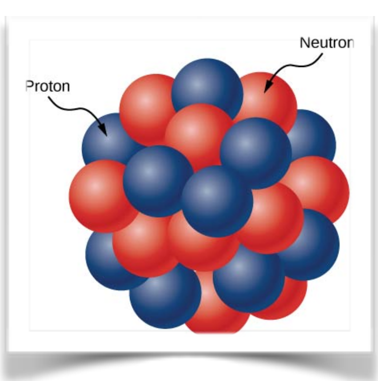
$$x_i \equiv (\mathbf{r}_i, s_{iz}, t_{iz}) \qquad i \in (1, \cdots, A) \qquad A = N + Z$$

- Many-nucleon wave function $\Psi(x_1, \cdots, x_n)$

- In principle 4^A amplitudes each a function of $3A$ coordinates

Imposing charge conservation we have $2^A \dfrac{N!}{A!Z!}$ amplitudes

How do we go to A>12?



Schrodinger equation solved with ab initio methods up to $^{12}\mathrm{C}$

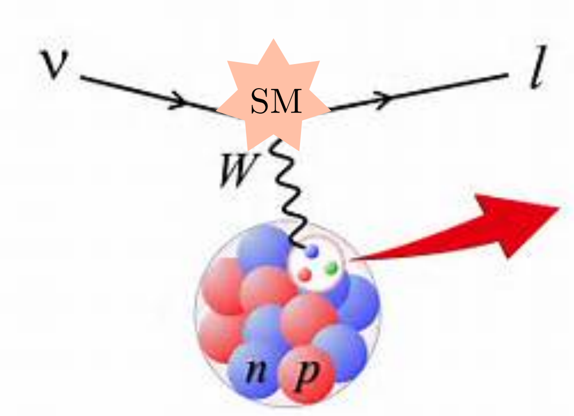
Electroweak nuclear scattering

- Nuclear electroweak scattering
  - Interactions described at ‘low’ energies by

$$H_I = c\, L_\mu \, J^\mu$$

Leptonic current

Nuclear part has one- and two-body terms



  - Quantity connected with experiments is

$$\frac{d^2\sigma}{d\Omega_e dE_e} \propto L_{\mu\nu} \, R^{\mu\nu}$$

Hadronic tensor that contains all the information on the target structure

Leptonic tensor fully specified by the electron kinematic variables

Response functions

- The challenging quantity to calculate is

$$R^{\mu\nu}(\omega, \mathbf{q}) = \sum_X \langle 0|J^\mu(\omega, \mathbf{q})|X\rangle \, \langle X|J^\nu(\omega, \mathbf{q})|0\rangle \delta(E_0 + \omega - E_X)$$

Directly related to the cross section

- What can be calculated is related to

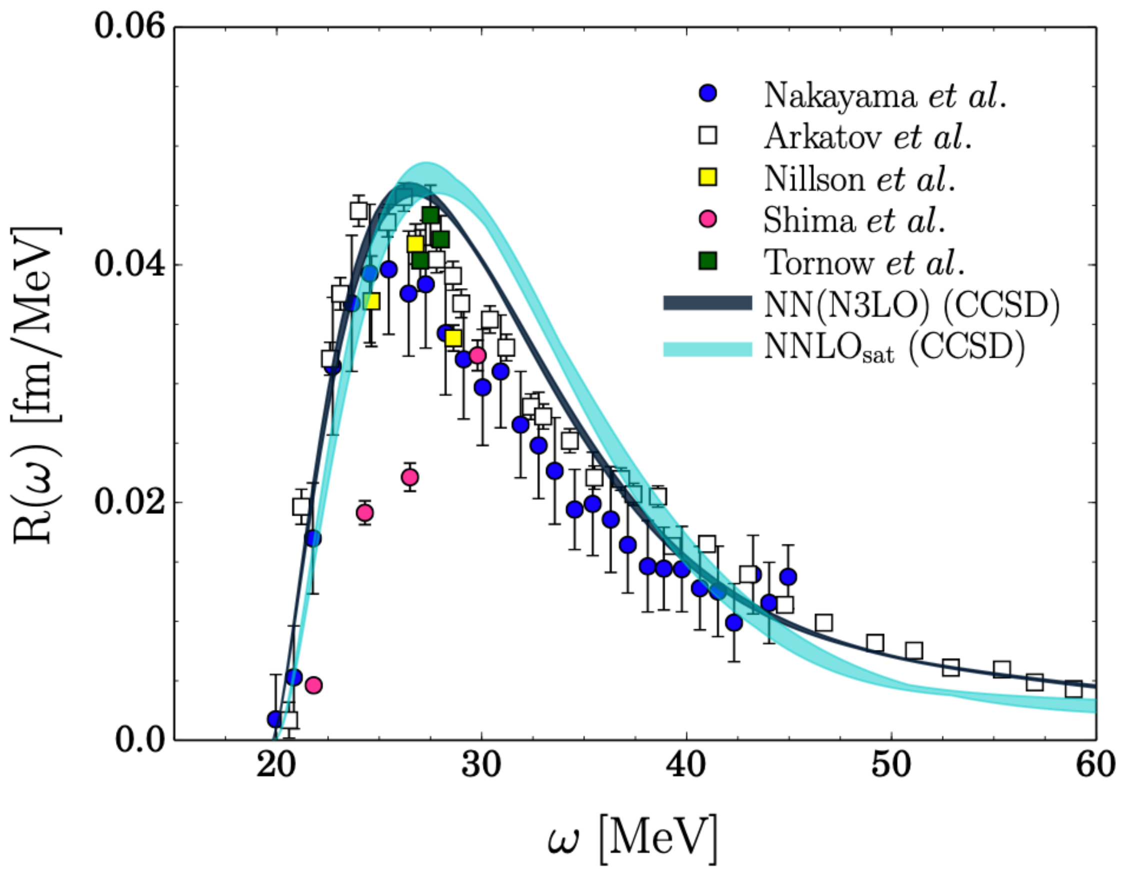
$$C^{\mu\nu}(t) = \int dt \, \langle 0|J^\mu(\omega, \mathbf{q}) e^{i(H-\omega)t} J^\nu(\omega, \mathbf{q})|0\rangle$$

- Classical calculation

  - done in euclidean time $t = it_E \longrightarrow e^{-Ht_E}$
  - go back to frequency domain (ill defined problem)

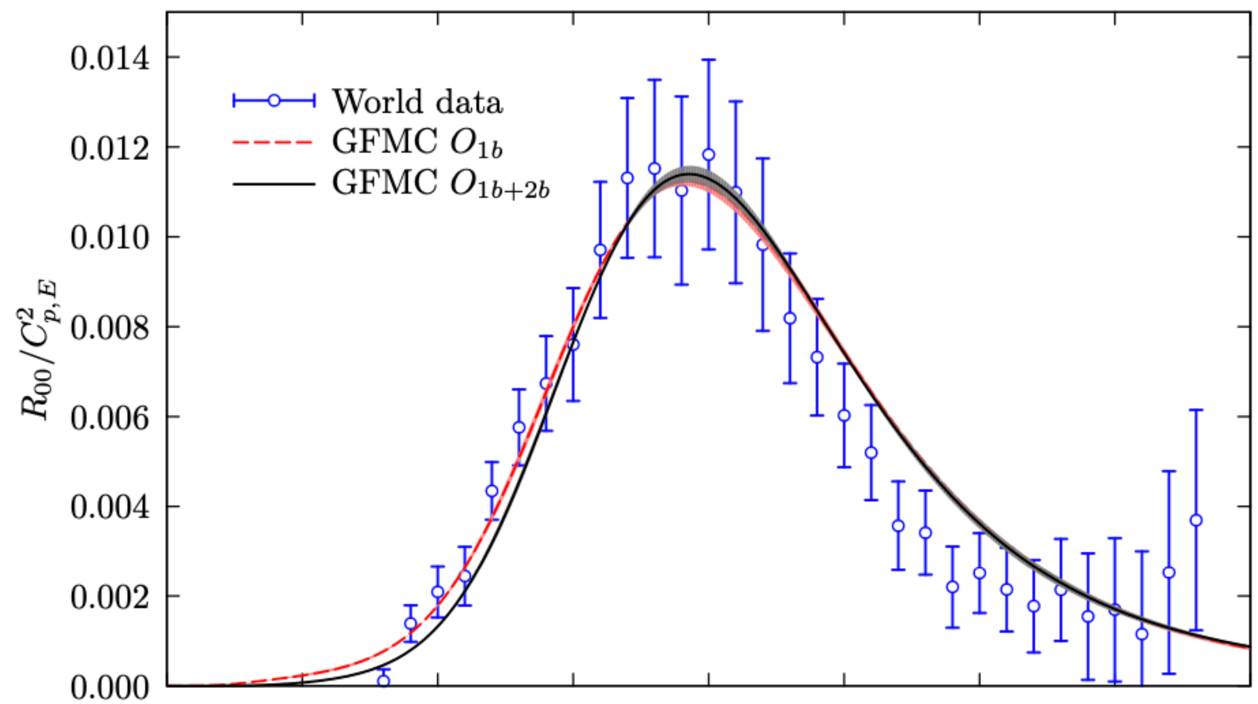
Alternative classical approaches ————> Integral transforms (not in this talk)

Response functions



Electric dipole polarizability from first principles calculations

M. Miorelli, S. Bacca, N. Barnea, G. Hagen, G. R. Jansen, G. Orlandini, and T. Papenbrock
Phys. Rev. C **94**, 034317 – Published 19 September 2016



Electromagnetic and neutral-weak response functions of ^{4}He and ^{12}C

A. Lovato, S. Gandolfi, J. Carlson, Steven C. Pieper, and R. Schiavilla
Phys. Rev. C **91**, 062501(R) – Published 4 June 2015

- How do we move to heavier nuclei? Are classical resources gonna be enough?
  - Exponential growth of # states with particle #Exponential growth of # states with particle #

Response functions on QC

Dynamic linear response quantum algorithm

Alessandro Roggero and Joseph Carlson
Phys. Rev. C **100**, 034610 – Published 13 September 2019

Spectral density estimation with the Gaussian Integral Transform

A. Roggero*
Institute for Nuclear Theory, University of Washington, Seattle, WA 98195, USA
(Dated: April 13, 2020)

$$R^{\mu\nu}(\omega, \mathbf{q}) = \sum_X \langle 0 | J^\mu(\omega, \mathbf{q}) | X \rangle \, \langle X | J^\nu(\omega, \mathbf{q}) | 0 \rangle \delta(E_0 + \omega - E_X)$$

Simulating physical phenomena by quantum networks

R. Somma, G. Ortiz, J. E. Gubernatis, E. Knill, and R. Laflamme
Phys. Rev. A **65**, 042323 – Published 9 April 2002

Quantum computing for neutrino-nucleus scattering

Alessandro Roggero, Andy C. Y. Li, Joseph Carlson, Rajan Gupta, and Gabriel N. Perdue
Phys. Rev. D **101**, 074038 – Published 27 April 2020

$$C^{\mu\nu}(t) = \int dt \, \langle 0 | J^\mu(\omega, \mathbf{q}) e^{i(H-\omega)t} J^\nu(\omega, \mathbf{q}) | 0 \rangle$$

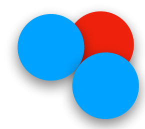
Following this approach

$\not{\pi}$ EFT lattice on qubits I

- Very simple nuclear interactions can be obtained by the LO pionless EFT

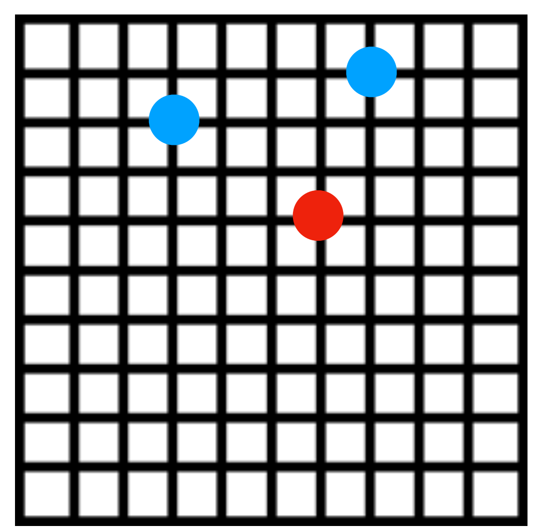
$$H = T + V_{2N} + V_{3N}$$

- Simple nucleus to study is $^{3}\mathrm{H}$



- How to formulate the problem in order to map to qubits?

  - Put the problem on a lattice



For N states

the number of qubits needed $\log_2 \mathrm{N}$

$$H = T + V_{2N} + V_{3N}$$

$T \rightarrow c^{\dagger}_{if} c_{if}$

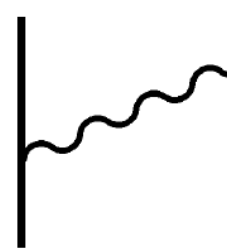
$V_{2N} \rightarrow c^{\dagger}_{if} c_{if} \; c^{\dagger}_{jf'} c_{jf'}$

$V_{3N} \rightarrow c^{\dagger}_{if} c_{if} \; c^{\dagger}_{jf'} c_{jf'} \; c^{\dagger}_{kf''} c_{kf''}$

Hubbard model-like

Responses

- We describe coupling with a nucleus using



$$\rho_f(i,j) = e_f \sum_i e^{iq_{i,j}x_i} c^\dagger_{i,f} c_{i,f}$$

Structure closely resembles

$$\mathbf{j}^{\rm LO}_{5,a}(\mathbf{q}) = -\frac{g_A}{2}\, \tau_{i,a}\, \boldsymbol{\sigma}_i\, {\rm e}^{i\mathbf{q}\cdot\mathbf{r}_i} + (i \rightleftharpoons j)\ ,$$

- The quantity we are after is the response, that in time domain becomes

$$S_f(i,j)(t) = \langle U^\dagger(t)\rho_f(i,j)U(t)\rho_f(i,j)\rangle$$

(i,j) → Site location

$U(t)$ → e^{-iHt}

Classical calculation for H of dimension NxN:

- Diagonalize H:
  - $O(N^2)$ storing, $O(N^3)$ operations

For approximate diagonalization better scalings

$\not\pi$ EFT lattice on qubits I

- How do we put this on a quantum computer?

Quantum computing for neutrino-nucleus scattering
Alessandro Roggero, Andy C. Y. Li, Joseph Carlson, Rajan Gupta, and Gabriel N. Perdue
Phys. Rev. D **101**, 074038 – Published 27 April 2020

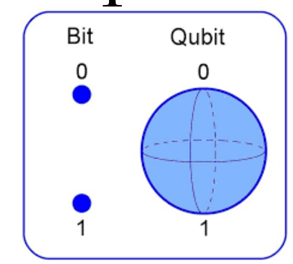
$$H = T + V_{2N} + V_{3N}$$

$$c^\dagger_{if} c_{if} \; c^\dagger_{jf'} c_{jf'} \; c^\dagger_{kf''} c_{kf''} \; \ldots$$

$$c_\alpha = \left(\prod_{k=1}^{n-1} \sigma_z^k \right) \sigma_-^n$$

Jordan-Wigner (1928)

$$H_{\text{qubits}}$$



- *Mapping between fermionic second quantized operators and Pauli matrices*

- Simple model that captures not trivial physics?

  Avoid symmetrization issues

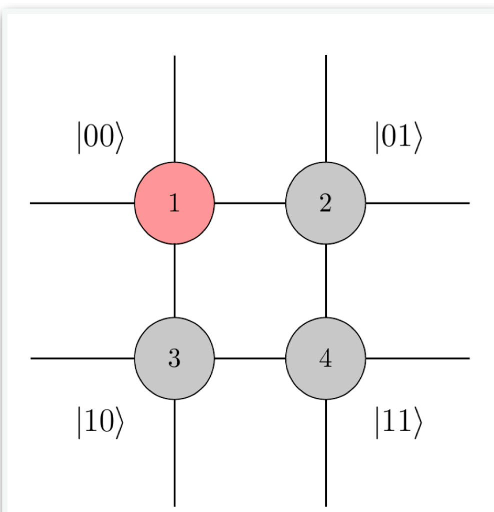
  Only two species

$\not\pi$ EFT lattice on qubits II

Quantum computing for neutrino-nucleus scattering

Alessandro Roggero, Andy C. Y. Li, Joseph Carlson, Rajan Gupta, and Gabriel N. Perdue
Phys. Rev. D **101**, 074038 – Published 27 April 2020

- We use a model where one nucleon is fixed at one site and the other two can move
  - Only two particles moving in a static field (particles of two different species)
    - States needed are only four in this case



Mapping to qubits for this case only four qubits are needed

- (Approximate) Ground state of the Hamiltonian
- Time evolution done with Trotterizzation

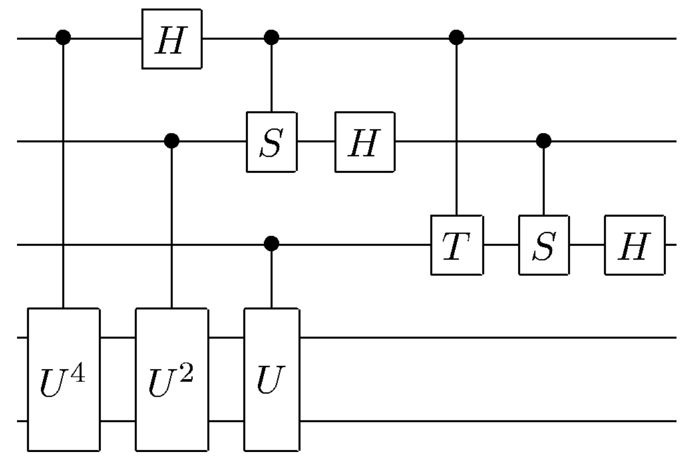
$$U(t) = e^{-itH} = e^{-it\sum_i H_i} \simeq \left[\Pi_i e^{-\frac{it}{r}H_i}\right]^r$$

Quantum Simulations in a nutshell

State preparation

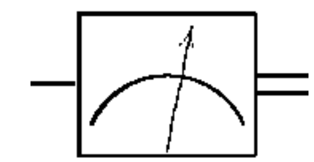
$|\psi_{\text{prep.}}\rangle$

$U\,|\psi_{\text{prep.}}\rangle$



Can realize all unitary matrices with a small set of unitary gates (Barenco et al.,Sleator et al., 1995)

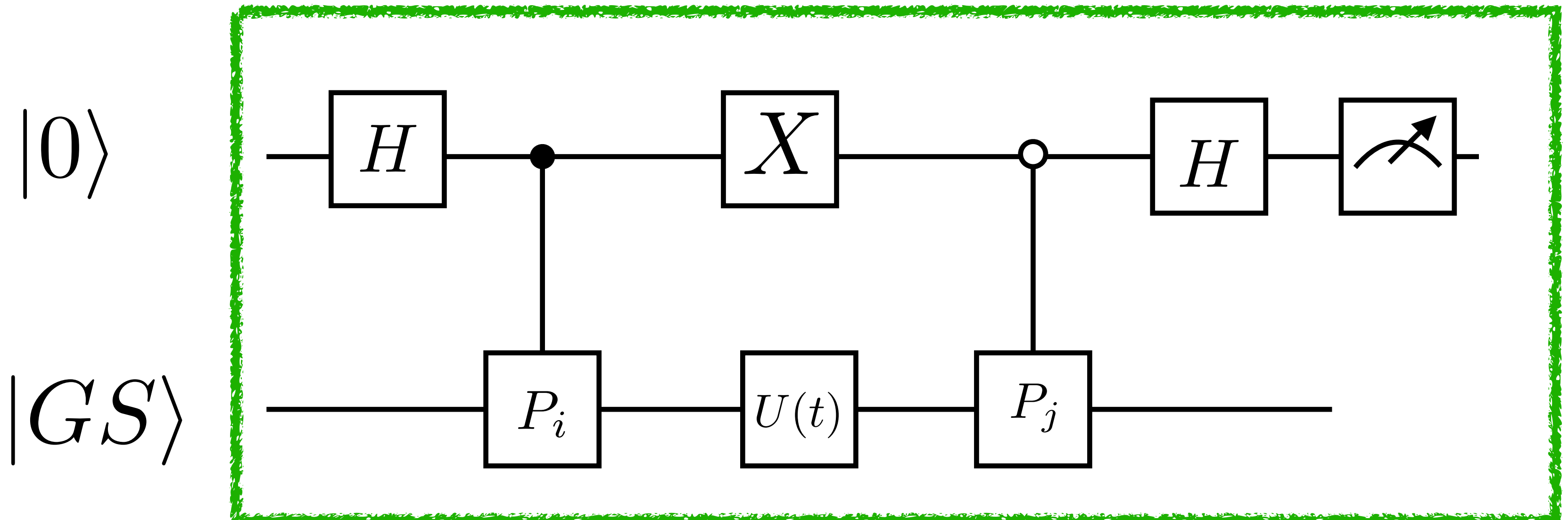
Measurements



- Three sources of error state preparation, time evolution, measurements
  - They should have all poly(N) scaling for precision epsilon
- The idea is to start small with a few qubits problem with a well-known solution

Responses on a quantum computer

- How do we compute the response on a quantum computer?



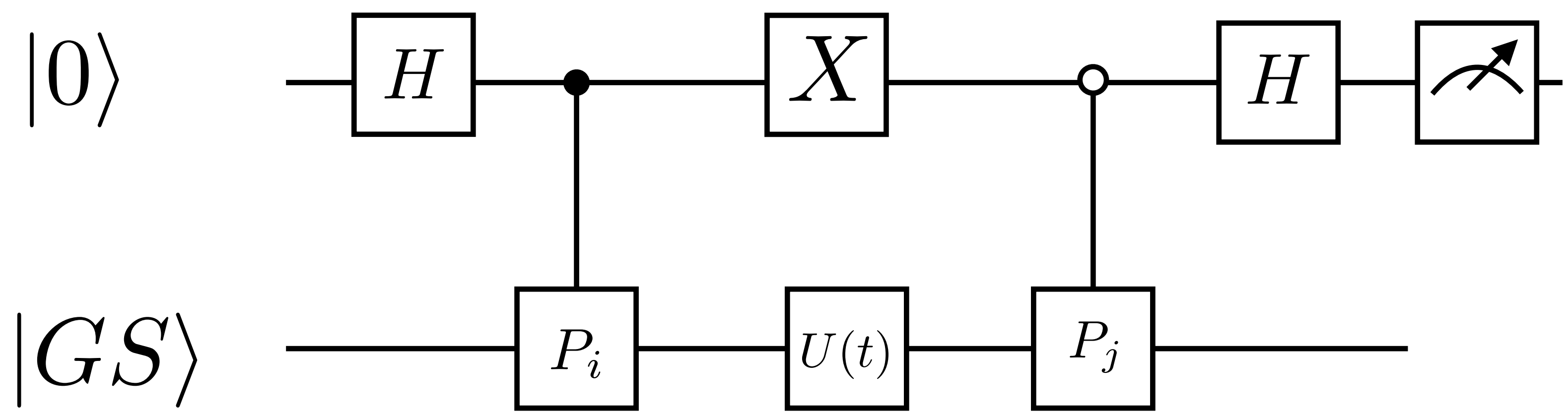
- Allows to calculate

$$S_f(i,j)(t) = \sum_{ij} a_{ij} \langle GS | U^\dagger(t) P_i U(t) P_j | GS \rangle$$

Tensor product of Pauli matrices

Time evolution of H over qubits

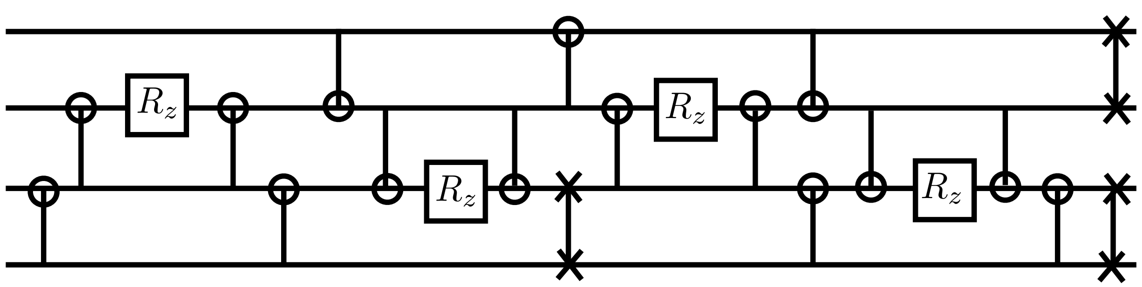
Responses on a quantum computer



$$U(t) = e^{-itH} = e^{-it\sum_i H_i} \simeq \left[\Pi_i e^{-\frac{it}{r}H_i}\right]^r$$

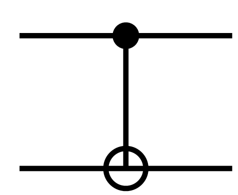
- One Trotter step

- Example circuit

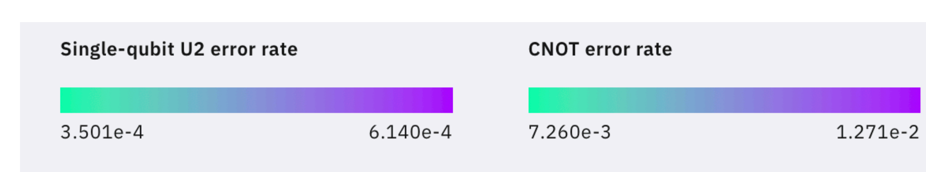


$$U_{3-\text{body}} = \Pi_{i\neq j\neq k} e^{-i\eta Z_i Z_j Z_k}$$

- On current quantum hardware major source of noise



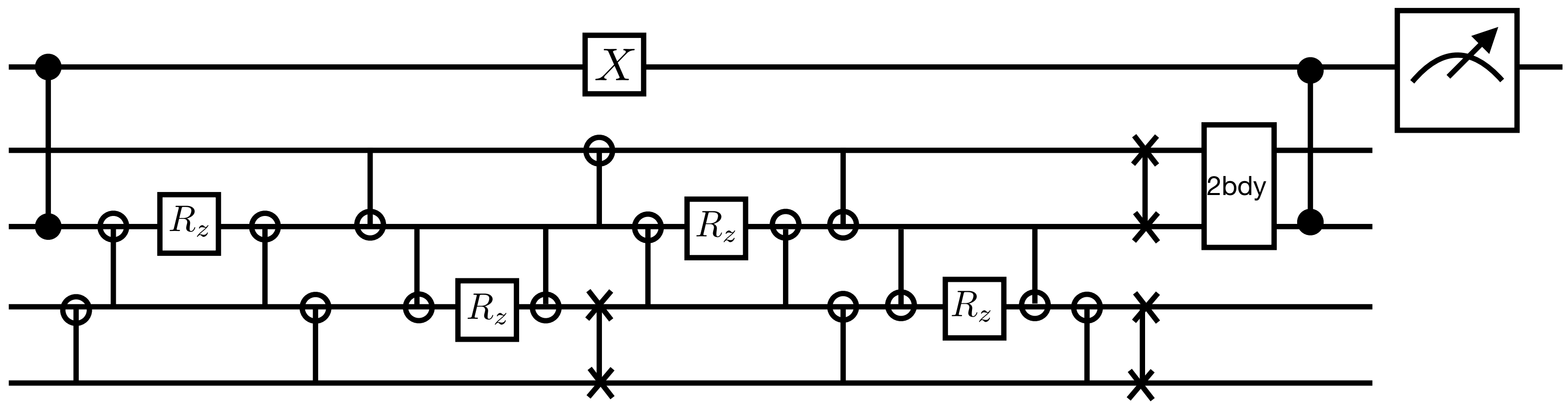
Ibmq Vigo



Responses on a quantum computer

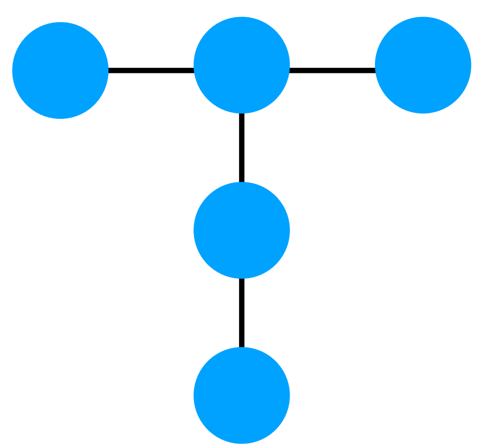
- Minimal (found) circuits with 26 Cnots

$$\langle GS_{\text{approx.}} | U^\dagger(t) Z_1 U(t) Z_1 | GS_{\text{approx}} \rangle$$

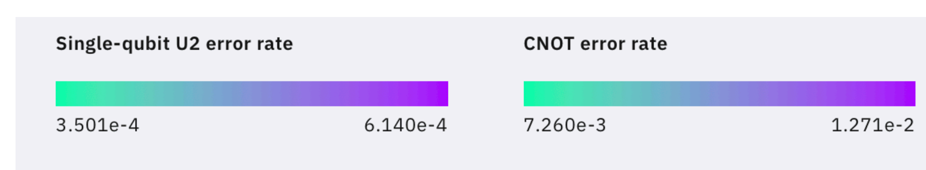


connectivity constraints taken into account

- Ibmq Vigo/Ourense 5 qubit machine



Properly map the problem



- Workflow of the calculation

Exact———> Simulator———> Real machine

Error mitigation

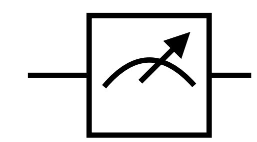
Letter | Published: 27 March 2019

Error mitigation extends the computational reach of a noisy quantum processor

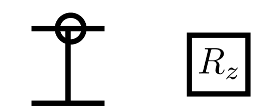
Abhinav Kandala, Kristan Temme, Antonio D. Córcoles, Antonio Mezzacapo, Jerry M. Chow & Jay M. Gambetta

Nature **567**, 491–495(2019) | Cite this article

- Readout error



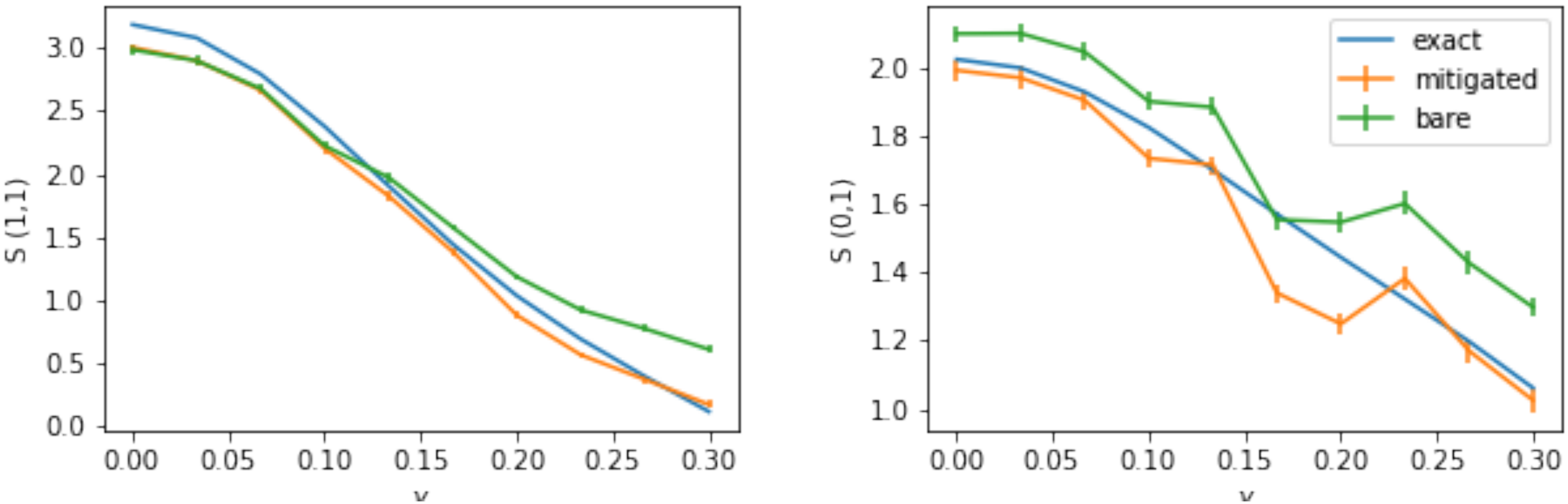
- Gate noise



- Strategy
  - Correct for readout (not difficult)
  - Correct for gate noise (adds a linear overhead)

Responses on a quantum computer

Ibmq Vigo virtual machine

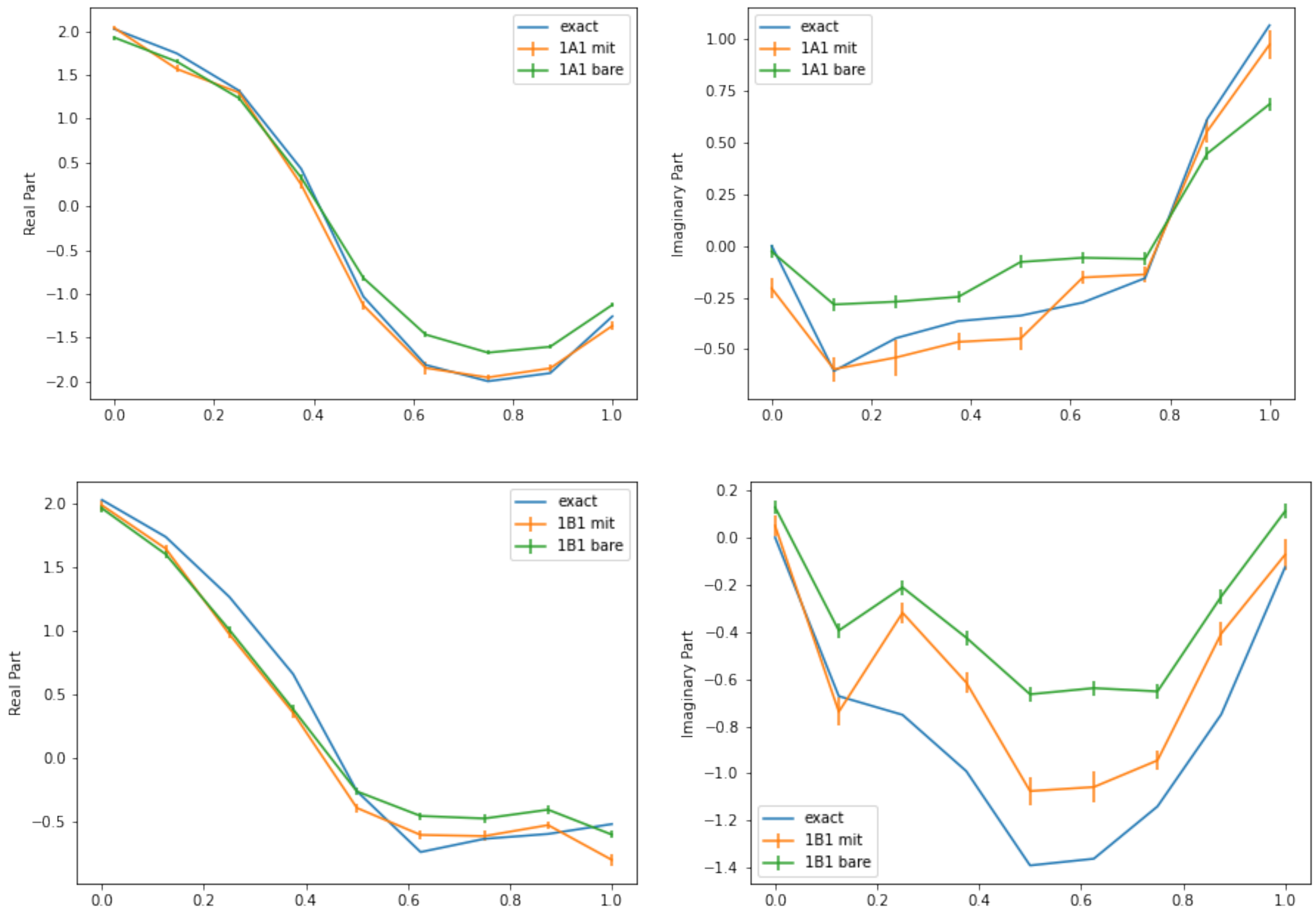


<u>Plots for real hardware next slide</u>

Responses on a quantum computer

Two different first order Trotterizzations   Ibmq Ourense

$S_f(0,1)$



Error mitigation brings results closer

Error mitigation I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- Readout error mitigation protocol
  - Obtain calibration matrix P with errors on the entries $\mathrm{Var}[P]$
  - Observable of interest is affected $\langle O \rangle = \sum_{i=1}^{N} a_i \, p_i$ → bare probabilities
  - Observable of interest is affected $\langle \widetilde{O} \rangle = \sum_{ij}^{N} a_i \left[P^{-1}\right]_{ij} [p_e]_j$
  - Caveat size of the calibration matrix exponential in the number of qubits, Exponential number of different measurements required
    - Independent errors on different qubits: N diagonal 2x2 blocks
      linear number of measurements required
  - Error propagation has been implemented (not present in current qiskit)

Error mitigation II

- For inversion probabilities we use three different methods
  - Richardson extrapolation

$$O(r) = O_F + \sum_{j=1}^{M} c_j r^j + \mathcal{O}(r^{M+1})$$

Computed at M+1 different noise values
Invert the linear system to obtain the error free observable

  - Exponential extrapolation

$$O(r) = O_F \quad e^{-\alpha r}$$
$$O(r') = O_F \quad e^{-\alpha r'}$$
$$\longrightarrow O_F = O(r) \left(\frac{O(r)}{O(r')} \right)^{r/(r-r')}$$

Summary

Classical calculation with realistic number of lattice sites to guide future simulations

Explore other error mitigation protocols

Explore automated circuit synthesis for larger circuits

Thank you

Scaling of classical diagonalization algorithms

Finding eigenvalues of a matrix, exact algorithms

Improving tradeoff between space and time

NxN matrix	Space complexity	Time complexity (flops)	Task
QR decomposition	$O(N^2)$	$O(N^3)$	Get all eigenvalues
Lanczos algorithm	$O(N^2)$	Number of times mat vec mult $\mathcal{O}(N^2 \log(N)/\epsilon)$ Matrix vector multiplication	Get only largest eigenvalue

Trotter scaling

From Childs et al.

$$H = \sum_{j=1}^{L} H_j$$

$$||U(t) - T(t,r)|| \leq \frac{(L\Lambda t)^2}{r} \exp^{L\Lambda|t|/r} \qquad \Lambda = max_j ||H_j||$$

Gate depth (almost) to implement approximate unitary with precision ϵ

$$r = max\{L|t|\Lambda, \frac{e(Lt\Lambda)^2}{\epsilon}\}$$

Other orders can improve but still get polynomial in time, $1/\epsilon$

Qubitization? Not here….

Scaling of classical matrix inversion algorithms

$$Ax = b \longrightarrow x = \boxed{A^{-1}} b \; ?$$

NxN matrix	Space complexity	Time complexity	Task
Gaussian elimination	$O(N^2)$	$O(N^3)$	Get all eigenvalues
In general		At least linear in N	