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Title: Quantum Computing for Quantum Dynamics in Nuclear Physics

Author(s): Baroni, Alessandro

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Quantum Computing for Quantum Dynamics in Nuclear Physics

Alessandro Baroni

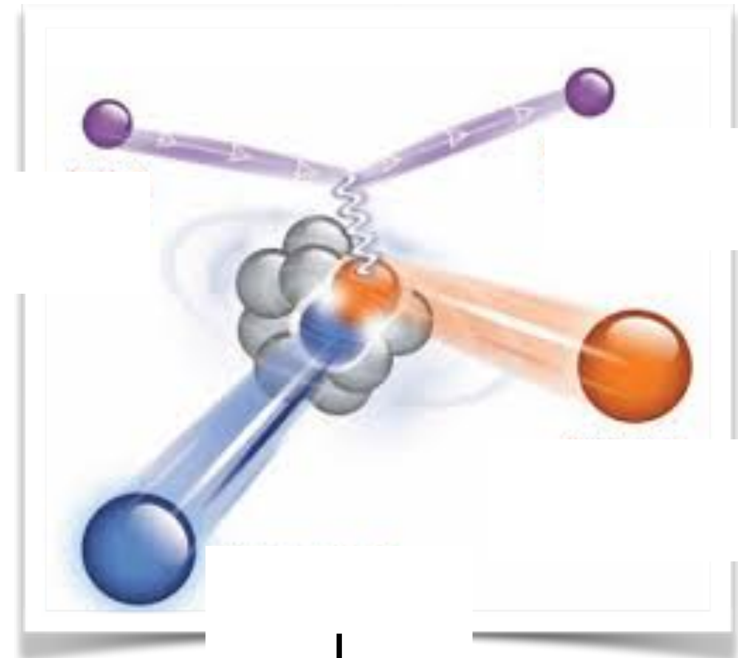
Los Alamos National Laboratory

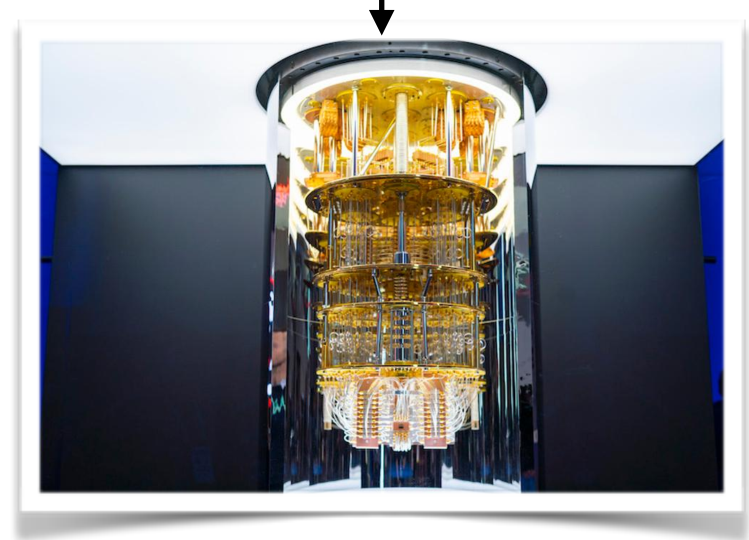
Collaborators

- J. Carlson, R. Gupta, I. Stetcu (LANL,USA)
- A. Roggero   (Univ. Trento, Italy/UW, USA)
- T. Papenbrock, C. Gu (ORNL, USA)
- G. Perdue, A. C. Li (Fermilab, USA)
- B. Hall (MSU, USA)

Outline

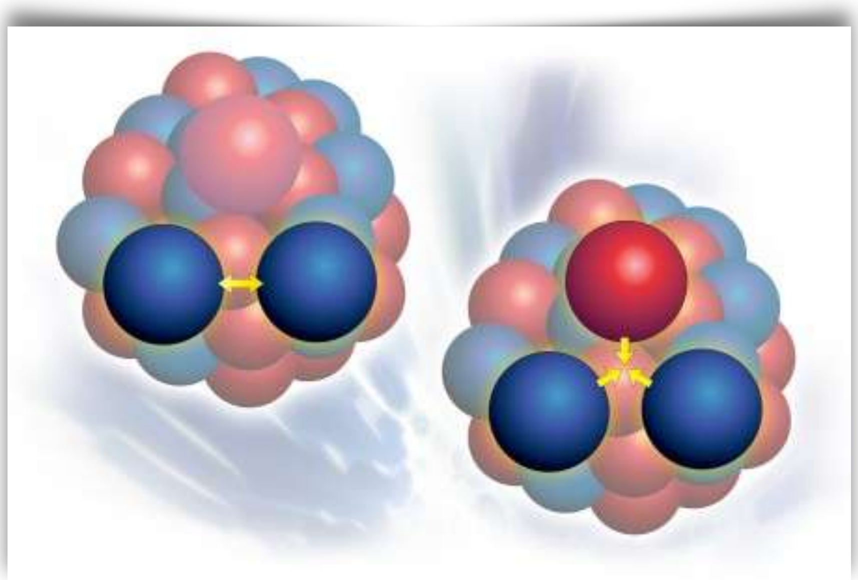
- Nuclear physics
- Quantum simulations
- Results on NISQ devices





Basic model

Nucleons interact between each others through many-body forces



Nuclear strong hamiltonian

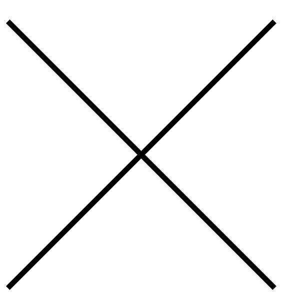
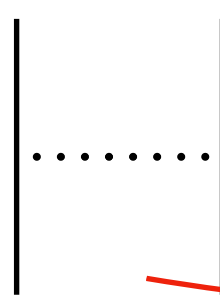
$$H = \sum_{i=1}^{N} \frac{p_i^2}{2m} + V_{2N} + V_{3N} + \cdots$$

Negligible >3 -body forces

Two and three body forces

Non-relativistic Kinetic term

Potentials derived in chiral EFT

$V_{2N} =$  +  + . . .

$$-\frac{g_A^2}{4f_\pi^2}\mathbf{t}_1\cdot\mathbf{t}_2\frac{\mathbf{s}_1\cdot\mathbf{k}\quad\mathbf{s}_2\cdot\mathbf{k}}{\mathbf{k}^2+m_\pi^2}$$

Scaling of classical resources

- Each nucleon has quantum numbers

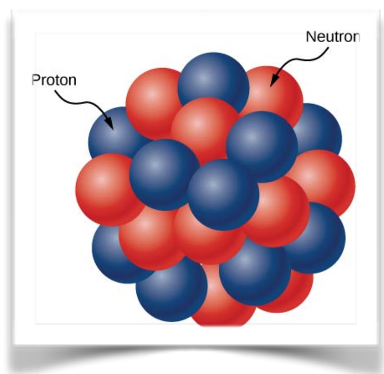
Number of nucleons

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

- 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

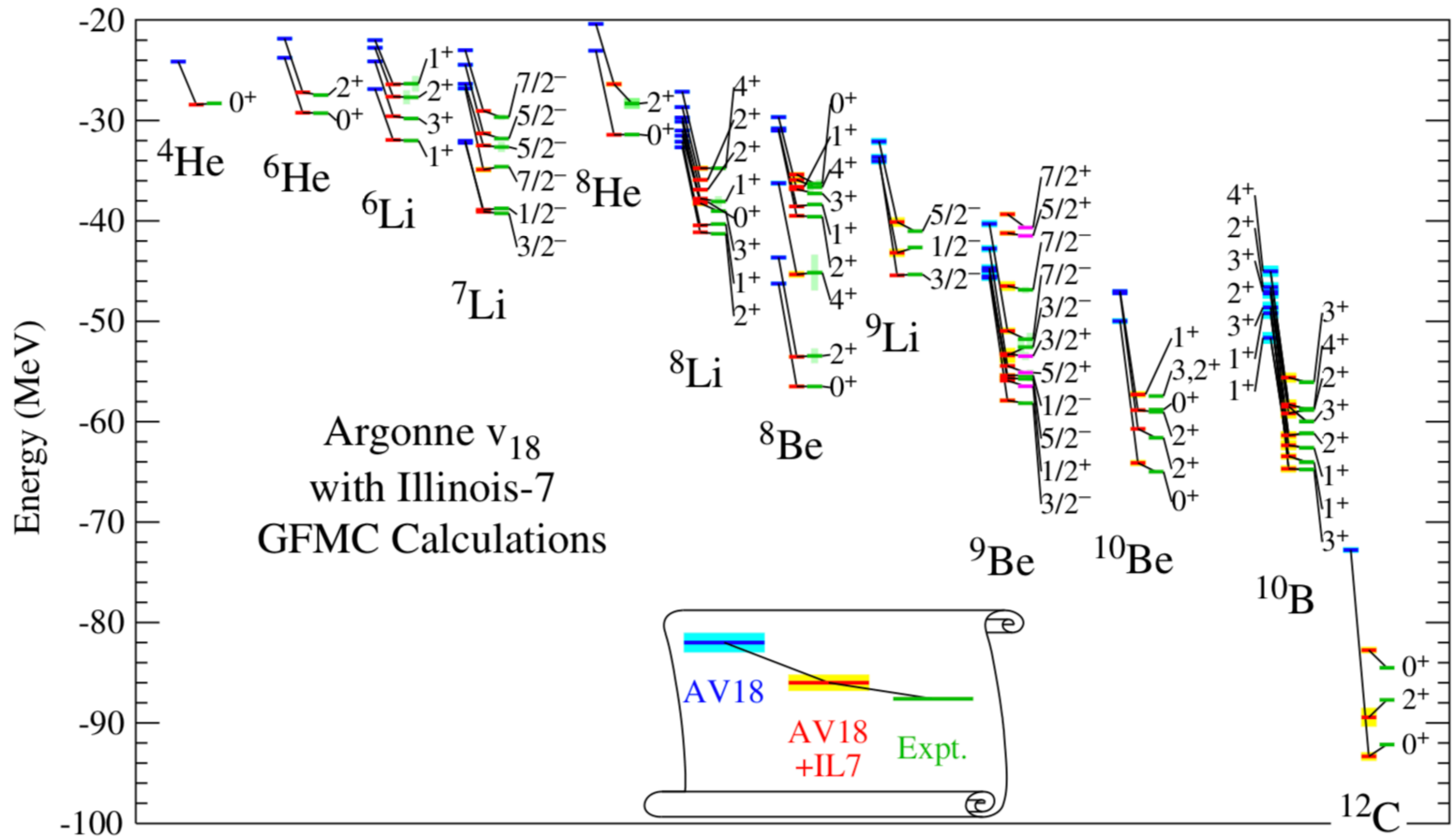
How do we go to A>12?



Energy spectra

- Energies are given from the solutions of the many body equation

$$H\Psi_n(x_1,\cdots,x_A) = E_n\Psi_n(x_1,\cdots,x_A)$$

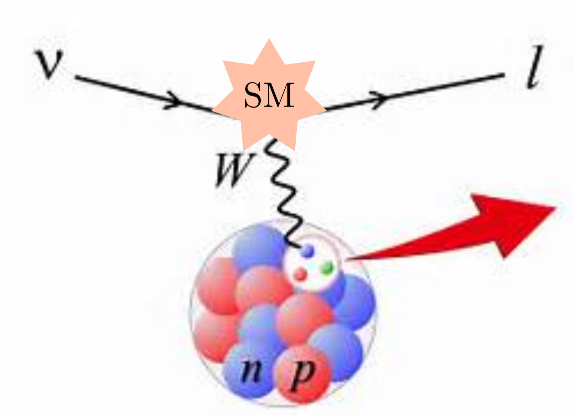


- Ground state energies and low lying energies are reproduced well up to ^{18}O

How do we go to A>>18?

Nuclear Dynamics

- Nuclear electroweak scattering



- Quantity connected with experiments is

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

Hadronic tensor that contains all the information on the target structure

Leptonic tensor fully specified by the electron kinematic variables

- The challenging quantity to calculate is

$$S(\omega, \mathbf{q}) = \sum_f |\langle 0|O(\mathbf{q})|f\rangle|^2 \; \delta(\omega - (E_f - E_0))$$

Directly related to the cross section

Response functions

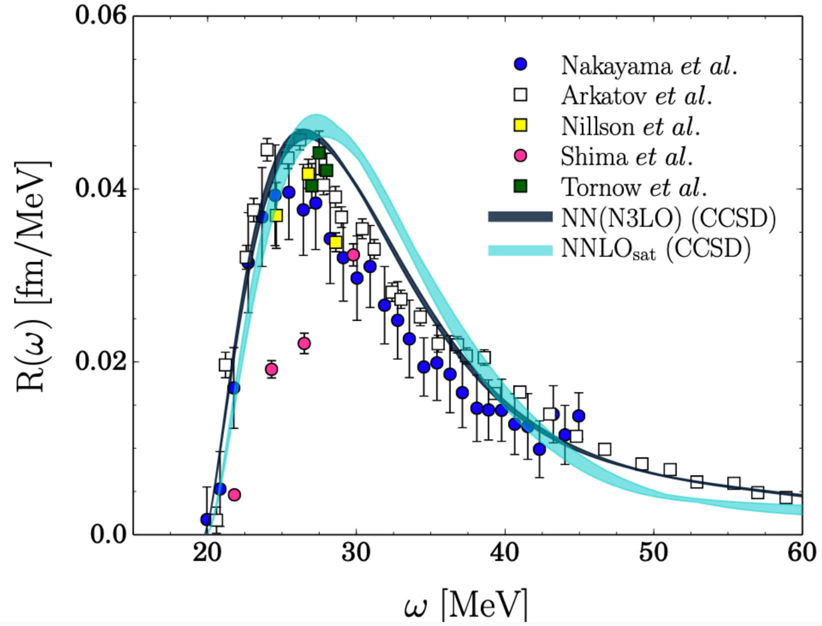
- What can be calculated is related to

$$S(\omega, \mathbf{q}) = \int \frac{dt}{2\pi} e^{i\omega t} \boxed{\langle 0|e^{iHt} O(\mathbf{q})^\dagger e^{-iHt} O(\mathbf{q})|0\rangle}$$

- Classical calculation

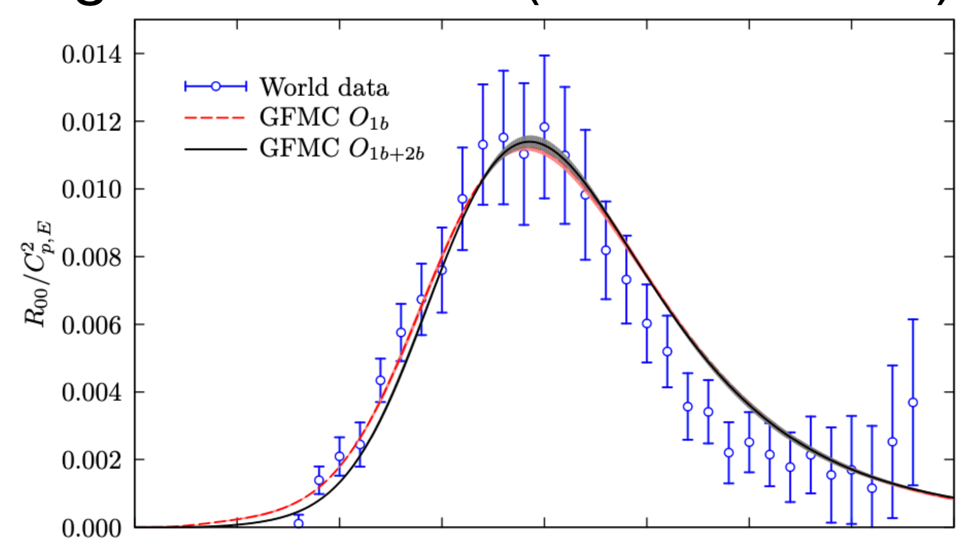
  - done in euclidean time $\quad t_E \longrightarrow e^{-Ht_E}$
  - go back to frequency domain (ill defined problem)

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



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

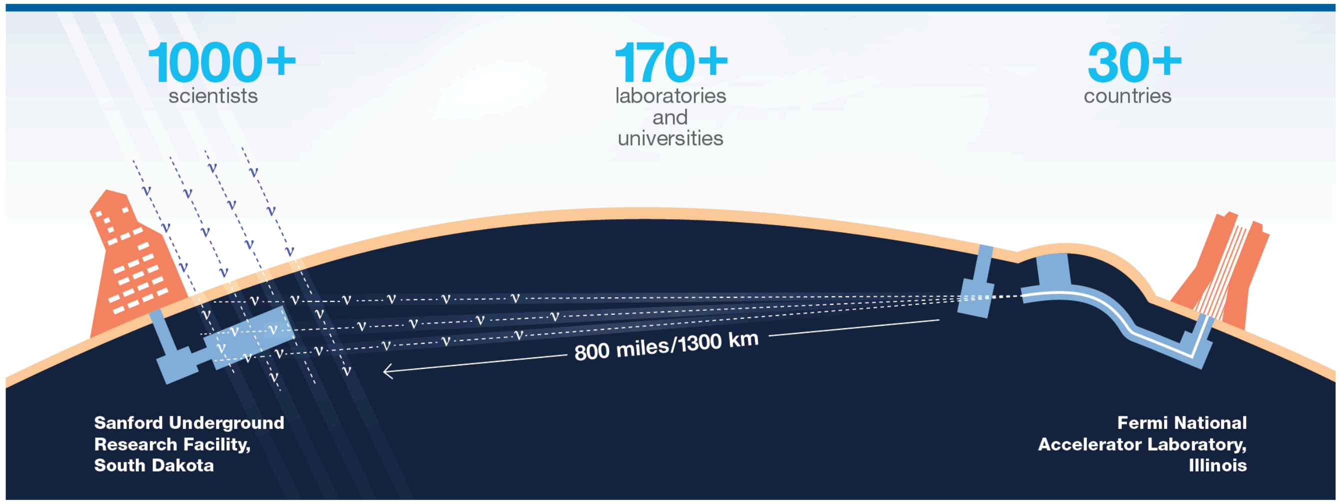


Electromagnetic and neutral-weak response functions of ^{4}He and ^{12}C

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

How can we tackle heavier nuclei?

- Many current experiments have nuclear targets with A>12



- Are current and near future computing resources enough?
  - Exponential growth of # states with particle #

- Can we do nuclear physics on a quantum computer?
  - Explore application of nuclear problems on current quantum computer

Response functions on QC

Quantum eigenvalue estimation via time series analysis

Rolando D Somma

Theoretical Division, Los Alamos National Laboratory, Los Alamos, NM 87545, United States of America

E-mail: somma@lanl.gov

Keywords: quantum computing, quantum simulation, phase estimation

Dynamic linear response quantum algorithm

Alessandro Roggero and Joseph Carlson

Phys. Rev. C **100**, 034610 – Published 13 September 2019

$$S(\omega,\mathbf{q}) = \sum_f |\langle 0|O(\mathbf{q})|f\rangle|^2\ \delta(\omega - (E_f - E_0))$$

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

PRX QUANTUM **2**, 010317 (2021)

Quantum Computation of Finite-Temperature Static and Dynamical Properties of Spin Systems Using Quantum Imaginary Time Evolution

Shi-Ning Sun,[1] Mario Motta,[2] Ruslan N. Tazhigulov,[3] Adrian T.K. Tan,[1] Garnet Kin-Lic Chan,[3,*] and Austin J. Minnich[1,†]

$$\boxed{\langle 0|e^{iHt}O(\mathbf{q})^\dagger e^{-iHt}O(\mathbf{q})|0\rangle}$$

We will focus on this approach

Nuclear two point correlation functions on a quantum computer

A. Baroni,[1] J. Carlson,[1] R. Gupta,[1] Andy C. Y. Li,[2] G. N. Perdue,[2] and A. Roggero[3,4,5]

Response functions on a quantum computer

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In order to compute this quantity in principle we need

$|0\rangle$ Prepare the initial state → Calculated using VQE

> **Variational approaches to constructing the many-body nuclear ground state for quantum computing**
> I. Stetcu, A. Baroni, and J. Carlson
> *Los Alamos National Laboratory, Theoretical Division, Los Alamos, New Mexico 87545, USA*
> (Dated: October 13, 2021)

$O(\mathbf{q})|0\rangle$ Apply excitation operator to the initial state

Two main strategies:

- Apply the full operator →

> Editors' Suggestion
> Preparation of excited states for nuclear dynamics on a quantum computer
> Alessandro Roggero, Chenyi Gu, Alessandro Baroni, and Thomas Papenbrock
> Phys. Rev. C **102**, 064624 – Published 28 December 2020

- Expand expectation as sum of Pauli →

> **Nuclear two point correlation functions on a quantum computer**
> A. Baroni,[1] J. Carlson,[1] R. Gupta,[1] Andy C. Y. Li,[2] G. N. Perdue,[2] and A. Roggero[3,4,5]

e^{-iHt} Apply real the time evolution →

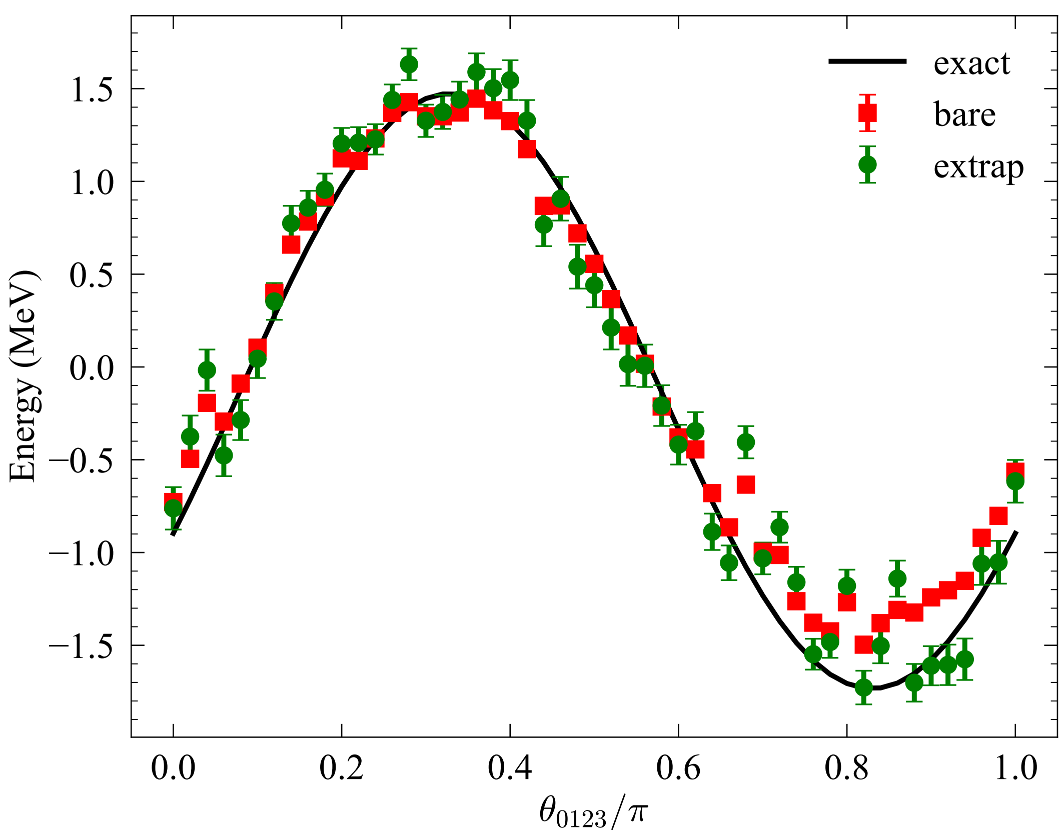
> Simulation of collective neutrino oscillations on a quantum computer
> Benjamin Hall, Alessandro Roggero, Alessandro Baroni, and Joseph Carlson
> Phys. Rev. D **104**, 063009 – Published 3 September 2021

VQE

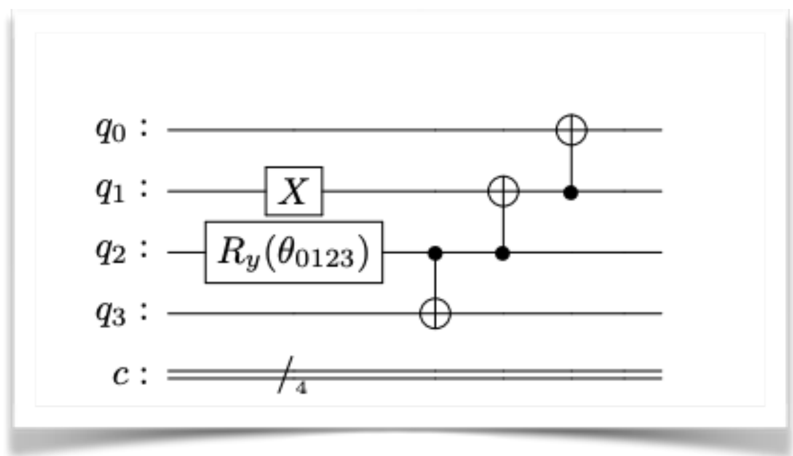
Apply UCCD to an initial HF state

$$U(\theta) = \sum_{i,m} \theta_{i,m} \left(a_i^\dagger a_m - a_m^\dagger a_i \right) + \sum_{i<j;m<n} \theta_{ij;mn} \left(a_i^\dagger a_j^\dagger a_n a_m - a_m^\dagger a_n^\dagger a_j a_i \right) + \cdots$$

$$E(\theta) = \langle HF | U^\dagger(\theta) H U(\theta) | HF \rangle$$



Toy Hamiltonian used has 18 terms



Error mitigation improves accuracy but not precision

Response functions on a quantum computer

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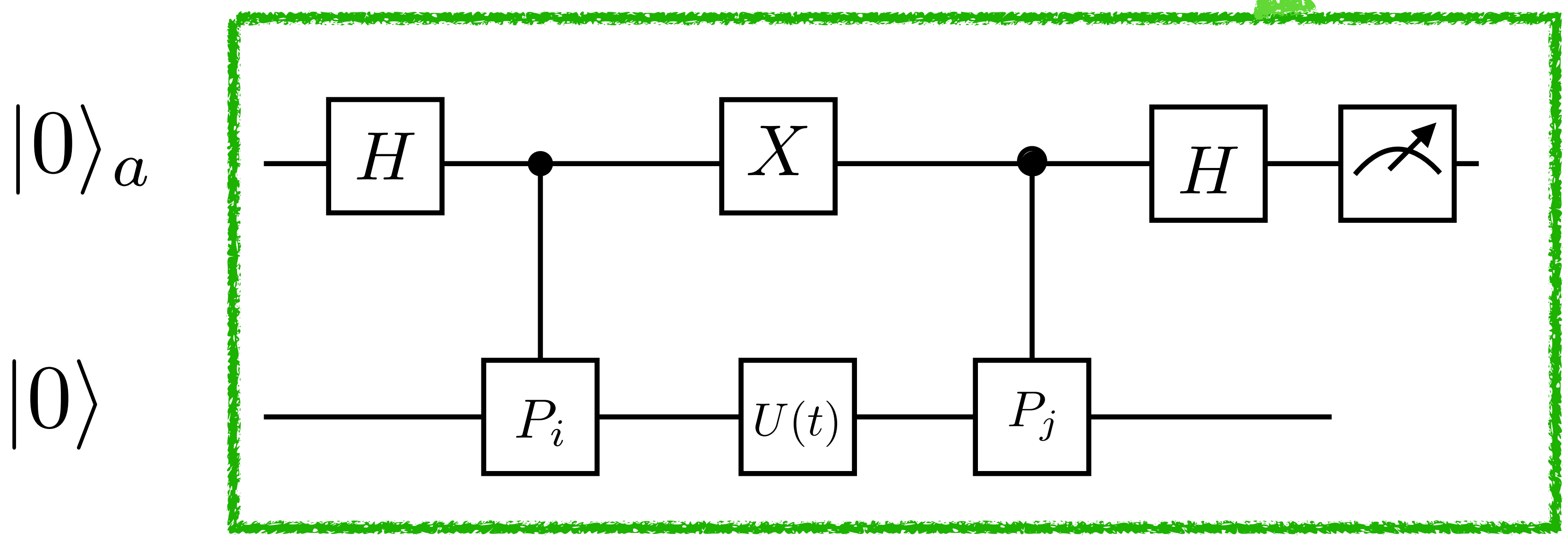
Real time correlators

We recall the well-known identity $$O(\mathbf{q}) = \sum_i \alpha_i P_i$$

$$\langle 0 | e^{iHt} O(\mathbf{q})^\dagger e^{-iHt} O(\mathbf{q}) | 0 \rangle = \sum_{ij} a_{ij} \boxed{\langle 0 | e^{iHt} P_i e^{-iHt} P_j | 0 \rangle}$$

We can compute this



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Phys. Rev. A **65**, 042323 – Published 9 April 2002

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

Lattice model

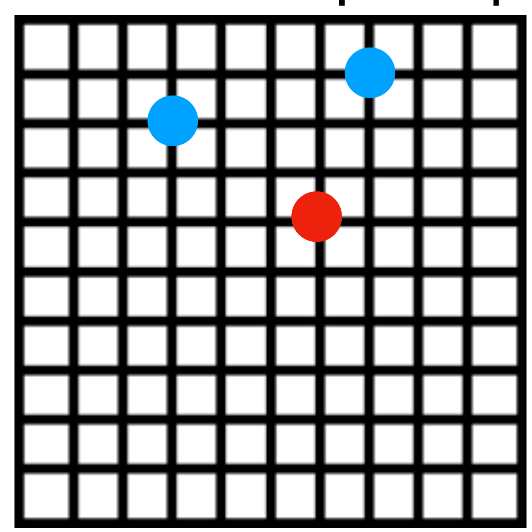
- Nuclear interactions can be obtained by the LO pionless EFT

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

    - lattice basis

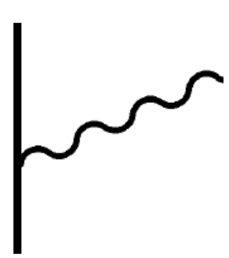
$$H = T + V_{2N} + V_{3N}$$

$$c^\dagger_{if}c_{jf} \qquad c^\dagger_{if}c_{if}\; c^\dagger_{jf'}c_{jf'} \qquad \cdots$$



Hubbard model-like with four fermion species and a three-body interaction

- We describe coupling with a nucleus using



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

Lattice model

$\eta = \text{identical fermions}$

$N = \text{single particle states}$

$D = \binom{N}{\eta}$

→ Jordan Wigner

$\# \text{ qubits} = N$

Antisimmetrizzation included automatically

→ First quantization

$\# \text{ qubits} = \eta \log_2(N)$

Antisimmetrizzation must be included explicitly

Gate complexity $\eta \log(\eta) \log(N)$

Fault-Tolerant Quantum Simulations of Chemistry in First Quantization

Yuan Su, Dominic W. Berry, Nathan Wiebe, Nicholas Rubin, Ryan Babbush

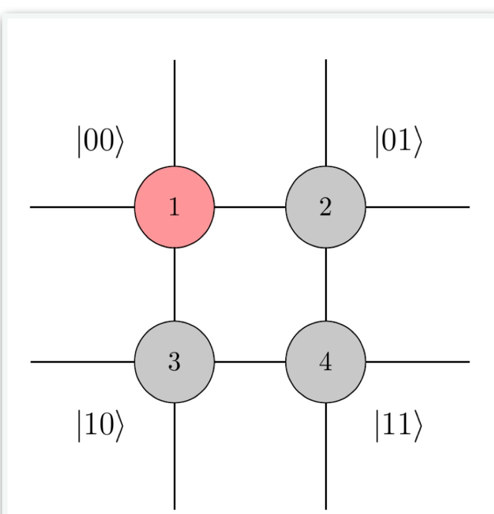
npj | Quantum Information www.nature.com/npjqi

ARTICLE OPEN

Improved techniques for preparing eigenstates of fermionic Hamiltonians

Dominic W. Berry[1], Mária Kieferová[1,2], Artur Scherer[1], Yuval R. Sanders[1], Guang Hao Low[3], Nathan Wiebe[3], Craig Gidney[4] and Ryan Babbush[5]

- For NISQ implementation what is the simplest non trivial problem?
  - 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

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

  - (Approximate) Ground state of the Hamiltonian

Error mitigation

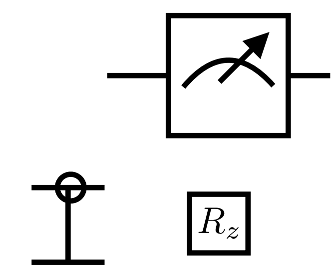
Letter | Published: 27 March 2019

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)
    - Size of the calibration matrix exponential in the number of qubits,
    - Independent errors on different qubits: N diagonal 2x2 blocks
      linear number of measurements required
    - Error propagation has been implemented (not present in current qiskit)
  - Correct for gate noise (adds a linear overhead)
    - Combined Richardson, polynomial and exponential extrapolation

Cloud Quantum Computing of an Atomic Nucleus*

E. F. Dumitrescu,[1] A. J. McCaskey,[2] G. Hagen,[3,4] G. R. Jansen,[5,3] T. D. Morris,[4,3] T. Papenbrock,[4,3,†] R. C. Pooser,[1,4] D. J. Dean,[3] and P. Lougovski[1,‡]

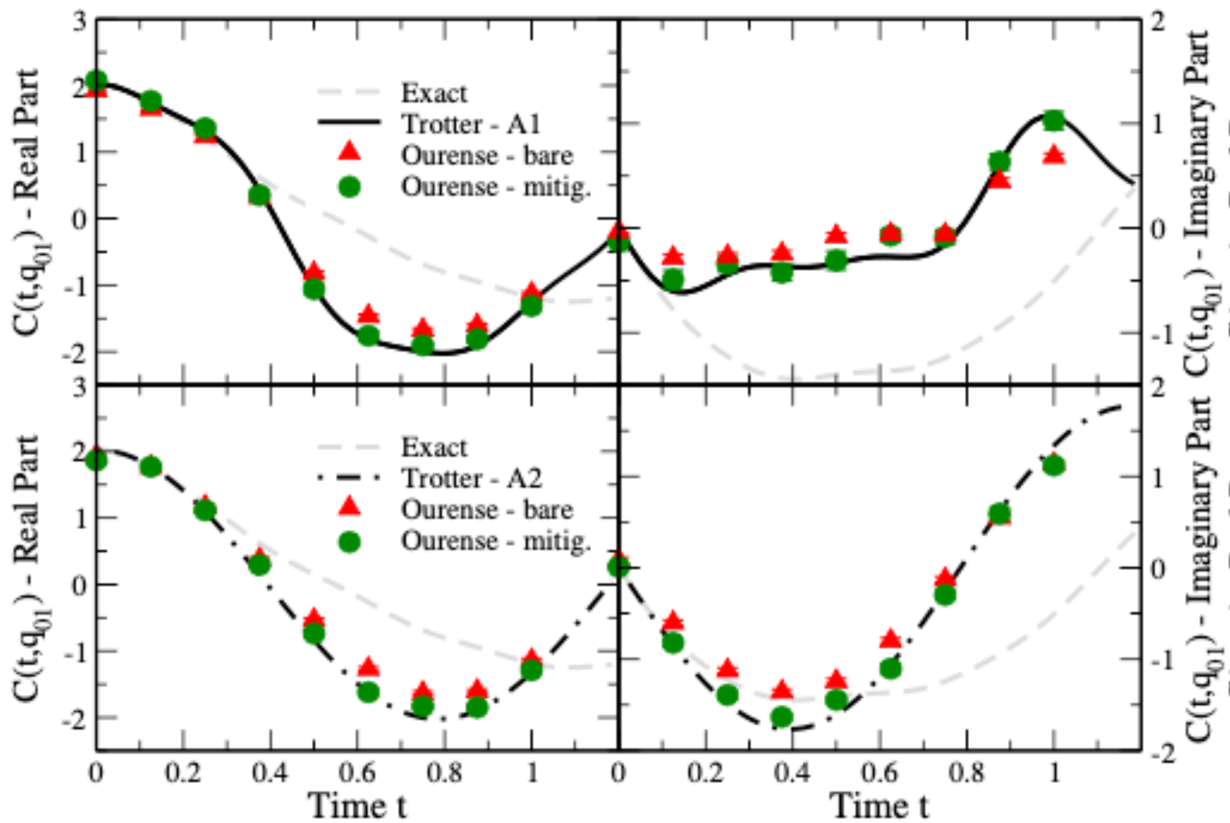
Preparation of excited states for nuclear dynamics on a quantum computer

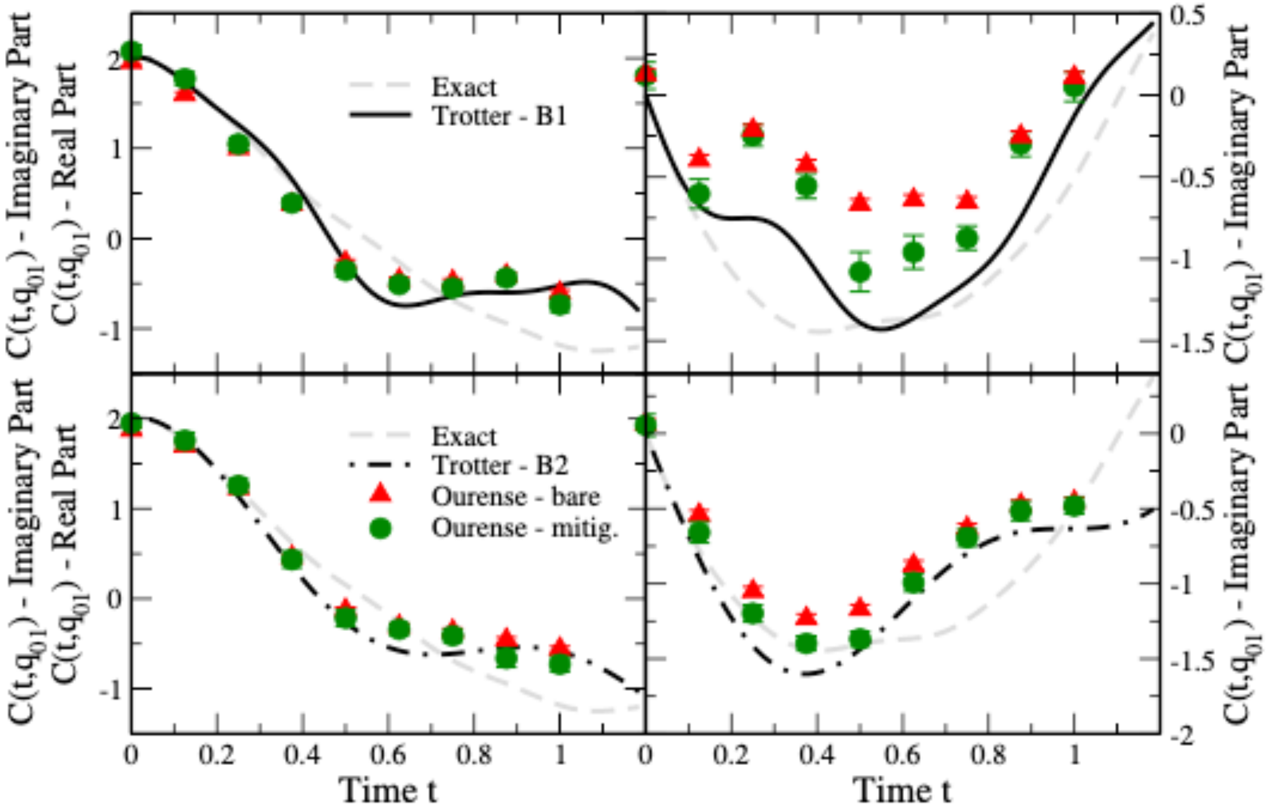
Alessandro Roggero, Chenyi Gu, Alessandro Baroni, and Thomas Papenbrock
Phys. Rev. C **102**, 064624 – Published 28 December 2020

Results

Ibmq real hardware

For a specific Trotterizzation





- ~32 circuits over 5 qubits optimization done by ‘hand’ with connectivity constraints 6-30 CNOTs
- Error mitigation (readout and zero-noise-extrapolation)

Response functions on a quantum computer

$$\boxed{\langle 0|e^{iHt}O(\mathbf{q})^\dagger e^{-iHt}O(\mathbf{q})|0\rangle}$$

In order to compute this quantity in principle we need

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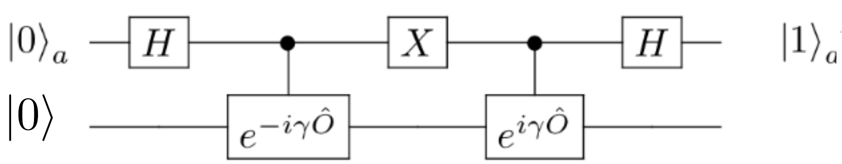
Application of the full excitation operator

$$O(\mathbf{q})|0\rangle$$

- Apply a time evolution-like operator
- Post-select the ancillary qubit



- Success probability

$$P_s = \langle 0|\sin^2(\gamma O)|0\rangle$$

- Fidelity of the state created

$$F = |\langle\psi_f|\widetilde{\psi}_f\rangle|^2$$

We observe that an hermitian operator can be written as linear combination of unitaries

$$O = \sum_i \alpha_i P_i$$

A subroutine of…


ARTICLE

Hamiltonian simulation using linear combinations of unitary operations

Authors: Andrew M. Childs, Nathan Wiebe Authors Info & Affiliations

Publication: Quantum Information & Computation • November 2012

- Success probability

$$P_s = \frac{\langle 0|O^2|0\rangle}{\Lambda^2}, \qquad \Lambda = \sum_i \alpha_i$$

- Fidelity of the state created is 1

Next slide

Application of the full excitation operator

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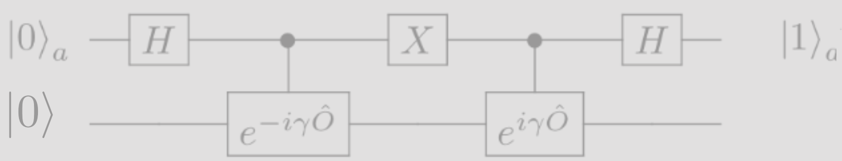
- Apply a time evolution-like operator
- Post-select the ancillary qubit



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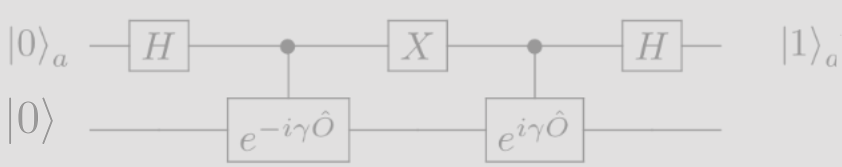

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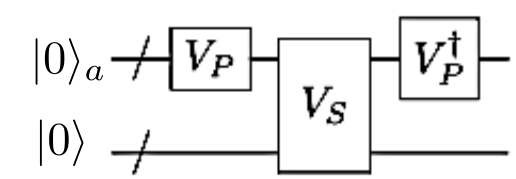
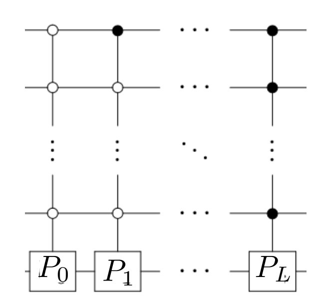
$$V_P|0\rangle_a = \sum_{k=0}^{L} \sqrt{\frac{\alpha_k}{\Lambda}}|k\rangle_a$$

$$\boxed{V_S} = \sum_{k=0}^{L} {}_a|k\rangle\langle k|_a \otimes P_k$$





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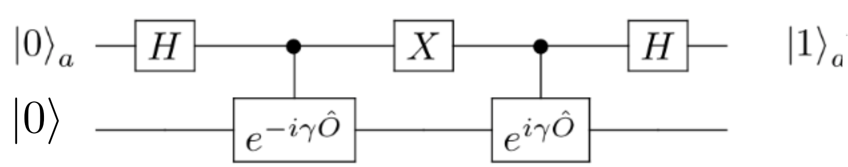
- Post-select the ancillary qubit



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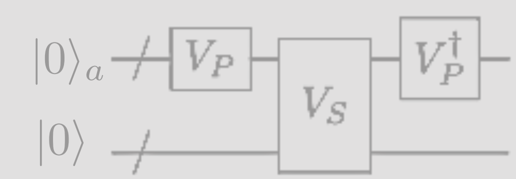
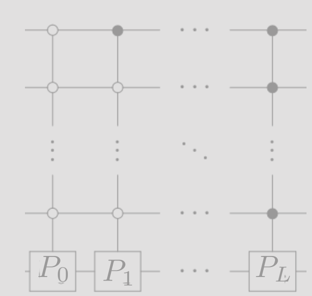
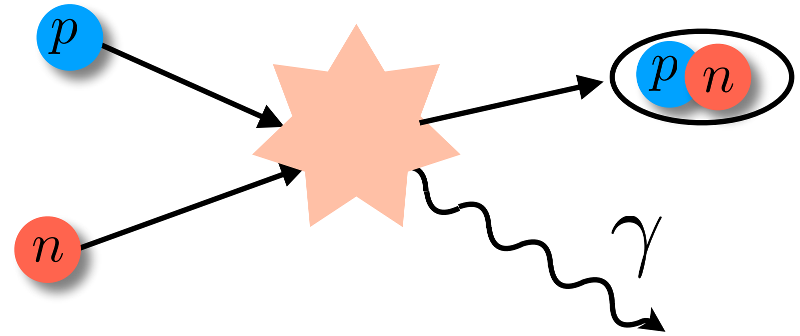


$$V_S = \sum_{k=0}^{L} {}_a|k\rangle\langle k|_a \otimes P_k$$



Neutron-proton em capture

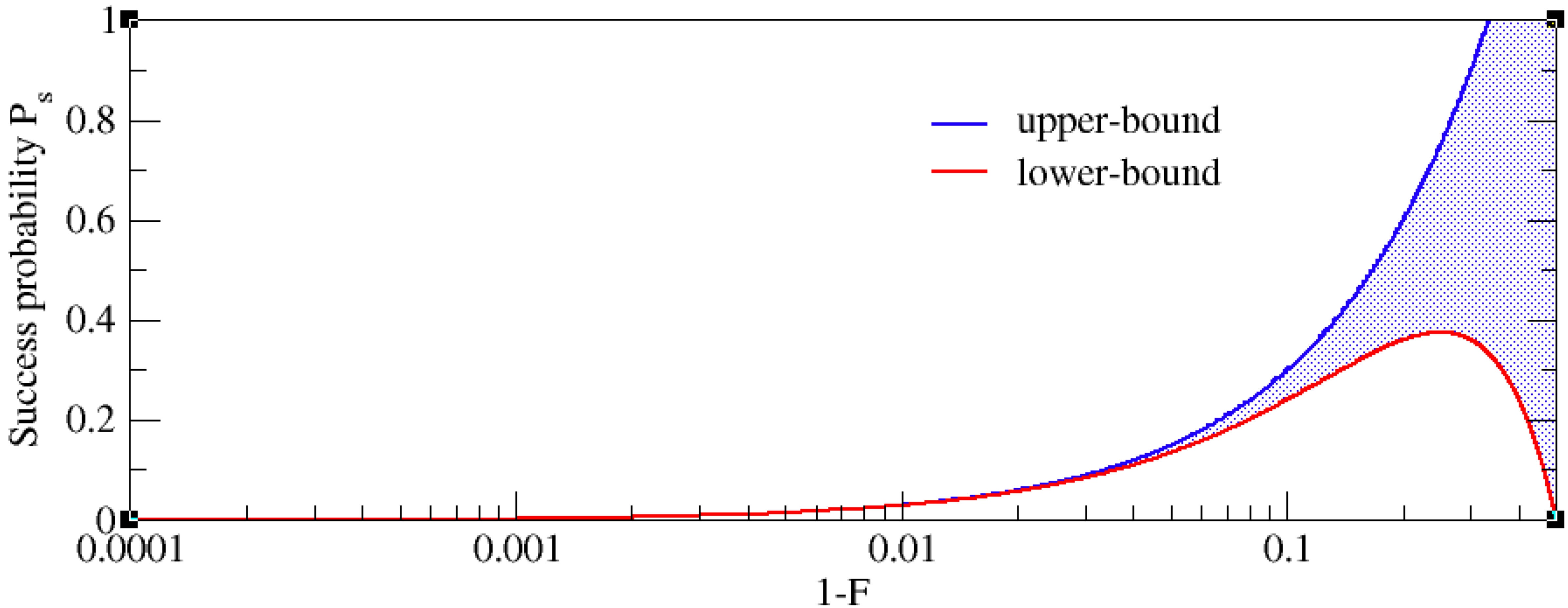


Editors' Suggestion

Preparation of excited states for nuclear dynamics on a quantum computer

Alessandro Roggero, Chenyi Gu, Alessandro Baroni, and Thomas Papenbrock

Phys. Rev. C **102**, 064624 – Published 28 December 2020



Tradeoff between success probability and fidelity

Response functions on a quantum computer

$$\langle 0|e^{iHt}O(\mathbf{q})^\dagger e^{-iHt}O(\mathbf{q})|0\rangle$$

In order to compute this quantity in principle we need

$|0\rangle$ Prepare the initial state → Calculated using VQE

Variational approaches to constructing the many-body nuclear ground state for quantum computing

I. Stetcu, A. Baroni, and J. Carlson
Los Alamos National Laboratory, Theoretical Division, Los Alamos, New Mexico 87545, USA
(Dated: October 13, 2021)

$O(\mathbf{q})|0\rangle$ Apply excitation operator to the initial state

Two main strategies:

- Apply the full operator →
- Expand expectation as sum of Pauli →

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Phys. Rev. C **102**, 064624 – Published 28 December 2020

Nuclear two point correlation functions on a quantum computer

A. Baroni,[1] J. Carlson,[1] R. Gupta,[1] Andy C. Y. Li,[2] G. N. Perdue,[2] and A. Roggero[3,4,5]

e^{-iHt} Apply real the time evolution →

Simulation of collective neutrino oscillations on a quantum computer

Benjamin Hall, Alessandro Roggero, Alessandro Baroni, and Joseph Carlson
Phys. Rev. D **104**, 063009 – Published 3 September 2021

Future directions

- Classical calculation with realistic number of lattice sites to guide future simulations
- Light nuclei on a quantum computer for benchmarking of current quantum hardware
  - Improve on error mitigation protocols
  - Explore automated circuit synthesis for larger circuits > 10 qubits
- Estimate resources needed for a first quantization mapping
- Perform fault tolerant resource estimates for $^{12}\mathrm{C}$ responses

Thank you

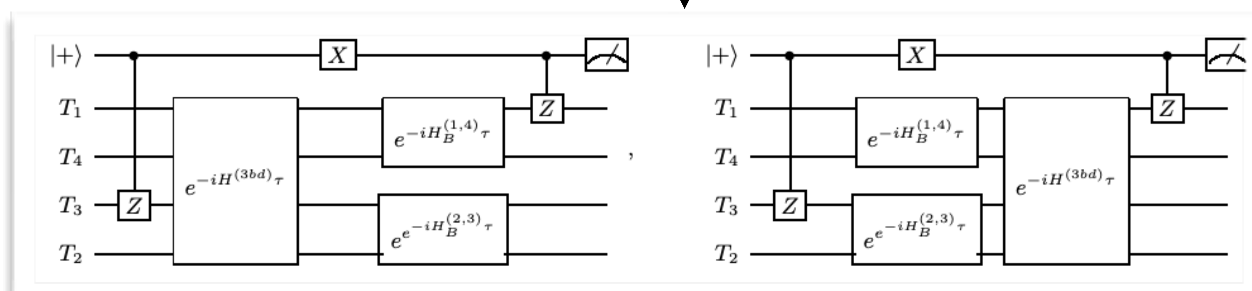
Splittings

$$H_A^{(1bd)} \equiv -2t\sum_{k=1}^{4} X_k \,,$$
$$H_A^{(2bd)} \equiv -\frac{U}{4}\left(Z_1Z_4 + Z_2Z_3\right) \,,$$
$$H^{(3bd)} \equiv -\frac{U}{4}\sum_{i<j<k} Z_iZ_jZ_k \,.$$

$$U_{A1}(\tau) = e^{-iH_A^{(1bd)}\tau}\, e^{-iH_A^{(2bd)}\tau - iH^{(3bd)}\tau}$$
$$U_{A2}(\tau) = e^{-iH_A^{(2bd)}\tau - iH^{(3bd)}\tau}\, e^{-iH_A^{(1bd)}\tau}$$

$$H_B^{(i,j)} = -2t(X_i + X_j) - \frac{U}{4} Z_iZ_j \,,$$

$$U_{B1}(\tau) = e^{-iH_B^{(1,4)}\tau} e^{-iH_B^{(2,3)}\tau} e^{-iH^{(3bd)}\tau}$$
$$U_{B2}(\tau) = e^{-iH^{(3bd)}\tau} e^{-iH_B^{(1,4)}\tau} e^{-iH_B^{(2,3)}\tau}$$



	A1	A2	B1	B2
$\langle Z_1(\tau)Z_1\rangle$	19	6	26	8
$\langle Z_1(\tau)Z_3\rangle$	25	9	28	11
$\langle Z_1(\tau)Z_2(\tau)Z_3Z_4\rangle$	25	15	28	15
$\langle Z_1(\tau)Z_2(\tau)Z_1Z_2\rangle$	30	9	29	13

Consistency check

Check consistency of extrapolations

$$(O_A, E_A) \quad \text{and} \quad (O_B, E_B) \quad \text{compatible} \longrightarrow \quad |O_A - O_B| \leq m\sqrt{E_A^2 + E_B^2} \quad m \geq 1\,.$$

If a result changes significantly
by adding one more order, the lower order
extrapolation is unlikely to have converged

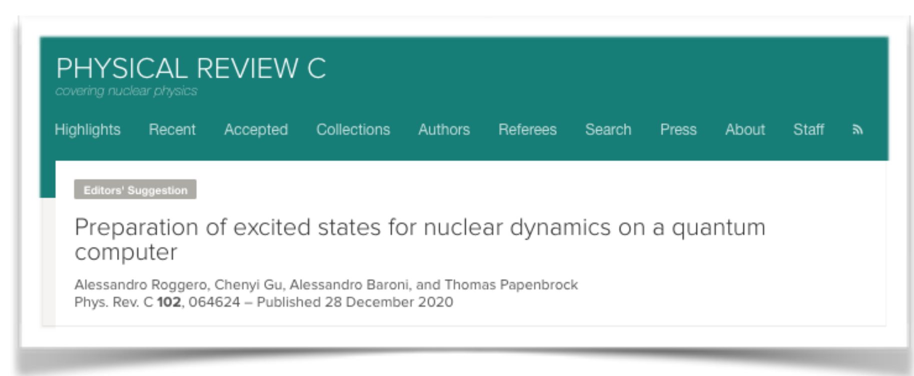
Determine lowest order result that is
compatible with higher orders

Algorithm 1 Consistency check

define BOOL array *ctest* of size $[N_{ex}^{max}]$
$error\_count \leftarrow 0$
for $i = 1$ to N_{ex}^{max} **do**
  $ctest[i] \leftarrow True$
  for $j = i+1$ to N_{ex}^{max} **do**
    if not $\left[(O_A, E_A) \stackrel{m}{==} (O_B, E_B)\right]$ **then**
      $ctest[i] \leftarrow False$
      $error\_count \leftarrow error\_count + 1$
      break
return array *ctest* and integer *error_count*

If no order passes the consistency
check return Failed

Attempt again removing the highest
order if fails again, mark definitely
as Failed


PHYSICAL REVIEW C
covering nuclear physics
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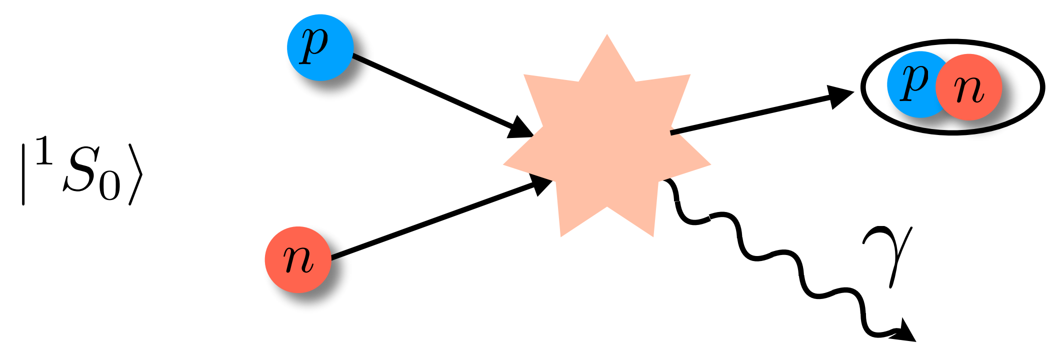
Neutron-proton em capture

A famous nuclear scattering process is thermal neutron-proton capture



$$|\mathrm{deuteron}\rangle = |^3S_1\rangle + |^3D_1\rangle$$

Main contribution

The excitation operator describing the transition is

$$\hat{O} = \hat{\mathbf{m}} \cdot \mathbf{n}_\gamma \longrightarrow \{|^1S_0\rangle\,,\ |^3S_1\rangle\} \longrightarrow \text{2x2 matrix}$$

Photon polarization

Simplest possible formulation
that allows to test various approaches
(Scale up later…)

Magnetic moment operator

$$\mathbf{m} = 2\mu_N \mathbf{l} + g_p \mu_N \mathbf{S}_p + g_n \mu_N \mathbf{S}_n$$

Neutron-proton em capture

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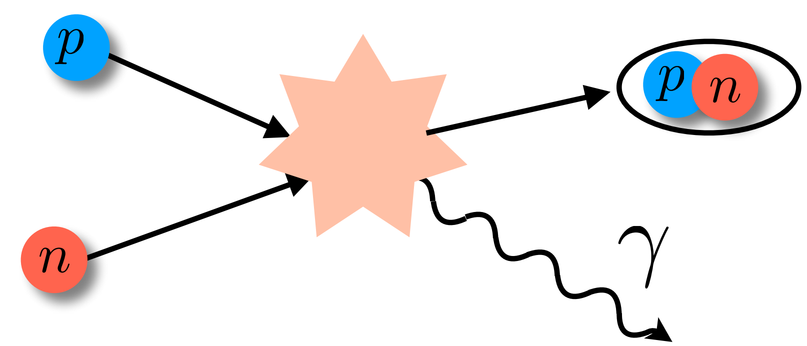
$|^1S_0\rangle$



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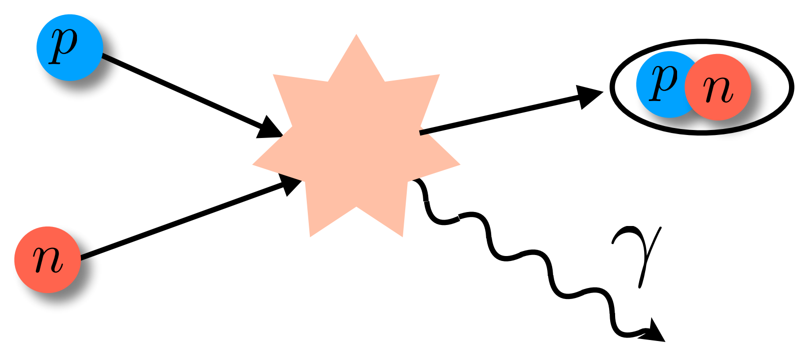

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Trotter scaling

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….

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Neutron-proton em capture

$$\mathbf{m} = 2\cancel{\mu_N}\mathbf{l} + g_p\mu_N\mathbf{S}_p + g_n\mu_N\mathbf{S}_n$$

$$\hat{O} = \hat{\mathbf{m}} \cdot \mathbf{n}_\gamma$$

XZ-plane

$$|i\rangle \equiv \frac{1}{2}\left(|p\uparrow n\downarrow\rangle + |n\uparrow p\downarrow\rangle - |p\downarrow n\uparrow\rangle - |n\downarrow p\uparrow\rangle\right)$$

$$|f\rangle \equiv \frac{1}{\sqrt{2}}\left(|n\uparrow p\uparrow\rangle - |p\uparrow n\uparrow\rangle\right).$$

$$O = \begin{pmatrix} \langle i|\hat{O}|i\rangle & \langle i|\hat{O}|f\rangle \\ \langle f|\hat{O}|i\rangle & \langle f|\hat{O}|f\rangle \end{pmatrix} = \alpha\mathbf{1} + \beta X + \gamma Z$$

Readout error

- Observable of interest is affected $$\langle O \rangle = \sum_{i=1}^{N} a_i p_i$$ bare probabilities

- Observable of interest is affected $$\langle \widetilde{O} \rangle = \sum_{ij}^{N} a_i \left[P^{-1}\right]_{ij} \left[p_e\right]_j$$

- 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)

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

Future directions

Open Access

Fault-Tolerant Quantum Simulations of Chemistry in First Quantization

Yuan Su, Dominic W. Berry, Nathan Wiebe, Nicholas Rubin, and Ryan Babbush
PRX Quantum **2**, 040332 – Published 11 November 2021

- Start with pionless EFT, only contact terms, two body terms (2+7), three body terms (1)
- Choose an appropriate basis Lattice, or Harmonic oscillator
  - Calculate explicitly the matrix elements
    Trying to get an analytical form

Pion-less effective field theory for atomic nuclei and lattice nuclei

A. Bansal, S. Binder, A. Ekström, G. Hagen, G. R. Jansen, and T. Papenbrock
Phys. Rev. C **98**, 054301 – Published 1 November 2018

- Perform first quantization mapping to qubits $\# \text{ qubits} = \eta \log_2(N)$
  - Antisymmetrizzation must be included explicitly

Gate complexity $\eta \log(\eta) \log(N)$

- Implement time evolution exploring all the available techniques
  - IP (Low, Wiebe, ..)
  - Trotter-Suzuki (Childs, Somma, ..)
  - Qubitization (Low,Chuang,..)
  - LCU (Wiebe, Childs, ..)

Gate error

- Correcting for gate errors

- 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

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

Combine extrapolations

After consistency check of results return the triple for each extrapolation method

$$(O_k^e, E_k^e, C_k)$$

Final result:

Global linear fit for each of the results of the extrapolation method

If successful return fitted observables

If not return average together all the triplets with the smallest error count

Toy model used

NN Interaction in pionless EFT at LO

S wave interaction S=0 T=1 nn scattering a<0

S=1 T=0 weakly bound state deuteron

NNN Interaction required to avoid collapse into deeply bound states

This model can 'easily' be put on a lattice basis

$$H = 2DtA - t\sum_{f=1}^{N_f}\sum_{\langle i,j\rangle}^{M}\left[c_{i,f}^\dagger c_{j,f} + c_{i,f}^\dagger c_{j,f}\right] + \frac{1}{2}C_0\sum_{f\neq f'}^{N_f}\sum_{i=1}^{M} n_{i,f}n_{i,f'} + \frac{D_0}{6}\sum_{f\neq f'\neq f''}^{N_f}\sum_{i=1}^{M} n_{i,f}n_{i,f'}n_{i,f''}\ ,$$

PAPER

Finite volume effects in low-energy neutron–deuteron scattering

A Rokash[1], E Epelbaum[1], H Krebs[1], D Lee[2] and U-G Meißner[3,4]

Published 3 December 2013 • © 2014 IOP Publishing Ltd

Journal of Physics G: Nuclear and Particle Physics, Volume 41, Number 1

Citation A Rokash *et al* 2014 *J. Phys. G: Nucl. Part. Phys.* **41** 015105

D space dimension

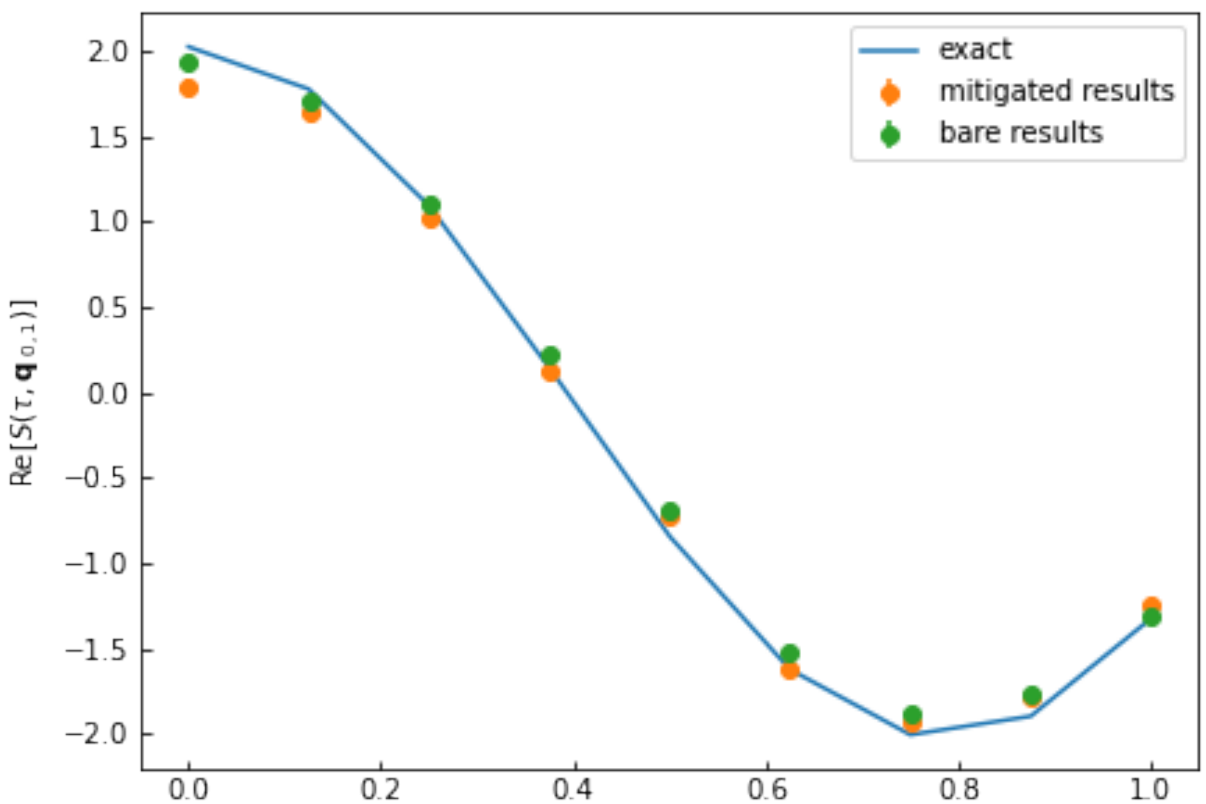
t [MeV]	C_0 [MeV]	D_0 [MeV]
10.5794	-98.2265511	127.839693

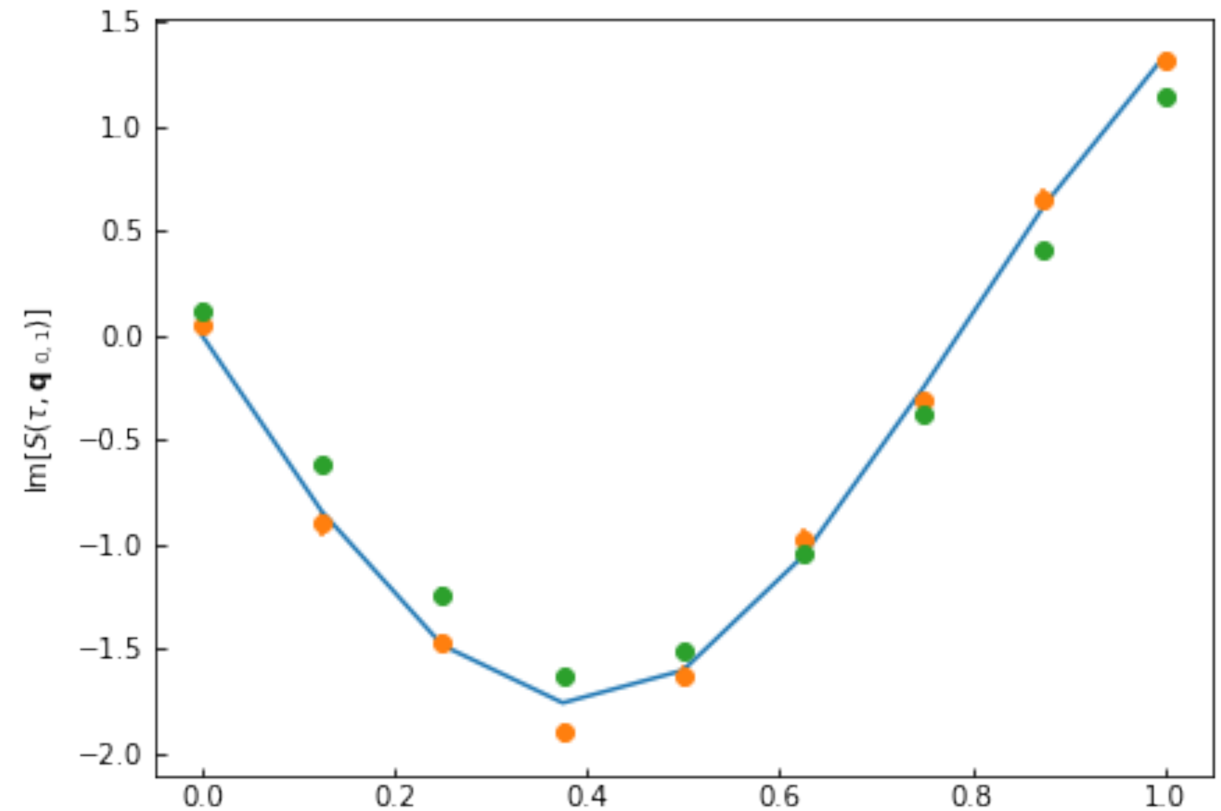
Lattice spacing 1.4 fm

Responses on a quantum computer

Ibmq Vigo real hardware

For a specific Trotterizzation





$$S(\tau, \mathbf{q}_{1,0}) = e_A^2 \langle Z_1(\tau) Z_1 \rangle + e_A e_B \langle Z_1(\tau) Z_3 \rangle + e_A e_B \langle Z_3(\tau) Z_1 \rangle + e_B^2 \langle Z_3(\tau) Z_3 \rangle$$

Scalings

$$||\overline{H_I(\mathbf{q}_k)}||_q = \left(\sum_{i=1}^{L} |\alpha_i(\mathbf{q}_k)|^q\right)^{1/q}, \quad \text{for } q \geq 1$$

$$H_I(\mathbf{q}_k) = \sum_{f=1}^{N_f} \rho_f(\mathbf{q}_i) = \sum_{f=1}^{N_f} e_f \sum_i e^{i\mathbf{q}_k \cdot \mathbf{r}_i} n_{i,f}$$

$$N \leq \frac{L^2}{\epsilon^2} \max_k \left[\sum_{i=1}^{L} \alpha_i^2(\mathbf{q}_k)\right]^2$$

Scaling of classical diagonalization algorithms

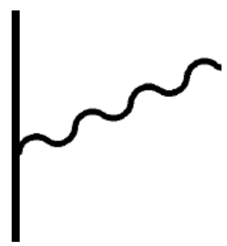
Finding eigenvalues of a matrix, exact algorithms

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 $\mathcal{O}(\underbrace{\boxed{N^2}}_{\text{Matrix vector multiplication}}\boxed{\log(N)/\epsilon})$	Get only largest eigenvalue

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

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

Site location

$$e^{-iHt}$$

Classical calculation for H of dimension NxN:

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

For approximate diagonalization better scalings

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	

Evolution of a qc

Richardson extrapolation finds justification into the Lindbald equation

$$\frac{\partial}{\partial t}\rho(t) = -i\left[K(t), \rho(t)\right] + \lambda \mathcal{L}\left(\rho(t)\right).$$

$\lambda \to 0$ Noiseless quantum computation

Cannot adjust the parameter
Assuming that the form of the Lindbald operator is invariant under time re scaling
And independent of K adding gates we can increase λ