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Real-time quantum Lanczos for nuclear structure

Calvin W. Johnson, San Diego State University

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"Nuclear and particle physics on a quantum computer," ECT*, June 5, 2023

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Collaborators

Amanda Bowman, SDSU M.S. student in Computational Science

Ionel Stetcu, Staff Scientist, Los Alamos

Motivation

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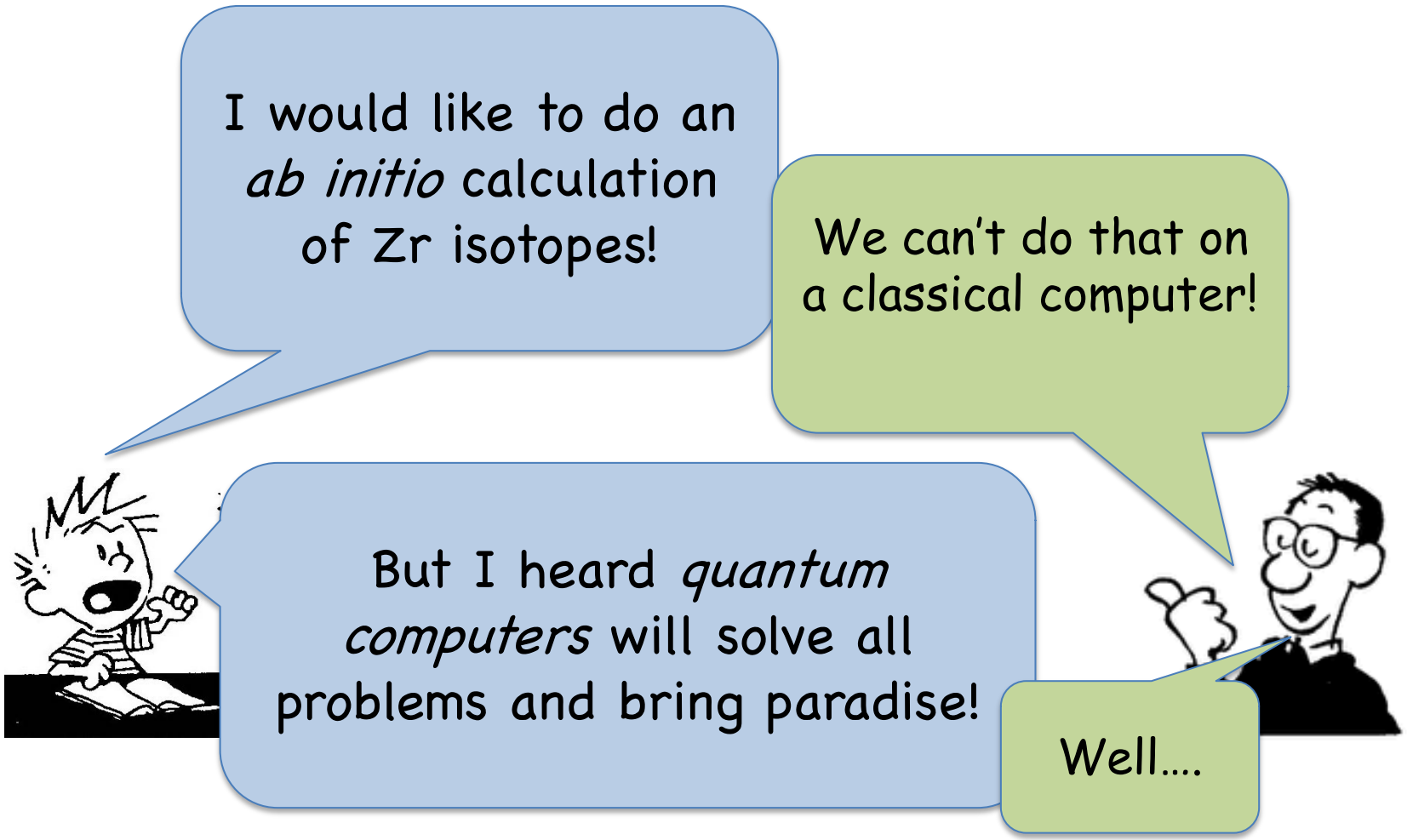

SCIENCE PROBLEMS FOR QUANTUM COMPUTING?

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- **Dark matter targets**: some targets for dark matter (e.g. ^{40}Ar) are in very large model spaces. (Similarly for neutrino targets)

* **Beta decays**: beta-delayed neutron emission in fission fragments; independently, look at beta decays of neutron-rich 'rare' nuclides.

* **Hadronic parity violation**: Experimental measurement of the anapole moment in heavy nuclides is underway (D. DeMille et al)

* **Inputs for reactions in medium to heavy nuclei**, including spectroscopic factors, needed for astrophysics

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All of these problems require
the quantum wave function of atomic nuclei

To answer this, we attempt to solve *Schrödinger's equation*:

$$\left(\sum_i -\frac{\hbar^2}{2m}\nabla^2 + U(r_i) + \sum_{i<j} V(\vec{r}_i - \vec{r}_j)\right)\Psi(\vec{r}_1, \vec{r}_2, \vec{r}_3 \ldots) = E\Psi$$

This differential equation is too difficult to solve directly

$$\left(\sum_i -\frac{\hbar^2}{2m}\nabla^2 + U(r_i) + \sum_{i<j} V(\vec{r}_i - \vec{r}_j)\right)\Psi(\vec{r}_1,\vec{r}_2,\vec{r}_3\ldots) = E\Psi$$

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Hence we turn to the matrix formalism (configuration-interaction):

expand in some (many-body) basis

$$\hat{\mathbf{H}}|\Psi\rangle = E|\Psi\rangle$$

$$|\Psi\rangle = \sum_{\alpha} c_{\alpha}|\alpha\rangle \qquad H_{\alpha\beta} = \langle\alpha|\hat{\mathbf{H}}|\beta\rangle$$

$$\sum_{\beta} H_{\alpha\beta} c_{\beta} = E c_{\alpha}$$

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But what do we use for the basis states?

Maria Mayer

$$\hat{\mathbf{H}}|\Psi\rangle = E|\Psi\rangle$$

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- How the basis states are represented

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Can only really solve 1D differential equation

$$\left(-\frac{\hbar^2}{2m}\frac{d^2}{dr^2} + U(r)\right)\phi_i(r) = \varepsilon_i\phi_i(r)$$

- How the basis states are represented

Can only really solve 1D differential equation

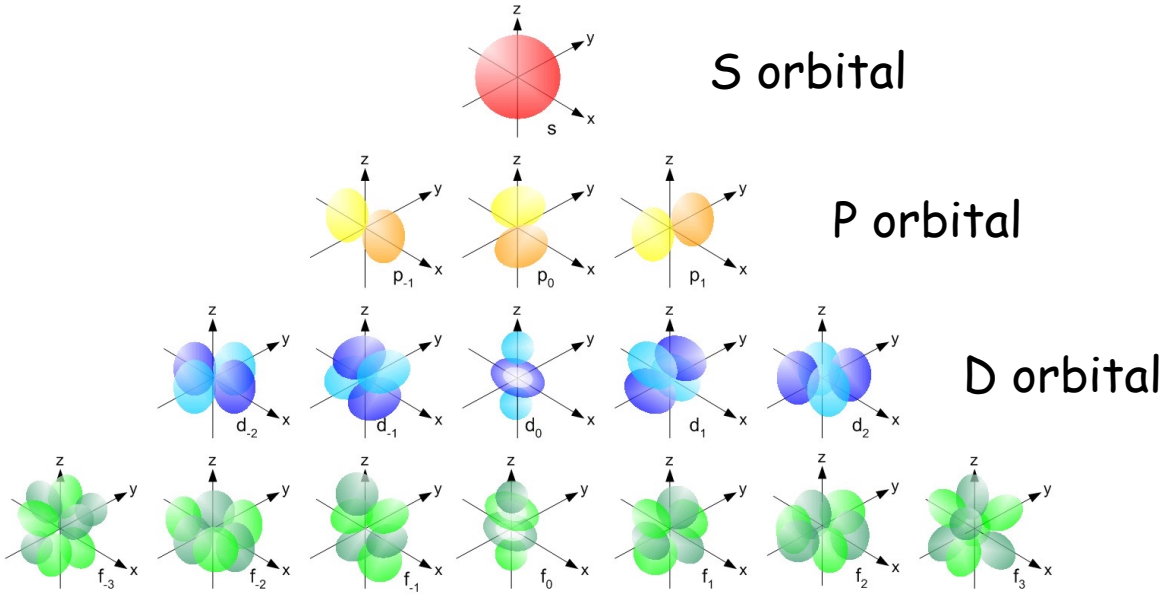
$$\left(-\frac{\hbar^2}{2m}\frac{d^2}{dr^2}+U(r)\right)\phi_i(r)=\varepsilon_i\phi_i(r) \Rightarrow \left\{\phi_i(\vec{r})\right\}$$

Single-particle wave functions labeled by, *e.g.*, n, j, l, m

Atomic case: 1s, 2s, 2p, 3s, 3p, 3d *etc*

Nuclear: $0s_{1/2}$, $0p_{3/2}$, $0p_{1/2}$, $0d_{5/2}$, $1s_{1/2}$, $0d_{3/2}$, *etc*

- This gives rise to the shell model



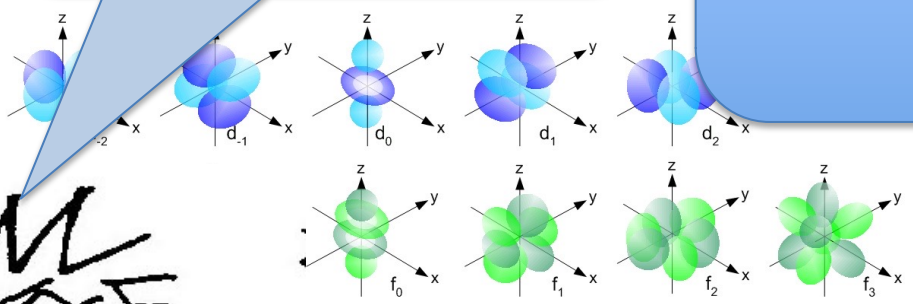
The **orbitals** are solutions to a one-particle Schrodinger eqn:

$$\left(-\frac{\hbar^2}{2m}\frac{d^2}{dr^2}+U(r)\right)\phi_i(r)=\varepsilon_i\phi_i(r)$$

- T… ell model

How do we get many-body states?

We just mash many single-particle states together!



T… re solutions to a one-particle Schrodinger e…

$$\left(\frac{d^2}{dr^2} + U(r)\right)\phi_i(r) = \varepsilon_i\phi_i(r)$$

- How the basis states are represented

Product wavefunction ("Slater Determinant")

$$\Psi(\vec{r}_1,\vec{r}_2,\vec{r}_3\ldots) = \phi_{n_1}(\vec{r}_1)\phi_{n_2}(\vec{r}_2)\phi_{n_3}(\vec{r}_3)\ldots\phi_{n_N}(\vec{r}_N)$$

Each many-body state can be *uniquely* determined by a list of "occupied" single-particle states = "occupation representation"

$$|\alpha\rangle = \hat{a}^+_{n_1}\hat{a}^+_{n_2}\hat{a}^+_{n_3}\ldots\hat{a}^+_{n_N}|0\rangle$$

- How the basis is represented

"occupation representation" $|\alpha\rangle = \hat{a}^+_{n_1} \hat{a}^+_{n_2} \hat{a}^+_{n_3} \ldots \hat{a}^+_{n_N} |0\rangle$

n_i	1	2	3	4	5	6	7
α=1	1	0	0	1	1	0	1
α=2	1	0	1	0	0	1	1
α=3	0	1	1	1	0	1	0

$$|\Psi\rangle = \sum_\alpha c_\alpha |\alpha\rangle$$

Each basis state a Slater determinant

~ a product of many 'orbitals'

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Nuclear Hamiltonian: $\hat{H} = \sum_i -\frac{\hbar^2}{2M}\nabla_i^2 + \sum_{i<j} V(r_i, r_j)$

At this point one generally goes to occupation representation:

$$\hat{H} = \sum_i \varepsilon_i \hat{a}_i^+ \hat{a}_i + \frac{1}{4}\sum_{ijkl} V_{ijkl} \hat{a}_i^+ \hat{a}_j^+ \hat{a}_l \hat{a}_k$$

single-particle energies

two-body matrix elements

Boring technical points **important** to our story:

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Nuclear Hamiltonian is rotationally invariant
-> total ang. mom. *J* and z-component *M* are 'good' q#s

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If the single-particle states have good *j*,*m*,
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(Good *J* emerges from diagonalizing *H*.)

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If the single-particle states have good *j,m*,
easy to construct many-body states with good M.
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Because we can generate such single-particle states with a rotationally invariant one-body Hamiltonian, we call this the *spherical basis*.

Boring technical point **important** to our story:

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However, *in principle*, we can choose
single-particle states that mix *j*,*m*.

In particular, deformed Hartree-Fock naturally leads to
states mixing *j* (and sometimes mixing *m* -> 'triaxial' states)

Boring technical point **important** to our story:

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However, *in principle*, we can choose
single-particle states that mix j,m.

In particular, deformed Hartree-Fock naturally leads to states mixing j (and sometimes mixing m -> 'triaxial' states)

The Hartree-Fock state is a single Slater determinant which has the lowest energy, i.e.,
let Ψ be a general Slater determinant:
Minimizing. $\frac{\langle\Psi|H|\Psi\rangle}{\langle\Psi|\Psi\rangle}$ leads to the Hartree-Fock equations.

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$$\hat{H} = \sum_i \varepsilon_i \hat{a}_i^+ \hat{a}_i + \frac{1}{4} \sum_{ijkl} V_{ijkl} \hat{a}_i^+ \hat{a}_j^+ \hat{a}_l \hat{a}_k$$

In the *spherical basis* (s.p. states with good j,m), many matrix elements $V_{\mathrm{ijkl}} = 0$ due to angular momentum selection rules.

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Coupled matrix element: $\langle aj_a, bj_b; J_{ab}|V|cj_c, dj_d; J_{cd}\rangle$

Uncoupled matrix element: $\langle j_1 m_1, j_2 m_2|V|j_3 m_3, j_3 m_3\rangle$
(uncoupled used Clebsch-Gordan coefficients)

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$$\hat{H} = \sum_i \varepsilon_i \hat{a}_i^+ \hat{a}_i + \frac{1}{4} \sum_{ijkl} V_{ijkl} \hat{a}_i^+ \hat{a}_j^+ \hat{a}_l \hat{a}_k$$

In the *spherical basis* (s.p. states with good j,m),
many matrix elements $V_{\mathrm{ijkl}} = 0$
due to angular momentum selection rules.

In the single-particle *Hartree-Fock* basis, there are
more nonzero matrix elements V_{ijkl}
due to mixing/breaking of symmetries.
(Overall symmetry is still conserved,
if you keep *all* matrix elements.)

This will be important later!

Hence we turn to the matrix formalism (configuration-interaction):

expand in some (many-body) basis

How can quantum computers help with this problem?

$$|\Psi\rangle = \sum_{\alpha}$$

$$H_{\alpha\beta} = \langle \alpha | \hat{\mathbf{H}} | \beta \rangle$$

$$\sum_{\beta} H_{\alpha\beta} c_{\beta} = E c_{\alpha}$$

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Nuclear shell model on a quantum computer

Lv, Wei, Xie, Long, arXiv:2205.12087 'Package' for computing shell model (not public)

Romero, Engel, Tang, Economou, PRC **105**, 064317 (2022). Advanced VQE for shell model.

Stetcu, Baroni, Carlson, arXiv: 2110.06098. Uses unitary coupled cluster for p-shell

Siwach, Arumugam, PRC **105**, 064318 (2022) Computing quadrupole moment of deuteron

Kiss, Grossi, et al, arXiv:2205.0864. Unitary coupled cluster for ^{6}Li (really: frozen α + deuteron all over again)

Talks this week: Romero (next talk)
Robin (Thursday); Perez-Obiol (Thursday) (entanglement)

How are we going to tackle nuclear structure on a quantum computer?

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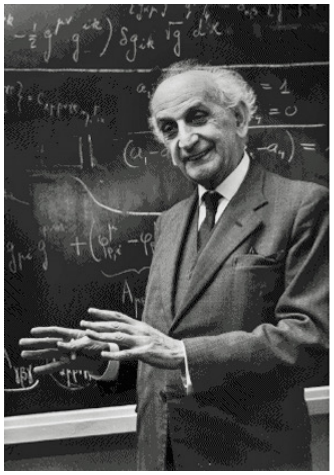
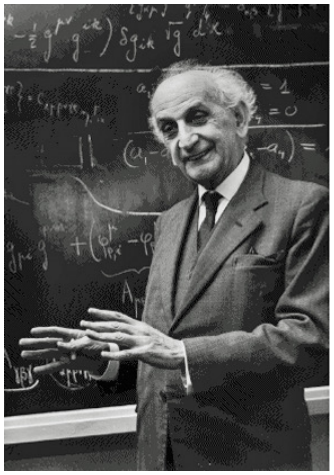
Can we adapt our current approaches to quantum computers?

- Lattice
- Coupled cluster → 'unitary' coupled cluster
- Advanced VQE (cf. next talk)
- **Configuration-interaction → Lanczos**



(Cornelius Lanczos)

The Lanczos Algorithm!



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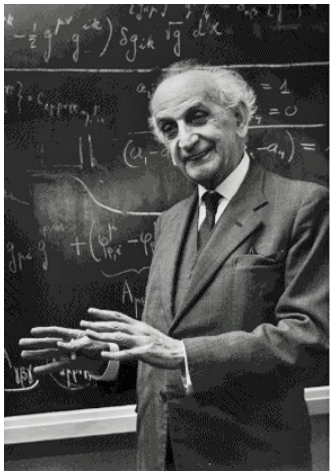
The Lanczos Algorithm!

Note: these quantum algorithms may not be practical on current machines, but reflect thinking about longer-term applications

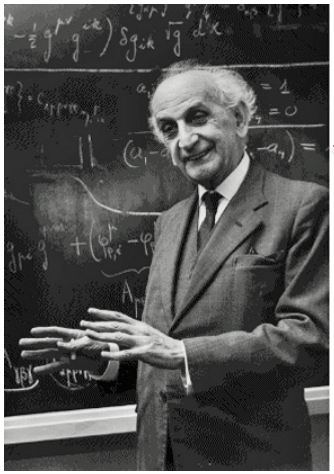


(Cornelius Lanczos)

$$\mathbf{A}\vec{v}_1 = \alpha_1\vec{v}_1 + \beta_1\vec{v}_2$$
$$\mathbf{A}\vec{v}_2 = \beta_1\vec{v}_1 + \alpha_2\vec{v}_2 + \beta_2\vec{v}_3$$
$$\mathbf{A}\vec{v}_3 = \beta_2\vec{v}_2 + \alpha_3\vec{v}_3 + \beta_3\vec{v}_4$$
$$\mathbf{A}\vec{v}_4 = \beta_3\vec{v}_3 + \alpha_4\vec{v}_4 + \beta_4\vec{v}_5$$

Starting from some initial vector (the "pivot") v_1 ,
the Lanczos algorithm iteratively creates
a new basis (a "Krylov space").

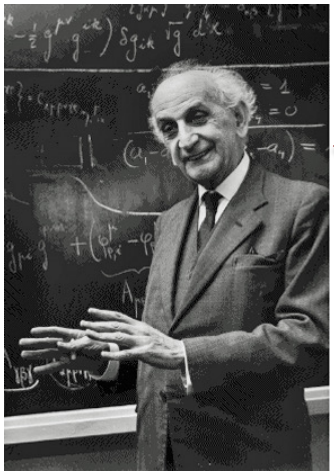
This is an example of a 'reduced basis method'



(Cornelius Lanczos)

This transforms the matrix A into a new basis, in which A is now tridiagonal

$$H \rightarrow \hat{H} = \begin{pmatrix} \alpha_1 & \beta_1 & & & \\ \beta_1 & \alpha_2 & \beta_2 & & \\ & \beta_2 & \alpha_3 & \beta_3 & \\ & & \ddots & \ddots & \ddots \end{pmatrix}$$



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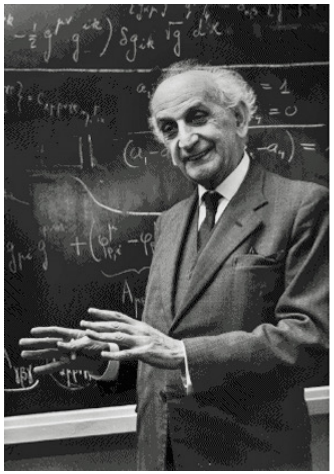
The extremal eigenvalues of the transformed, truncated matrix quickly converge to the extremal eigenvalues of the original matrix!



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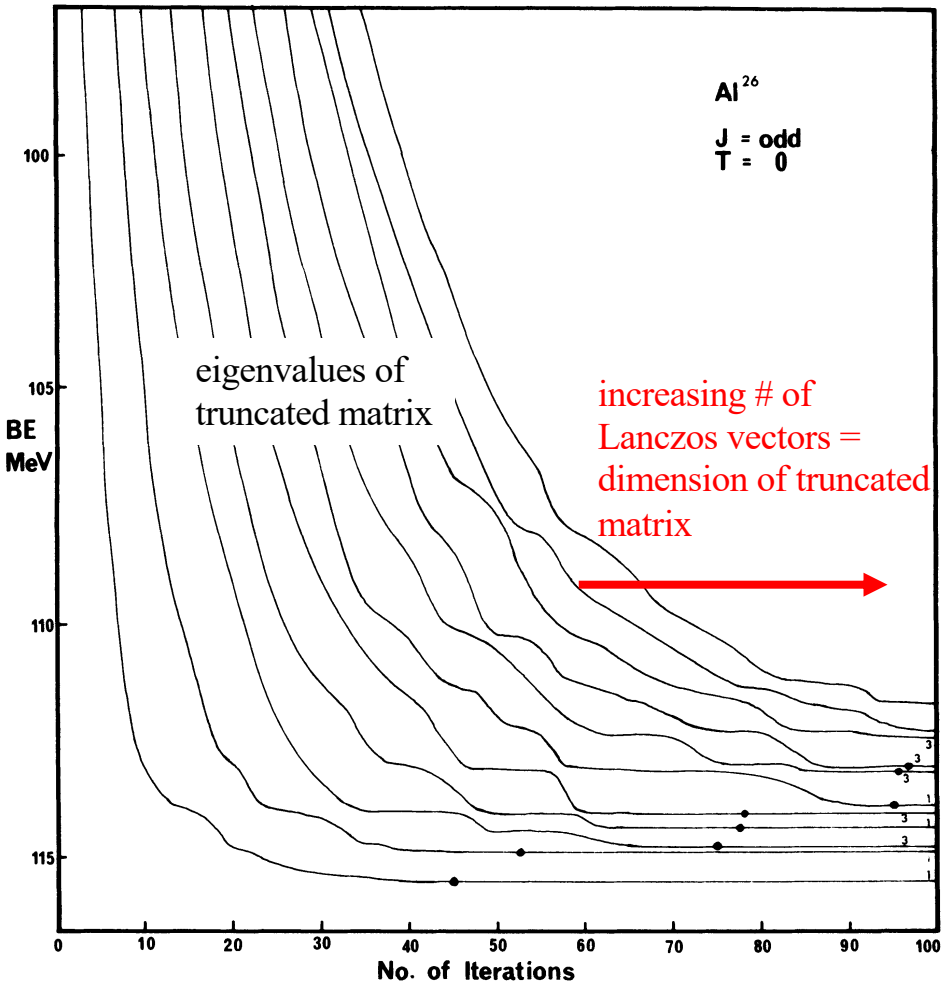
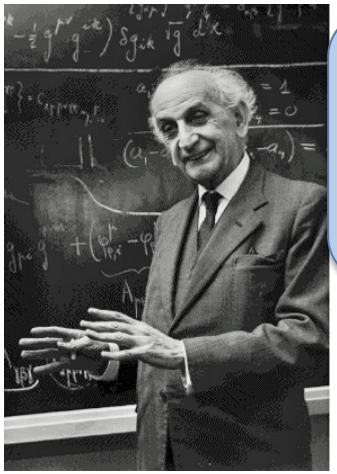


Whitehead, R. R., et al.
Advances in nuclear physics.
(1977) 123-176.

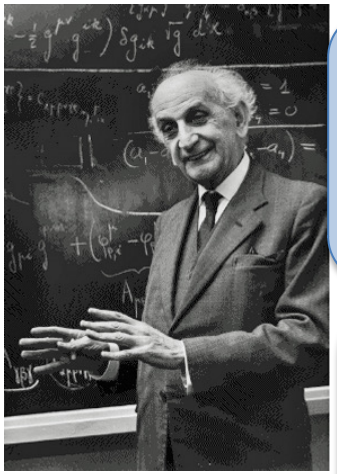
The one drawback of Lanczos is, due to round-off error, one must explicitly enforce orthogonality of Lanczos vectors

("reorthogonalization")



(Cornelius Lanczos)

But ordinary linear algebra is not straightforward on a quantum computer



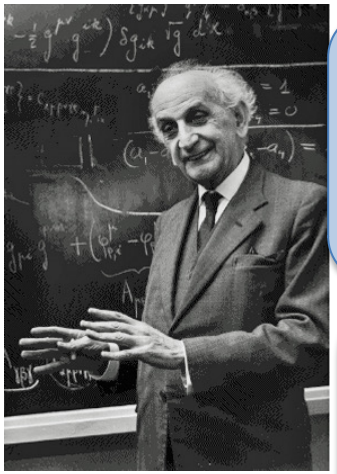
(Cornelius Lanczos)

But ordinary linear algebra is not straightforward on a quantum computer

We can take dot products: $\langle\Phi|\Psi\rangle$

compute matrix elements: $\langle\Phi|\hat{O}|\Psi\rangle$

and of course apply unitary transformations: $|\Phi\rangle = \hat{U}|\Psi\rangle$



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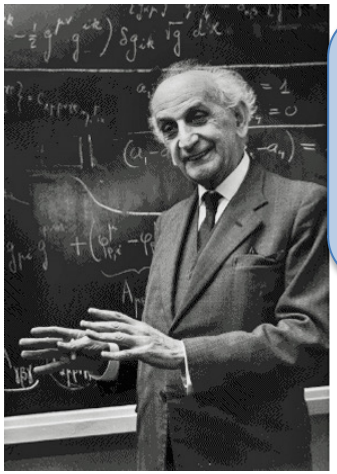
compute matrix elements: $\langle\Phi|\hat{O}|\Psi\rangle$
and of course apply unitary transformations: $|\Phi\rangle = \hat{U}|\Psi\rangle$

BUT: linear combinations: $|\Phi\rangle - a|\Psi\rangle$
(though possible) is not easy
(cf. linear combinations of unitaries (LCU))



(Cornelius Lanczos)

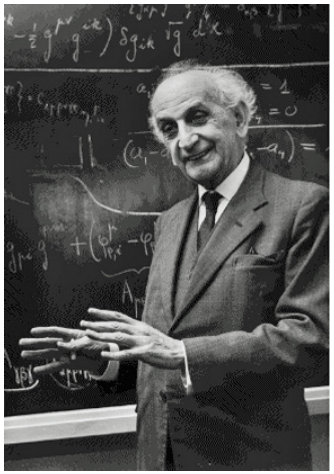
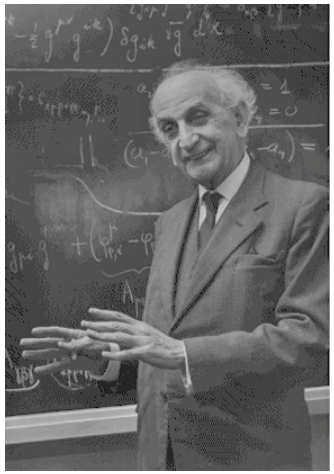
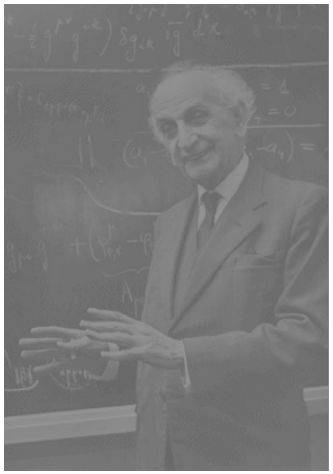
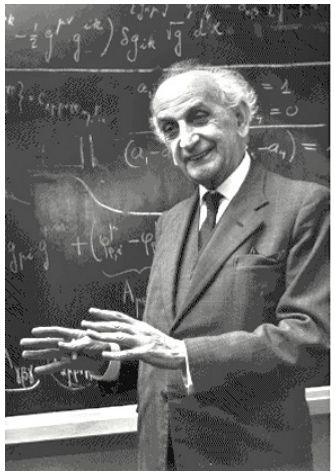
But ordinary linear algebra is not straightforward on a quantum computer

Let's do a hybrid approach:

some parts on a quantum machine

and some parts on a classical machine

Quantum Lanczos in imaginary time

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Motta, *et al*, Nature Physics **16**, 205 (2020)
McArdle *et al*, npj Quantum Inf. 5, 75 (2019)

Quantum Lanczos in imaginary time

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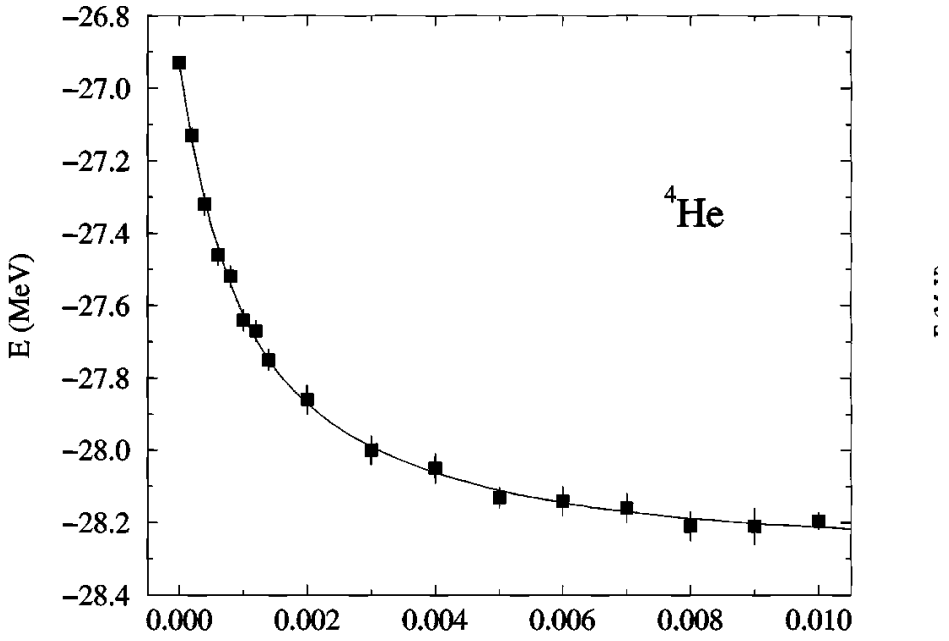
Imaginary-time evolution is the workhorse of "Quantum Monte Carlo" on classical computers

$$\lim_{\tau\to\infty} e^{-\tau\hat{H}}|\psi_{trial}\rangle \propto |\Psi_{gs}\rangle$$



Quantum Lanczos in imaginary time

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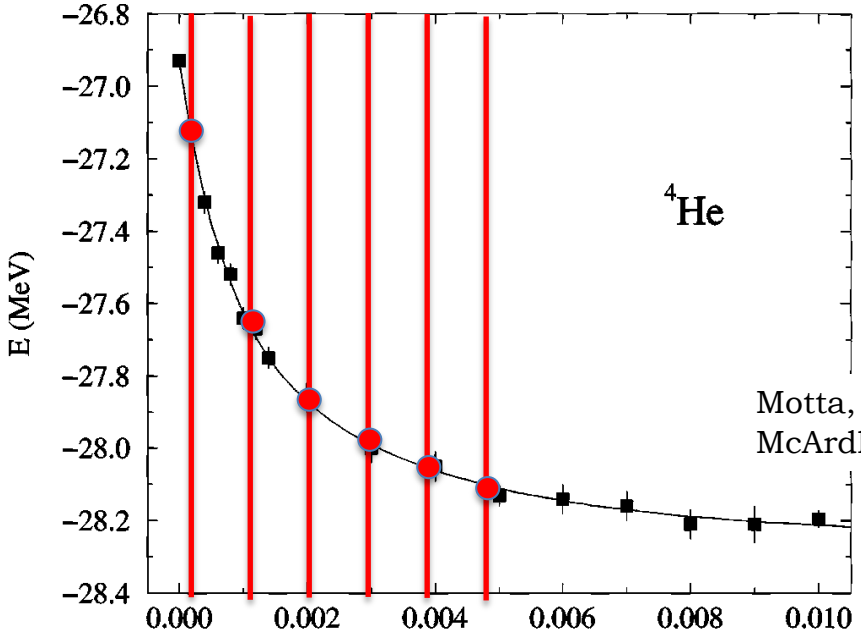
Key idea of "Quantum Lanczos": take states at different 'times' to form a non-orthogonal **reduced** basis

$$|\psi_n\rangle = e^{-n\Delta\tau\hat{H}}|\psi_0\rangle \qquad N_{mn} = \langle\psi_m|\psi_n\rangle \qquad H_{mn} = \langle\psi_m|\hat{H}|\psi_n\rangle$$



imaginary time τ (MeV^{-1})

In this reduced basis, solve generalized eigenvalue problem:

$$\hat{H}\vec{v} = E\,\hat{N}\vec{v}$$

Motta, *et al*, Nature Physics **16**, 205 (2020)
McArdle *et al*, npj Quantum Inf. 5, 75 (2019)

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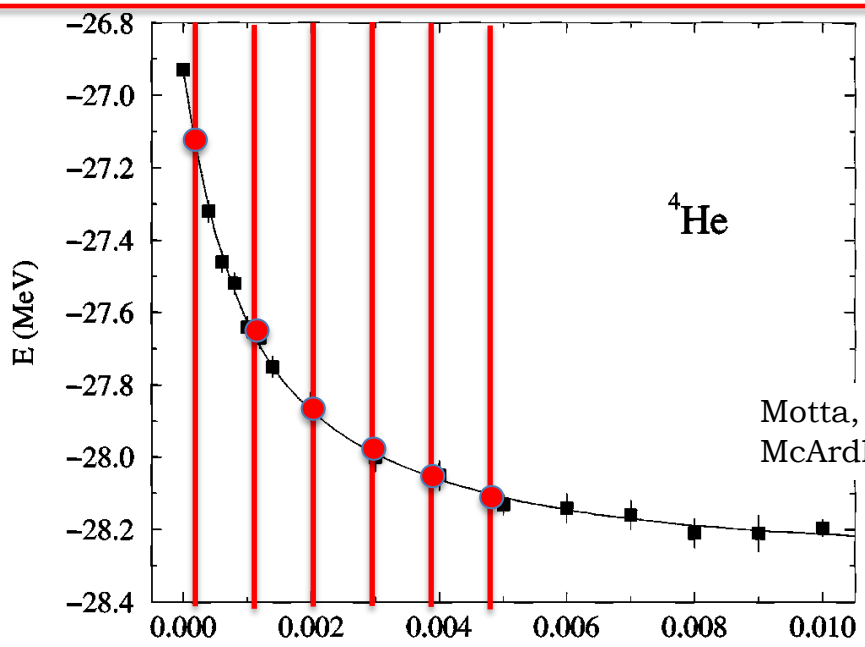
Do this on a quantum machine



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Do this on a classical machine

Motta, *et al*, Natu)20)
McArdle *et al*, npj 2019)

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Do this on a quantum machine

BUT:
imaginary time evolution is *not* unitary!

In this reduced basis, solve generalized eigenvalue problem:

$$\hat{H}\vec{v} = E\,\hat{N}\vec{v}$$

Do this on a classical machine

Instead one has to find a unitary operator that approximates imaginary time evolution

Quantum Lanczos in imaginary time

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That is, some **U** such that

$$U|\psi\rangle \approx e^{-\Delta\tau \hat{H}} |\psi\rangle$$

BUT:
imaginary time evolution
is *not* unitary!

Instead one has to find a unitary operator that approximates imaginary time evolution

Quantum Lanczos in imaginary time

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That is, some **U** such that

$$U|\psi\rangle \approx e^{-\Delta\tau \hat{H}}\,|\psi\rangle$$

That unitary approximation will be state dependent and not trivial to find!

but see Jouzdani, CWJ, Mucciolo, and Stectu, PRA **106**, 062435 (2022) for improvements

BUT:
imaginary time evolution is *not* unitary!

Instead one has to find a unitary operator that approximates imaginary time evolution

Quantum Lanczos in real time

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Quantum computers are good at unitary transformations so why not use **real time evolution?**

Quantum Lanczos in real time

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Parrish and McMahon, arXiv:1909.08925
"Quantum Filter Diagonalization"

Key idea of "Quantum Lanczos": take states at different 'times' to form a non-orthogonal **reduced** basis

$$|\psi_n\rangle = e^{-in\Delta t\hat{H}}|\psi_0\rangle \qquad N_{mn} = \langle\psi_m|\psi_n\rangle \qquad H_{mn} = \langle\psi_m|\hat{H}|\psi_n\rangle$$

In this reduced basis, solve generalized eigenvalue problem:

$$\hat{H}\vec{v} = E\,\hat{N}\vec{v}$$

Quantum Lanczos in real time

Parrish and McMahon, arXiv:1909.08925
"Quantum Filter Diagonalization"

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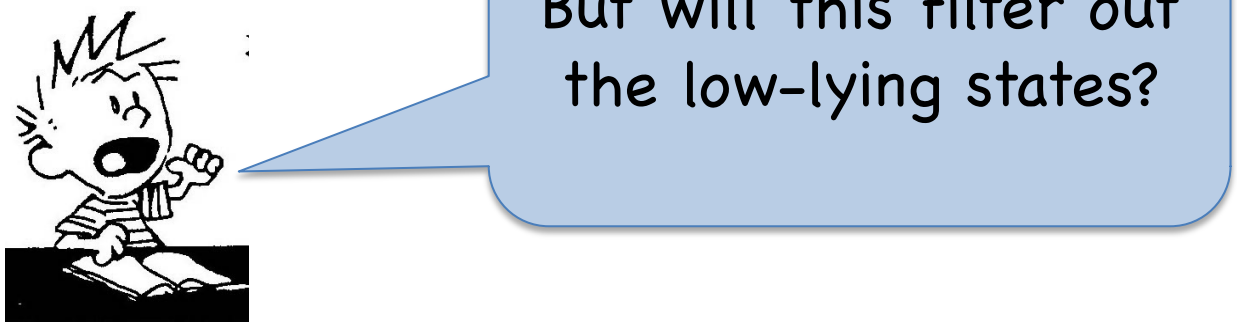

Quantum Lanczos in real time

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We took several steps to investigate this approach

Lanczos on a classical computer

Baseline

Quantum Lanczos in real time

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Lanczos on a classical computer

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Comparison of real- and imaginary-time evolution with synthetic data (working in eigenbasis)

Does basic idea work?

Quantum Lanczos in real time

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Partial emulation using bit & Pauli string representation

Checking technical details (HF vs spherical basis, Trotterization)

Quantum Lanczos in real time

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Full Qiskit emulation

Not done

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Checking technical details (HF vs spherical basis, Trotterization)

Full Qiskit emulation

Not done

Run on quantum computer

Not done

Quantum Lanczos in real time

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Lanczos on a classical computer

Baseline

Comparison of real- and imaginary-time evolution with synthetic data (working in eigenbasis)

Does basic idea work?

For this step, we fully diagonalized a nuclear Hamiltonian (USDB) in a valence space to get all the eigenenergies: $\hat{H}|\phi_n\rangle = E_n\ |\phi_n\rangle$

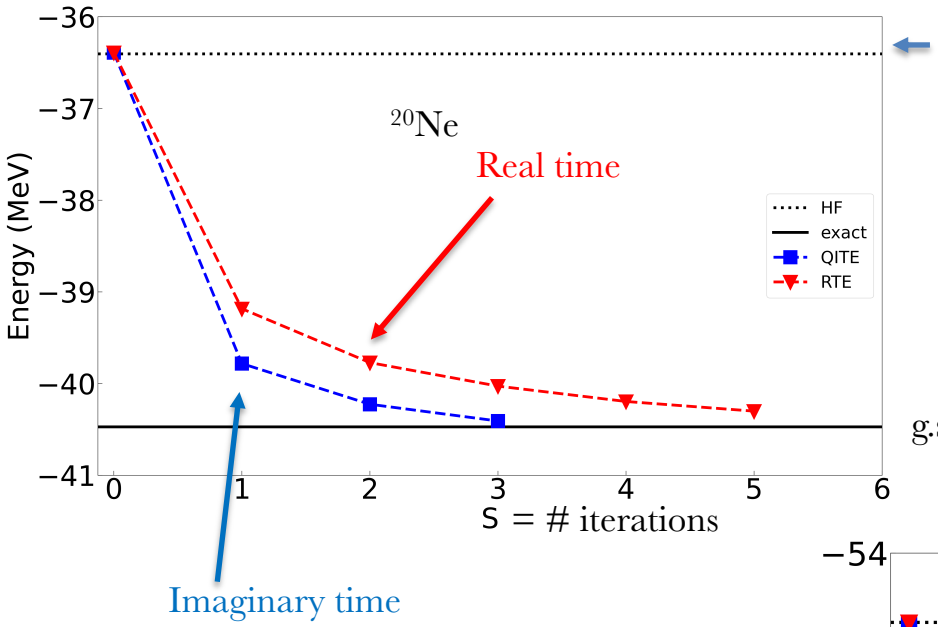
We then generated a random trial vector

$$|\psi_{trial}\rangle = \sum_n c_n\ |\phi_n\rangle$$

Evolution in the energy basis is easy:

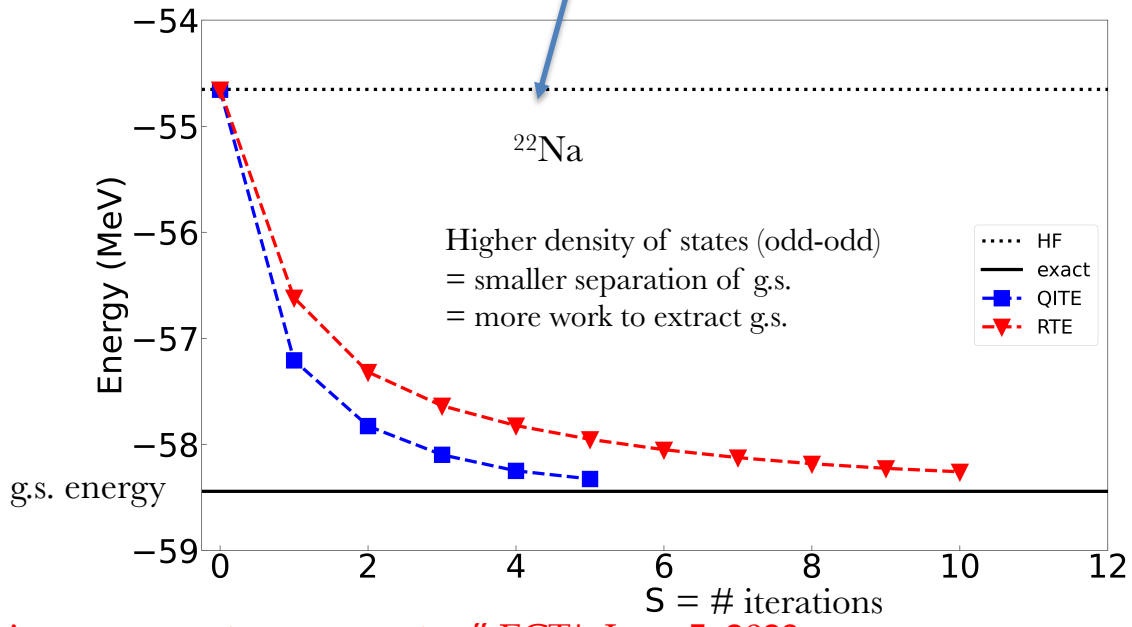
$$e^{-i\hat{H}t}|\psi_{trial}\rangle = \sum_n c_n\ e^{-iE_nt}|\phi_n\rangle$$

Quantum Lanczos in real time



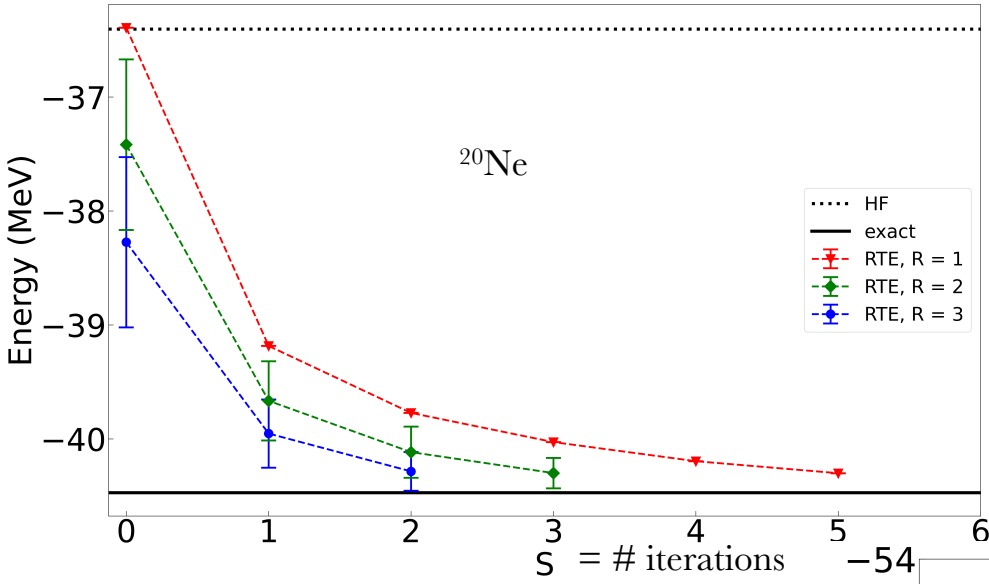
Initial state: We evolved in imaginary time a random state until $< H > = E_{HF}$

g.s. energy



Here $\Delta t = \Delta\tau = 0.1\ \text{MeV}^{-1}$

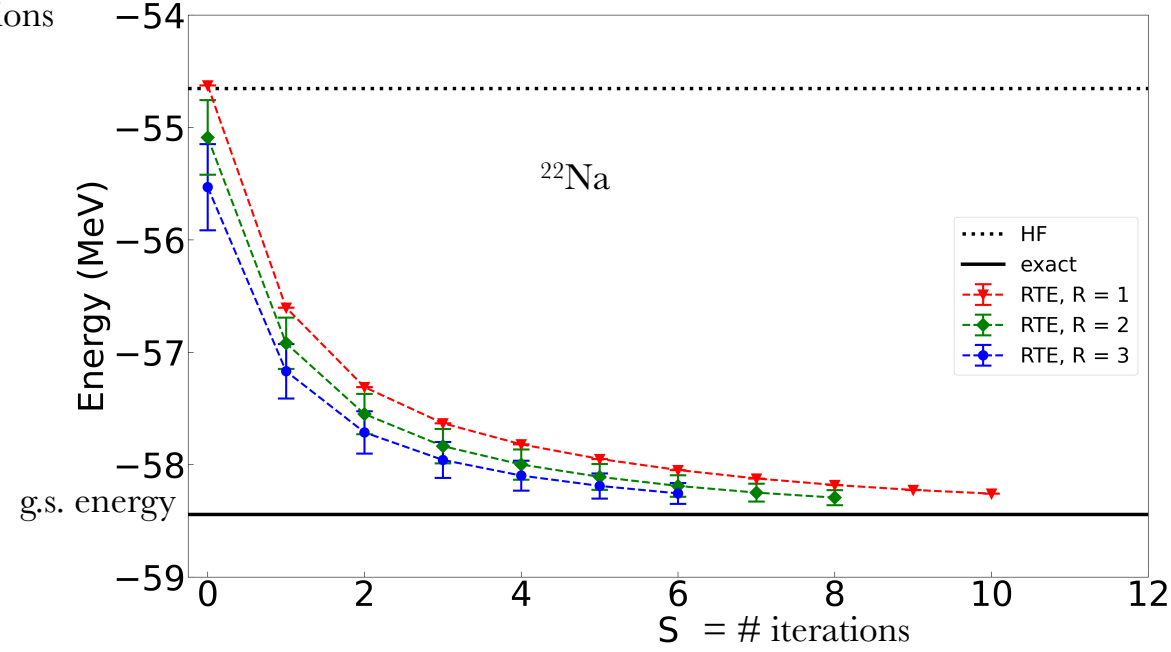
Quantum Lanczos in real time



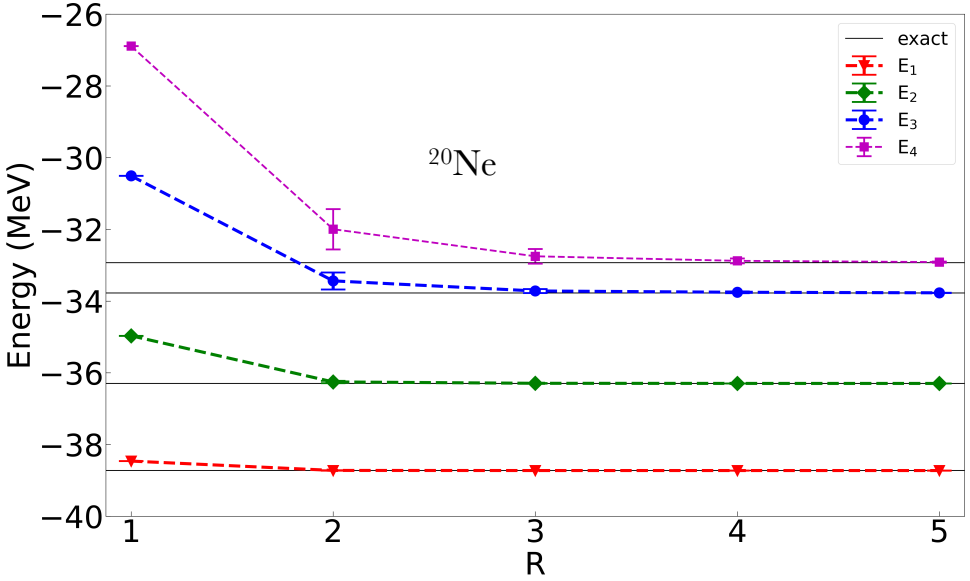
Use of multiple reference states improves convergence (Stair, Huang, Evangelista, *J. Chem. Theory Comput.* **16**, 2236 (2022))

Here $\Delta t = \Delta\tau = 0.1$ MeV^{-1}

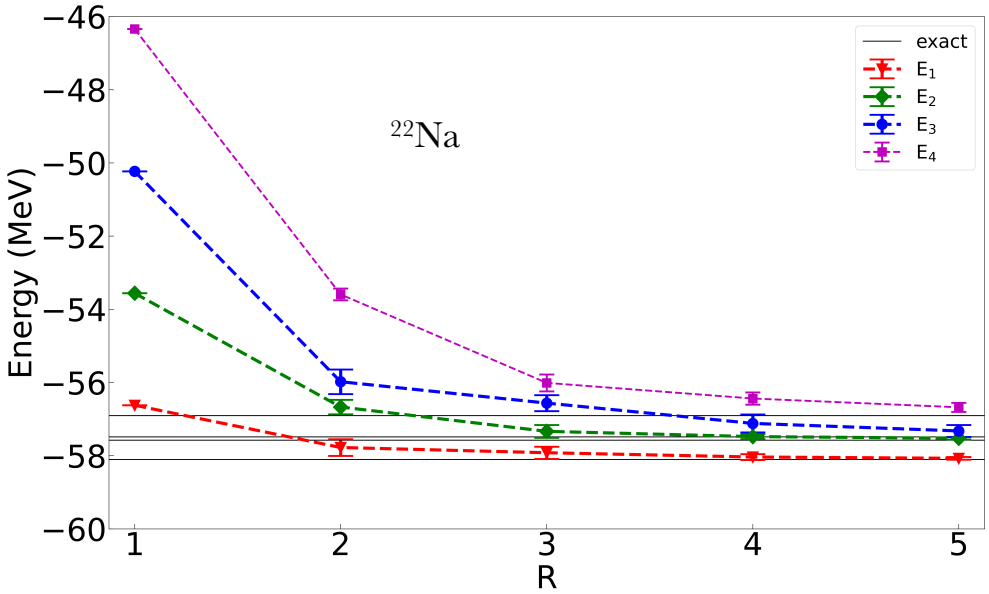
R = # of reference states



Quantum Lanczos in real time



We can also get excited states

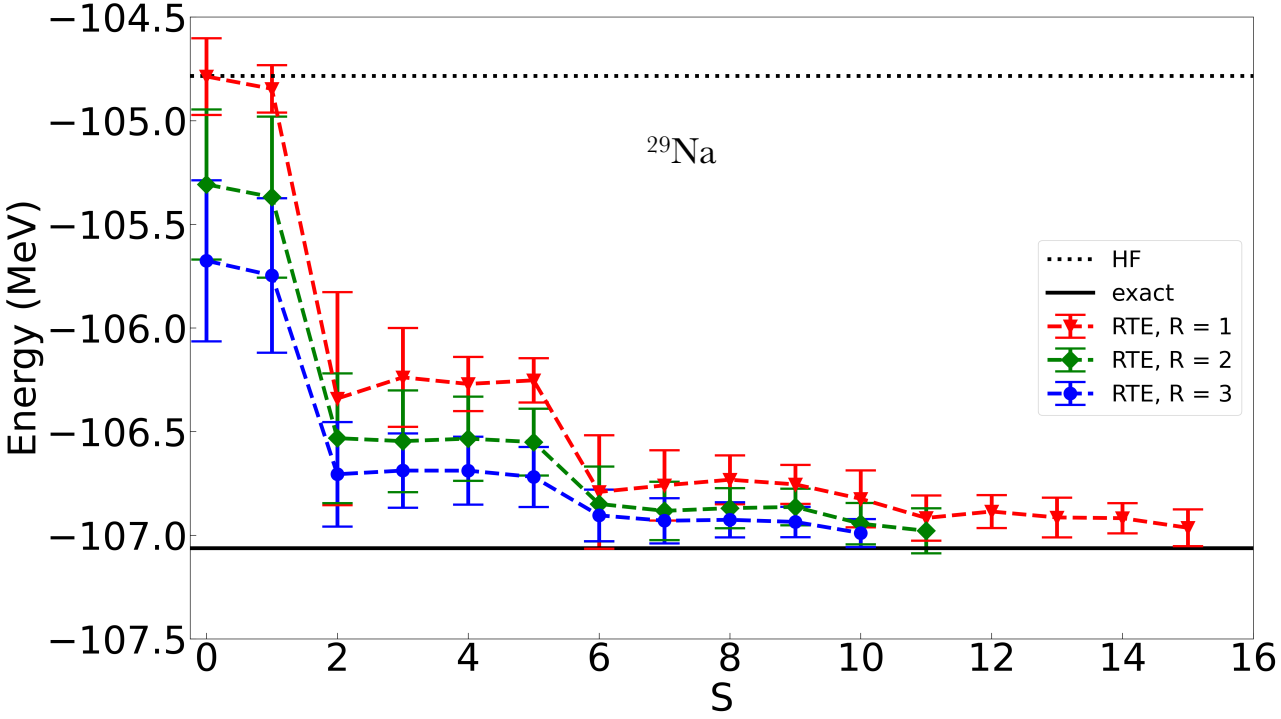


Here $\Delta t = \Delta\tau = 0.1\ \text{MeV}^{-1}$

Number of iterations fixed at S = 9

R = # of reference states

Quantum Lanczos in real time



Here $\Delta t = \Delta\tau = 0.1\ \text{MeV}^{-1}$

R = # of reference states
S = # of iterations

We added noise (1%) to check robustness of solving generalized eigenvalue equation

Quantum Lanczos in real time

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Lanczos on a classical computer

Comparison of real- and imaginary-time evolution with synthetic data (working in eigenbasis)

Does basic idea work?

Yes!
Basic idea works!

Quantum Lanczos in real time

SAN DIEGO STATE UNIVERSITY

Lanczos on a classical computer

→ Comparison of real- and imaginary-time evolution with synthetic data (working in eigenbasis)

→ Partial emulation using bit & Pauli string representation

Checking technical details (HF vs spherical basis, Trotterization)

For this next step, we generated the full wave function using operators, e.g., $\hat{a}_1^\dagger \hat{a}_3^\dagger \hat{a}_6^\dagger \hat{a}_{11}^\dagger |0\rangle$, and the Hamiltonian,

$$\hat{H} = \sum_{ij} \langle i| \hat{T} |j\rangle \, \hat{a}_i^\dagger \hat{a}_j + \frac{1}{4} \sum_{ijkl} \langle ij| \hat{V} |kl\rangle \, \hat{a}_i^\dagger \hat{a}_j^\dagger \hat{a}_l \hat{a}_k,$$

These were mapped to Pauli strings. We then simulated time-evolution, but using the operators directly, not using gates in Qiskit.

(Instead, these were applied in basis of all possible bitstrings | 0001 > etc.

Quantum Lanczos in real time

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example: ^{14}N in $0p_{1/2}$ -shell

Jordan-Wigner mapping

$$\hat{a}_0^\dagger = \frac{1}{2}(X_0 - iY_0) \qquad \text{proton, m= + ½}$$

$$\hat{a}_1^\dagger = \frac{1}{2}(Z_0X_1 - iZ_0Y_1) \qquad \text{proton, m = -1/2}$$

$$\hat{a}_2^\dagger = \frac{1}{2}(Z_0Z_1X_2 - iZ_0Z_1Y_2) \qquad \text{neutron, m= + ½}$$

$$\hat{a}_3^\dagger = \frac{1}{2}(Z_0Z_1Z_2X_3 - iZ_0Z_1Z_2Y_3), \qquad \text{neutron, m = -1/2}$$

Quantum Lanczos in real time

SAN DIEGO STATE UNIVERSITY

example: ^{14}N in $0p_{1/2}$ -shell

Jordan-Wigner mapping

$$\begin{aligned}\hat{H} = {} & c_0 I + c_1 Z_0 + c_2 Z_1 + c_3 Z_2 + c_4 Z_3 + c_5 Z_0 Z_3 + c_6 Z_1 Z_2 \\ & + c_7 Z_0 Z_2 + c_8 Z_1 Z_3 + c_9 Y_0 Y_1 Y_2 Y_3 + c_{10} X_0 X_1 X_2 X_3 \\ & + c_{11} Y_0 Y_1 X_2 X_3 + c_{1,2} X_0 X_1 Y_2 Y_3 + c_{13} Y_0 X_1 Y_2 X_3 \\ & + c_{14} X_0 Y_1 X_2 Y_3 + c_{15} X_0 Y_1 Y_2 X_3 + c_{16} Y_0 X_1 X_2 Y_3,\end{aligned}$$

Luckily, this can be automated in Qiskit and other packages!

Quantum Lanczos in real time

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^{8}Be in full 0p-shell

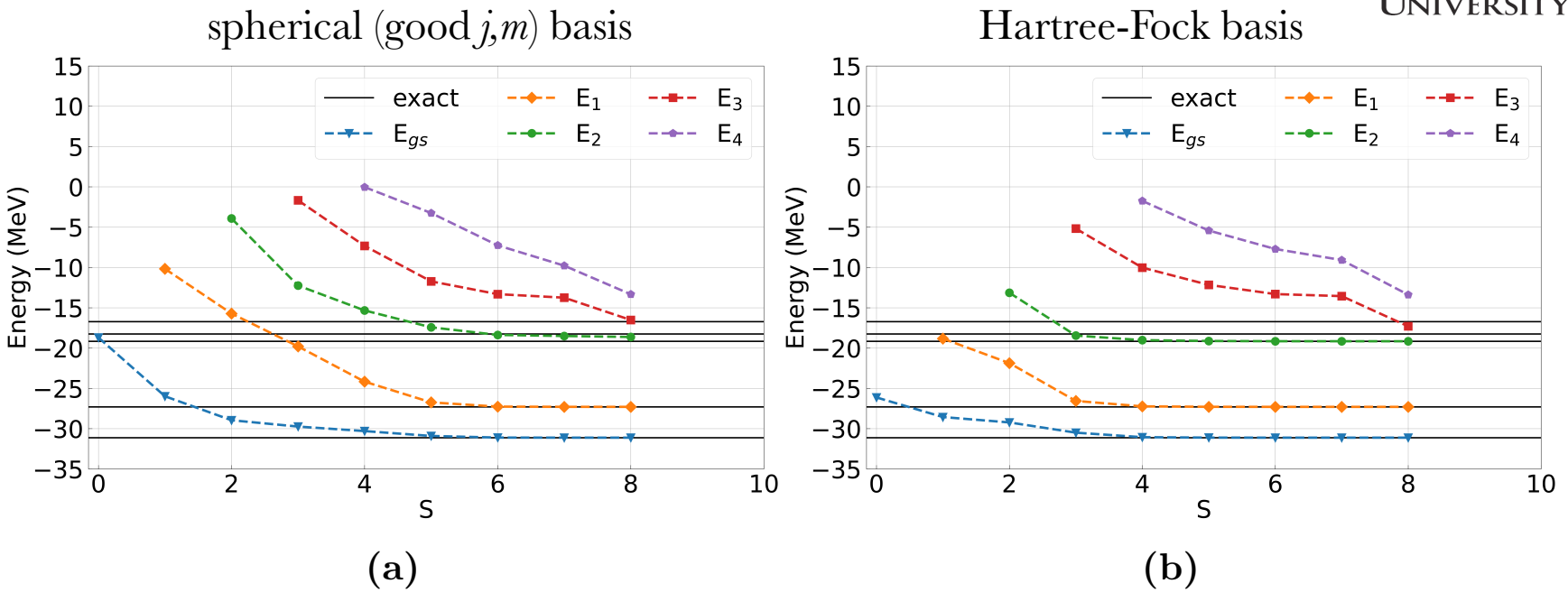

Figure 8.1. Numerical simulations of the QLanczos algorithm with exact real-time evolution to solve for the lowest five energy states of the valence particles of ^{8}Be (two protons and two neutrons in the full p-shell). The simulation was run using a single reference state; (a) the lowest energy configuration in the spherical basis and (b) the Hartree-Fock state. A fixed number of real-time evolution iterations was used ($S = 8$) with a time step size of $\Delta t = 0.1$.

Quantum Lanczos in real time

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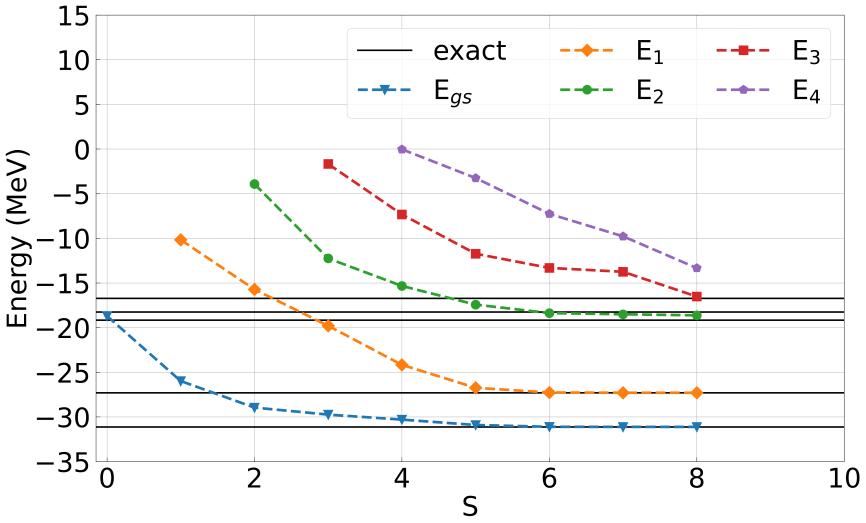
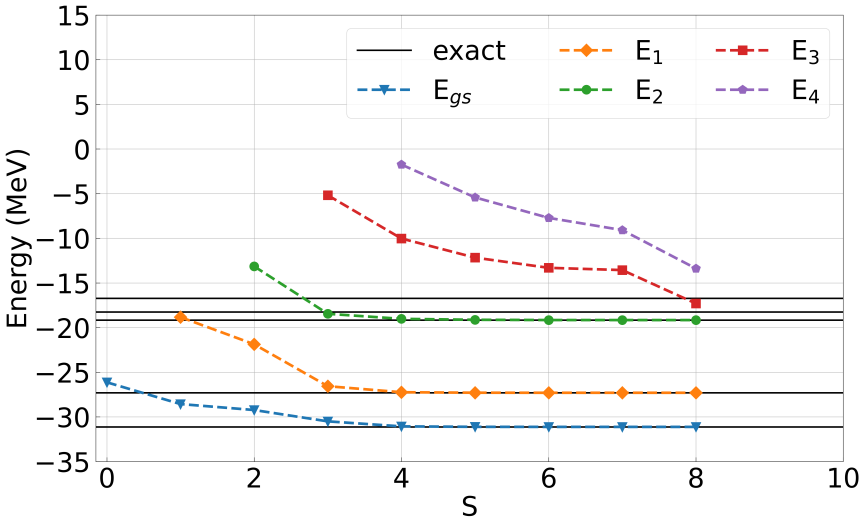
^{8}Be in full 0p-shell

spherical (good j,m) basis



Hartree-Fock basis



H requires 975 Pauli strings and ~ 24,000 gates

H requires 2,431 Pauli strings and ~ 61,000 gates

Fi … tir … of … run using a single reference state; (a) the lowest energy configuration in the spherical basis and (b) the Hartree-Fock state. A fixed number of real-time evolution iterations was used ($S = 8$) with a time step size of $\Delta t = 0.1$.

Quantum Lanczos in real time

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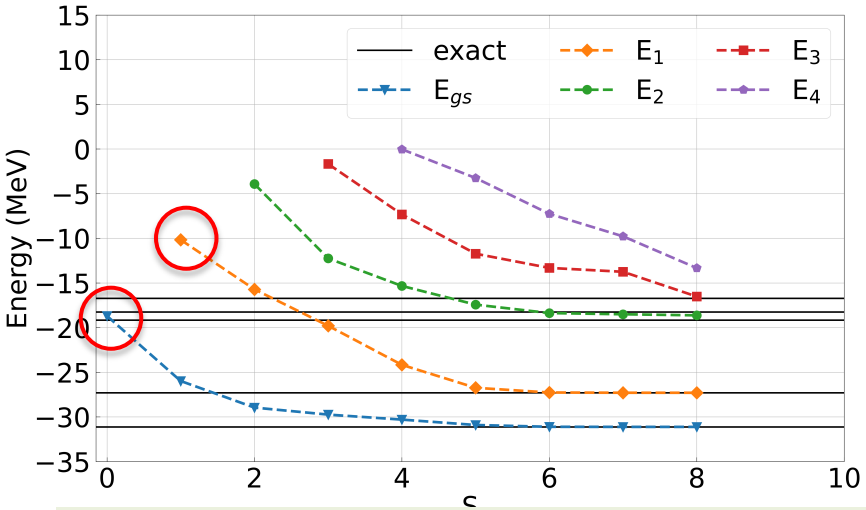

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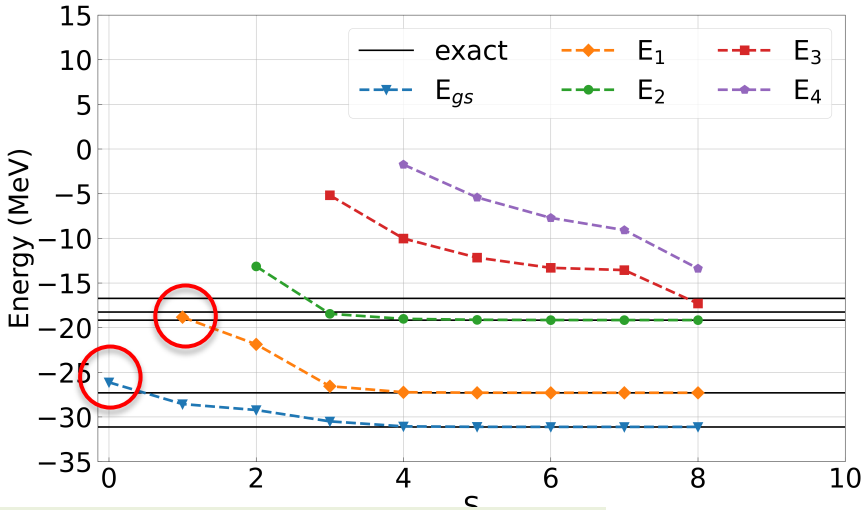

This is very similar to classical Lanczos:
the choice of initial reference state (pivot)
can affect the convergence of the first 1-3 states
but soon has no effect

Fig… …n exact real-time… …nce particles of… …ulation was ru… …ation in the spherical basis and (b) the Hartree-Fock state. A fixed number of real-time evolution iterations was used ($S = 8$) with a time step size of $\Delta t = 0.1$.

Quantum Lanczos in real time

SAN DIEGO STATE UNIVERSITY

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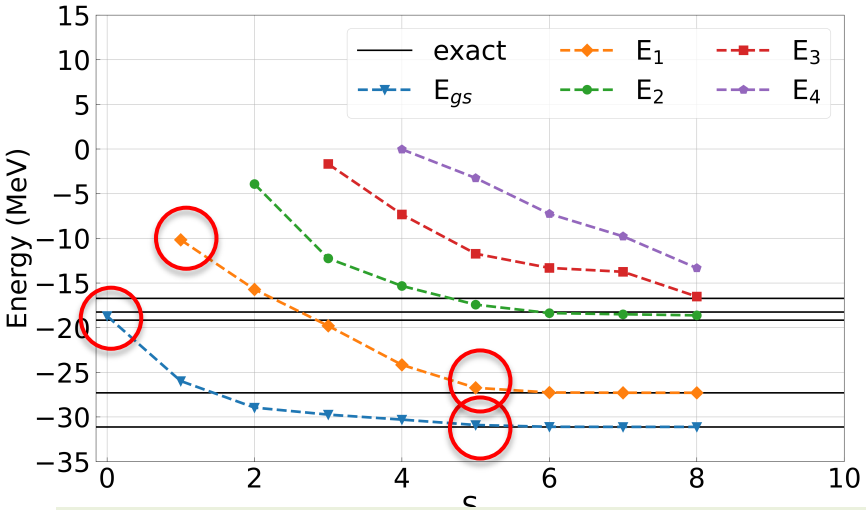

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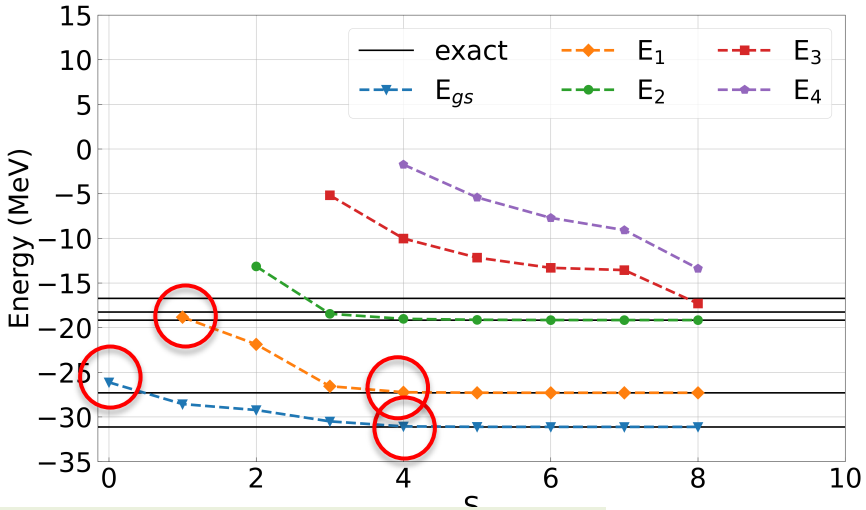

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Quantum Lanczos in real time

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We can investigate the importance of Trotterization

$$e^{-i\hat{H}\Delta tk} \approx \left(\prod_m e^{-ic_m P_m \Delta tk/N} \right)^N = U_k,$$

example: ^{14}N in 0p$_{1/2}$ -shell

$$\begin{aligned} U_k = & \exp(-ic_0 I \Delta tk) \exp(-ic_1 Z_0 \Delta tk) \exp(-ic_2 Z_1 \Delta tk) \\ & \exp(-ic_3 Z_2 \Delta tk) \exp(-ic_4 Z_3 \Delta tk) \exp(-ic_5 Z_0 Z_3 \Delta tk) \\ & \exp(-ic_6 Z_1 Z_2 \Delta tk) \exp(-ic_7 Z_0 Z_2 \Delta tk) \exp(-ic_8 Z_1 Z_3 \Delta tk) \\ & \exp(-ic_9 Y_0 Y_1 Y_2 Y_3 \Delta tk) \exp(-ic_{10} X_0 X_1 X_2 X_3 \Delta tk) \\ & \exp(-ic_{11} Y_0 Y_1 X_2 X_3 \Delta tk) \exp(-ic_{12} X_0 X_1 Y_2 Y_3 \Delta tk) \\ & \exp(-ic_{13} Y_0 X_1 Y_2 X_3 \Delta tk) \exp(-ic_{14} X_0 Y_1 X_2 Y_3 \Delta tk) \\ & \exp(-ic_{15} X_0 Y_1 Y_2 X_3 \Delta tk) \exp(-ic_{16} Y_0 X_1 X_2 Y_3 \Delta tk) \end{aligned}$$

Quantum Lanczos in real time

SAN DIEGO STATE UNIVERSITY

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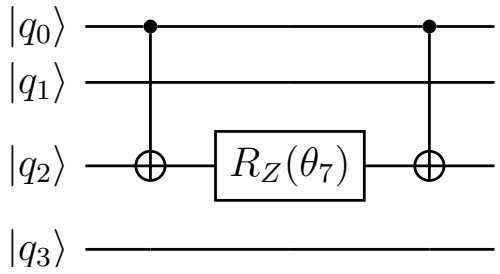
example: ^{14}N in 0p$_{1/2}$ -shell

For example, the circuit to compute $\exp(-ic_7 Z_0 Z_2 \Delta tk)$, is



where $\theta_7 = c_7 \Delta tk$.

Quantum Lanczos in real time

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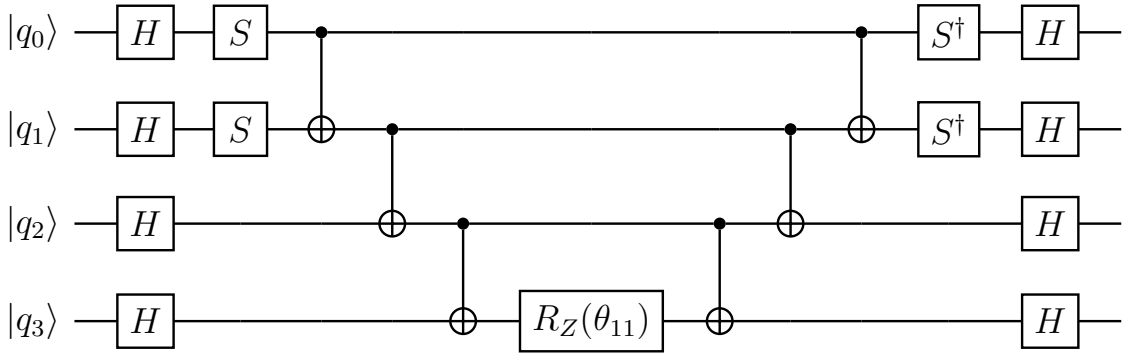
We can investigate the importance of Trotterization

$$e^{-i\hat{H}\Delta tk} \approx \left(\prod_m e^{-ic_m P_m \Delta tk/N} \right)^N = U_k,$$

example: ^{14}N in 0p$_{1/2}$ -shell

For example, the circuit for $\exp(-ic_{11}Y_0Y_1X_2X_3\Delta tk)$, is



where $\theta_{11} = c_{11}\Delta tk$.

Quantum Lanczos in real time

^{8}Be in full 0p-shell

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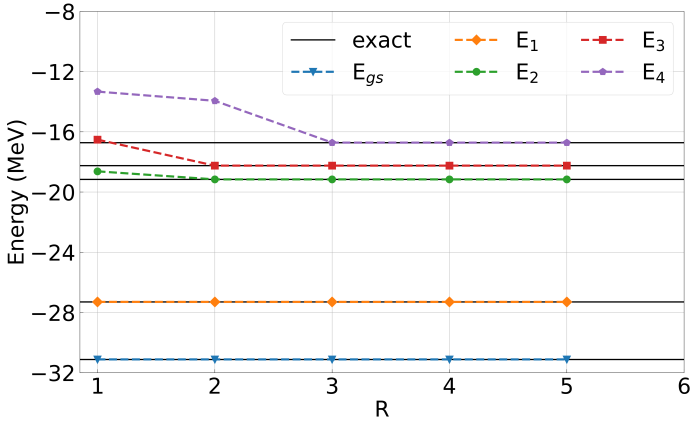
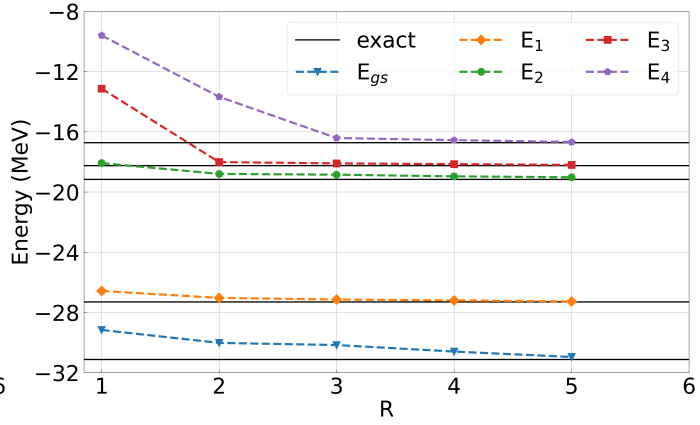
exact time evolution

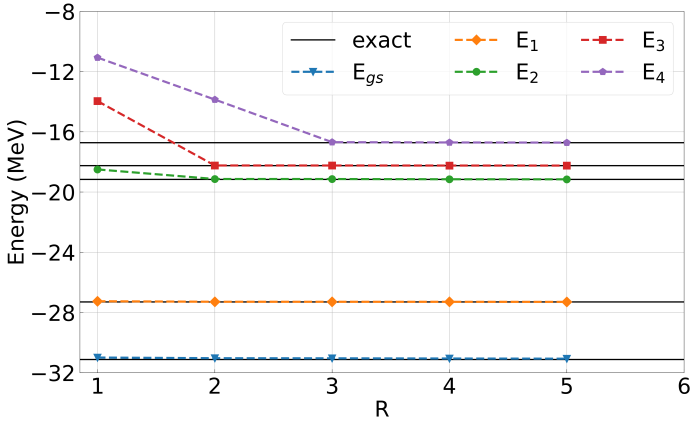


(a)

Trotter steps = 1

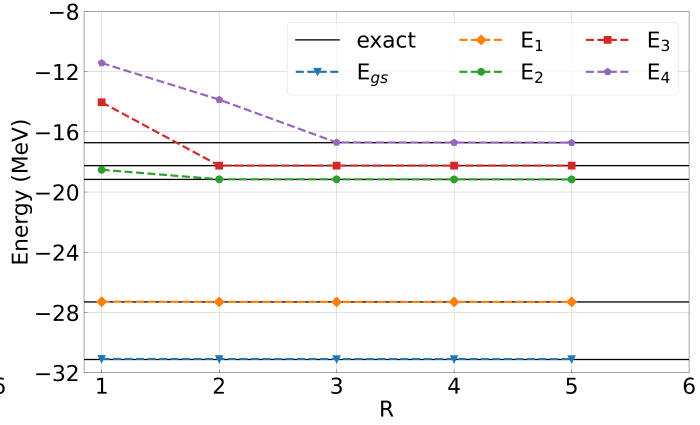


(b)



Trotter steps = 4

(c)



(d)

Trotter steps = 8

$\Delta t = 0.1\ \text{MeV}^{-1}$

R = # of reference states
S = # of iterations = 8

Quantum Lanczos in real time

^{8}Be in full 0p-shell

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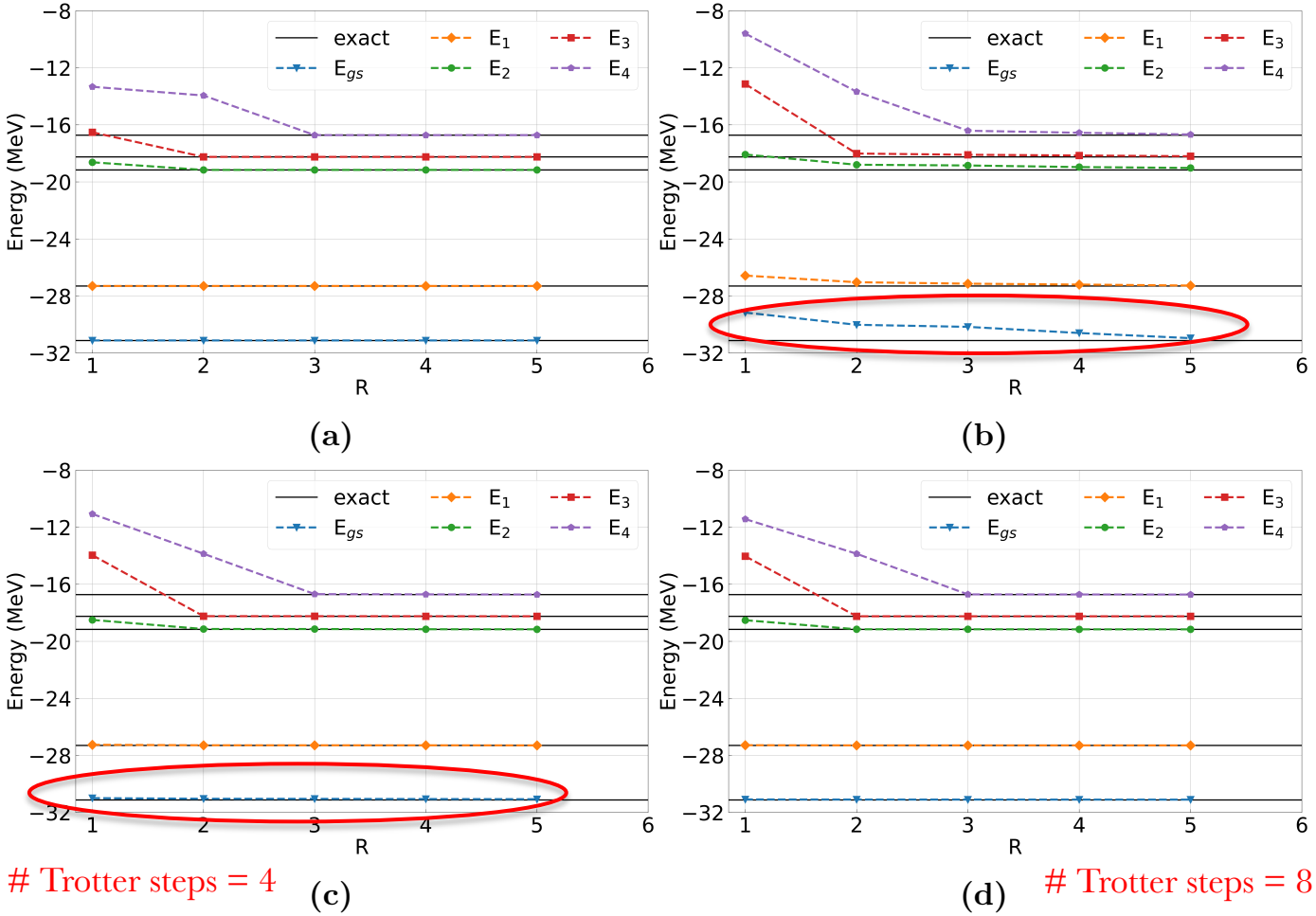
exact time evolution

Trotter steps = 1



Trotter steps = 4

Trotter steps = 8

$\Delta t = 0.1$ MeV^{-1}

R = # of reference states
S = # of iterations = 8

For this Δt,
2-4 Trotter steps
seems optimal

Quantum Lanczos in real time

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Lanczos on a classical computer

Comparison of real- and imaginary-time evolution with synthetic data (working in eigenbasis)

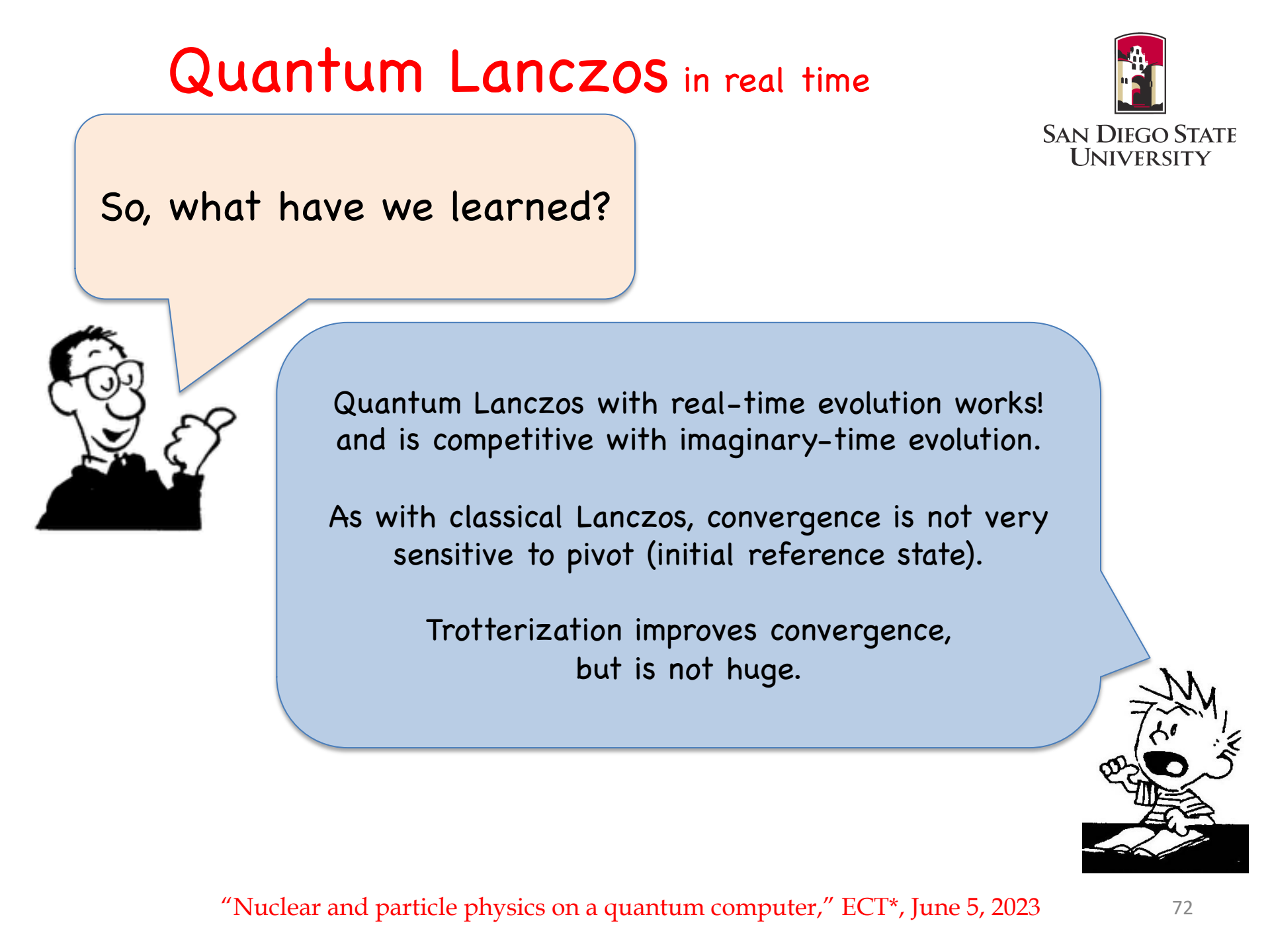
Partial emulation using bit & Pauli string representation

Full Qiskit emulation — Not done

Run on quantum computer — Not done

^{8}Be in full 0p shell requires 975 Pauli strings and ~ 24,000 gates

Quantum Lanczos in real time

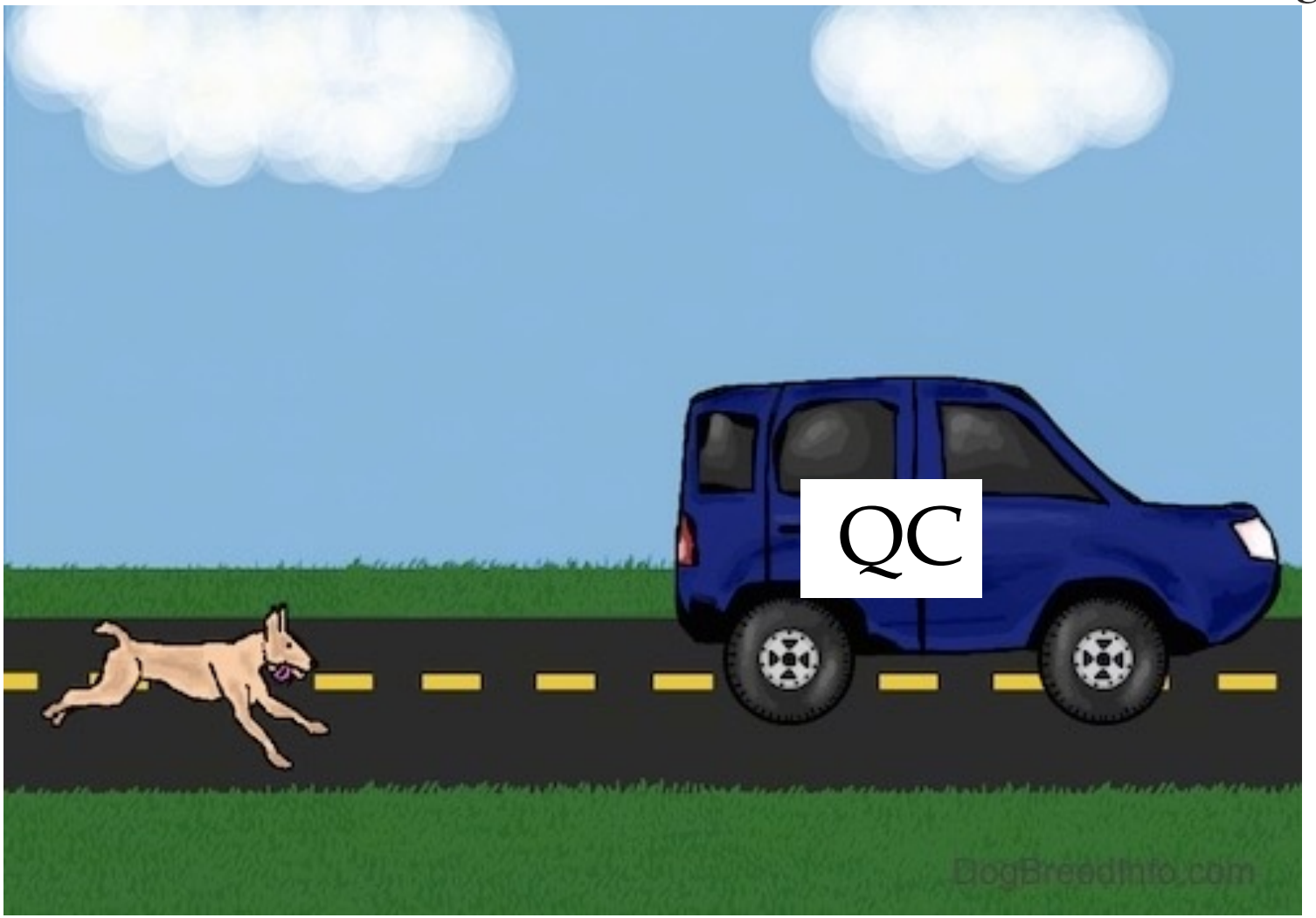


So, what have we learned?

Quantum Lanczos with real-time evolution works!
and is competitive with imaginary-time evolution.

As with classical Lanczos, convergence is not very sensitive to pivot (initial reference state).

Trotterization improves convergence,
but is not huge.


QC

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Let's look at the data requirements in more detail

Consider ^{12}C, $N_{max}=8$

M-scheme dimension 0.6 billion

55 single-particle orbitals (n l j)
440 single particle states (n l j m) | 0 1 1 0 0 1 … >

Let's look at the data requirements in more detail

Consider ^{12}C, $N_{max}=8$

M-scheme dimension 0.6 billion

55 single-particle orbitals (n l j)
440 single particle states (n l j m) | 0 1 1 0 0 1 … >

= estimate # of qubits needed

Let's look at the data requirements in more detail

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Consider ^{12}C, $N_{max}=8$

M-scheme dimension 0.6 billion

 # J-coupled 2-body matrix elements: ~ 1.5 million

$< a\ b\ J\ |\ H\ |\ c\ d\ J >$

 # uncoupled 2-body matrix elements ~ 10 million

$V_{ijkl}\ a^+_i\ a^+_j\ a_l\ a_k$

 # many-body matrix elements: ~ 1.2 trillion

(or 5 Tb storage)

Let's look at the data requirements in more detail

SAN DIEGO STATE UNIVERSITY

Consider ^{12}C, $N_{max}=8$

M-scheme dimension 0.6 billion *by superposition*

~~*# J-coupled 2-body matrix elements*: ~ 1.5 million~~
~~< a b J | H | c d J >~~ *input*

***# uncoupled 2-body matrix elements* ~ 10 million!** $\mathbf{V_{ijkl}\ a^+_i\ a^+_j\ a_l\ a_k}$ = # 'Pauli strings'

~~*# many-body matrix elements:* ~ 1.2 trillion~~
~~(or 5 Tb storage)~~ *not relevant?*

Let's look at the data requirements in more detail

SAN DIEGO STATE UNIVERSITY

Consider ^{12}C, $N_{max}=8$

M-scheme dimension 0.6 billion *by superposition*

 # uncoupled 2-body matrix elements ~ 10 million! $\mathbf{V_{ijkl}\ a^{+}_{i}\ a^{+}_{j}\ a_{l}\ a_{k}}$ = # 'Pauli strings'
= # of terms to be evaluated in a quantum circuit
(or, # of separate quantum circuits to be evaluated!)

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We're still a long ways from catching the car we want!

Lessons learned

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Quantum computing requires a new way of thinking—how to use unitary transformation as the basis for *processing*

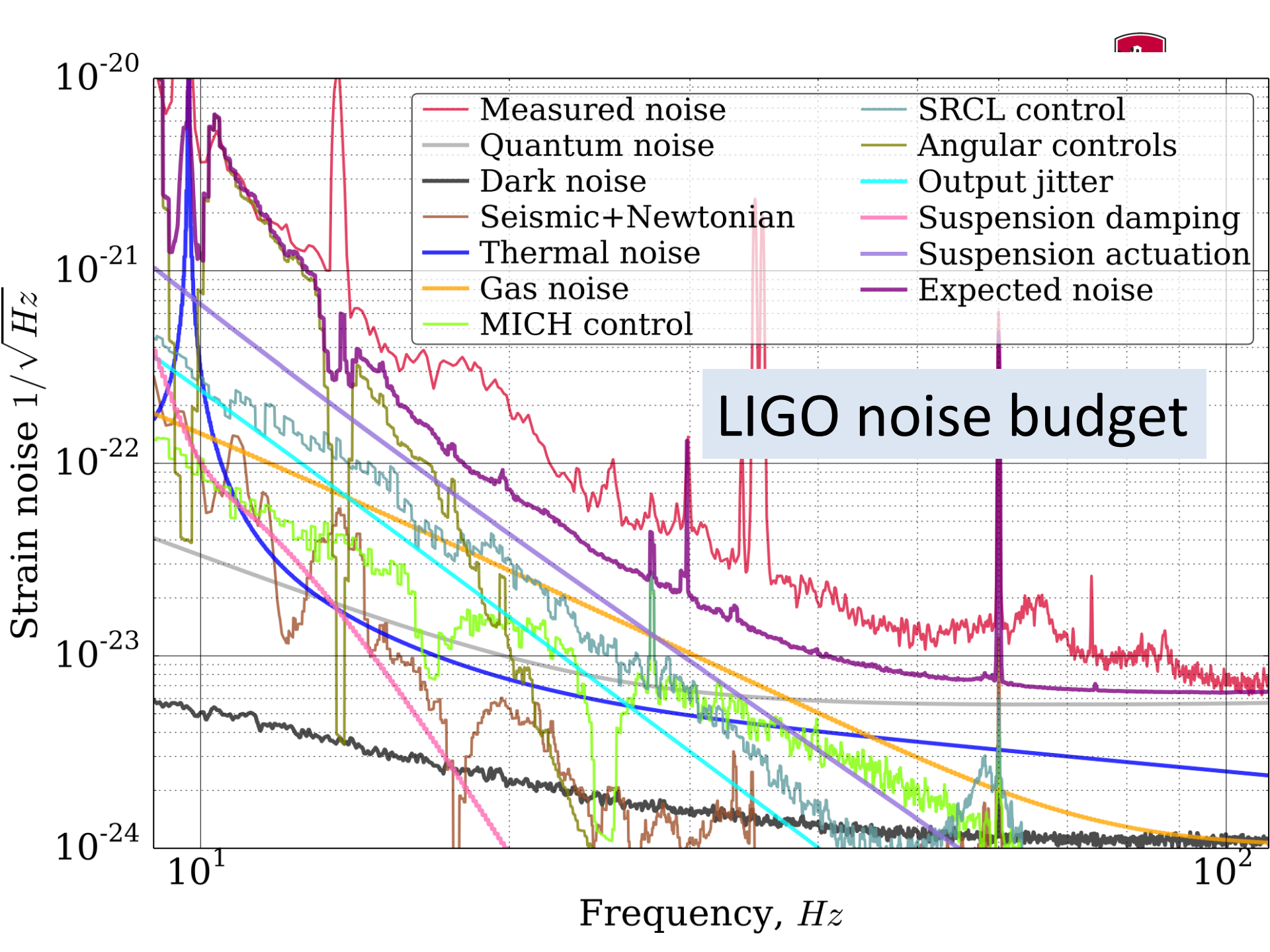
The eigenpair problem is important in nuclear and other fields—on classical machines, the **Lanczos algorithm** is often the method of choice.

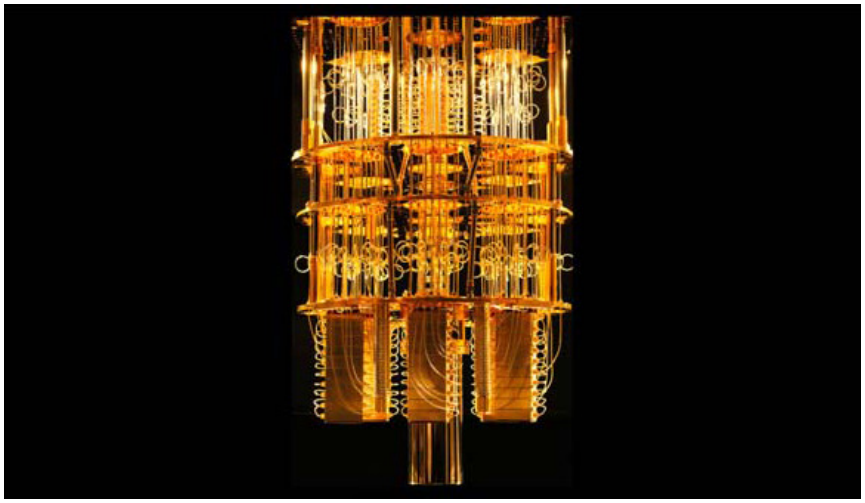
A **real-time version** of the quantum Lanczos algorithm works well and can compete with the imaginary-time version.

Multiple reference states improves performance; so does modest Trotterization.

To tackle problems our community cares about, we will need on the order of $> 10^{5\text{-}7}$ logical qubits (with error correction, $10^{6\text{-}9}$ physics qubits)

Nonetheless, science has stared down seemingly insurmountable challenges before


Measured noise
Quantum noise
Dark noise
Seismic+Newtonian
Thermal noise
Gas noise
MICH control
SRCL control
Angular controls
Output jitter
Suspension damping
Suspension actuation
Expected noise
LIGO noise budget
Strain noise $1/\sqrt{Hz}$
10^{-20}
10^{-21}
10^{-22}
10^{-23}
10^{-24}
10^{1}
10^{2}
Frequency, Hz



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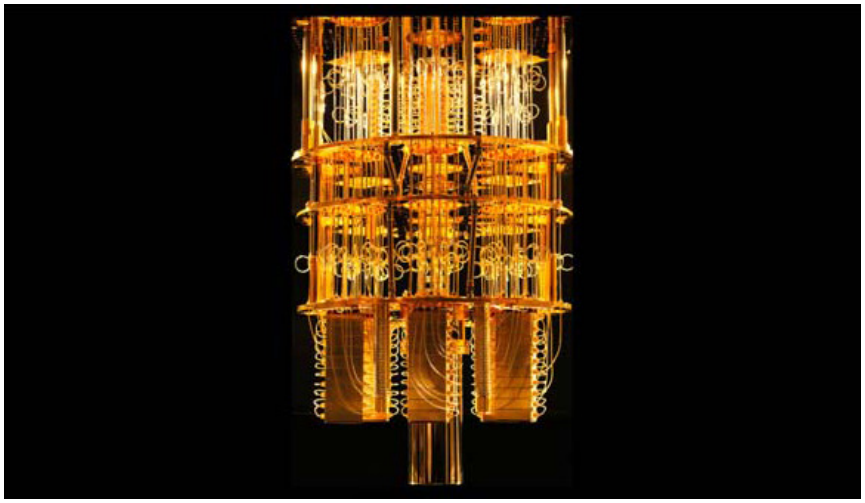

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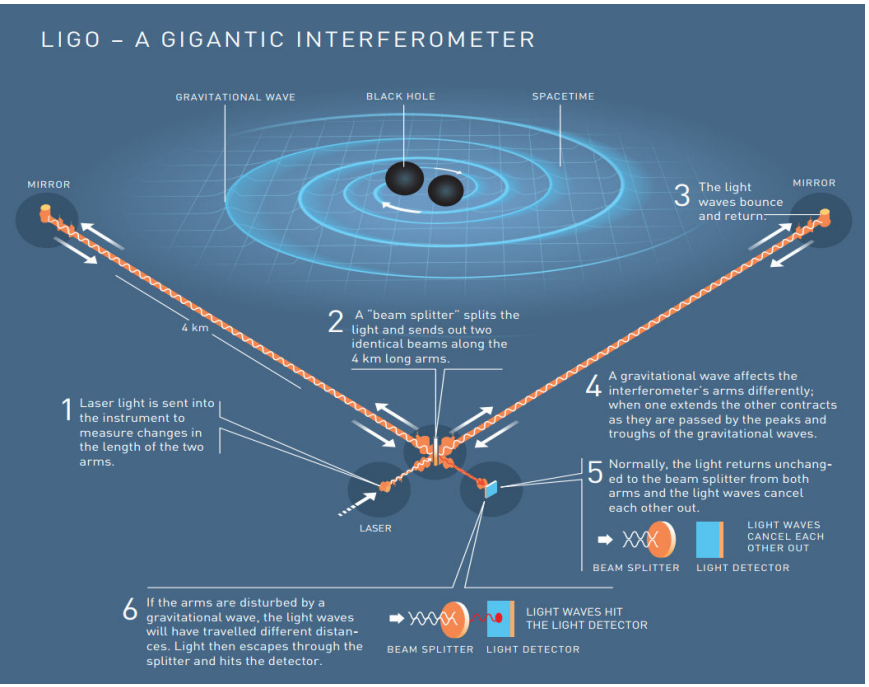
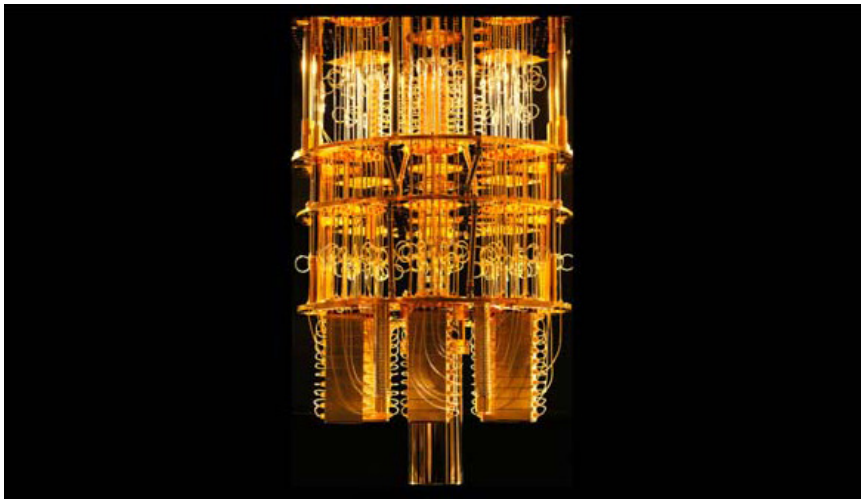

LIGO – A GIGANTIC INTERFEROMETER
GRAVITATIONAL WAVE
BLACK HOLE
SPACETIME
MIRROR
MIRROR
3 The light waves bounce and return.
4 km
2 A "beam splitter" splits the light and sends out two identical beams along the 4 km long arms.
1 Laser light is sent into the instrument to measure changes in the length of the two arms.
4 A gravitational wave affects the interferometer's arms differently; when one extends the other contracts as they are passed by the peaks and troughs of the gravitational waves.
5 Normally, the light returns unchanged to the beam splitter from both arms and the light waves cancel each other out.
LASER
LIGHT WAVES CANCEL EACH OTHER OUT
BEAM SPLITTER
LIGHT DETECTOR
6 If the arms are disturbed by a gravitational wave, the light waves will have travelled different distances. Light then escapes through the splitter and hits the detector.
LIGHT WAVES HIT THE LIGHT DETECTOR
BEAM SPLITTER
LIGHT DETECTOR



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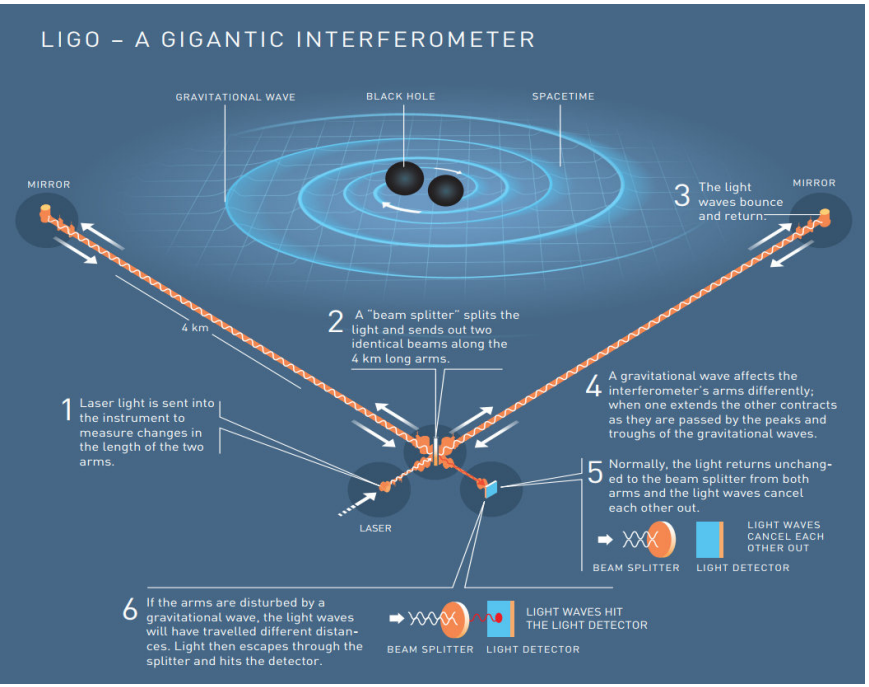
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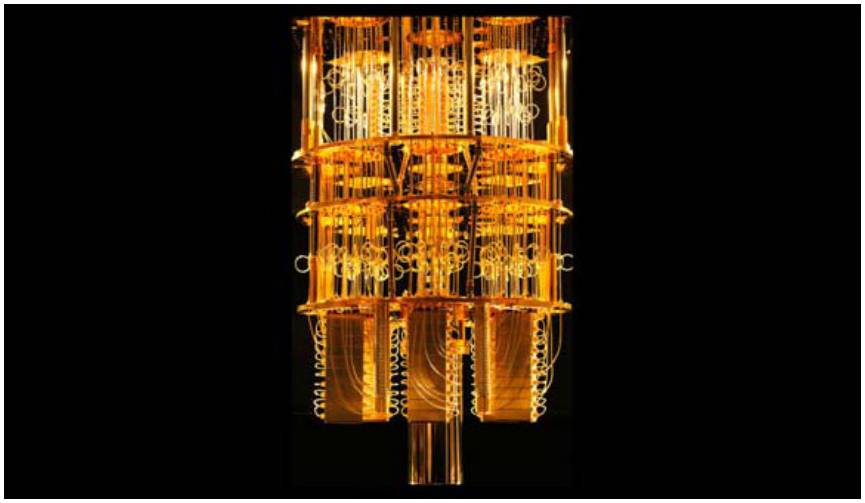
or



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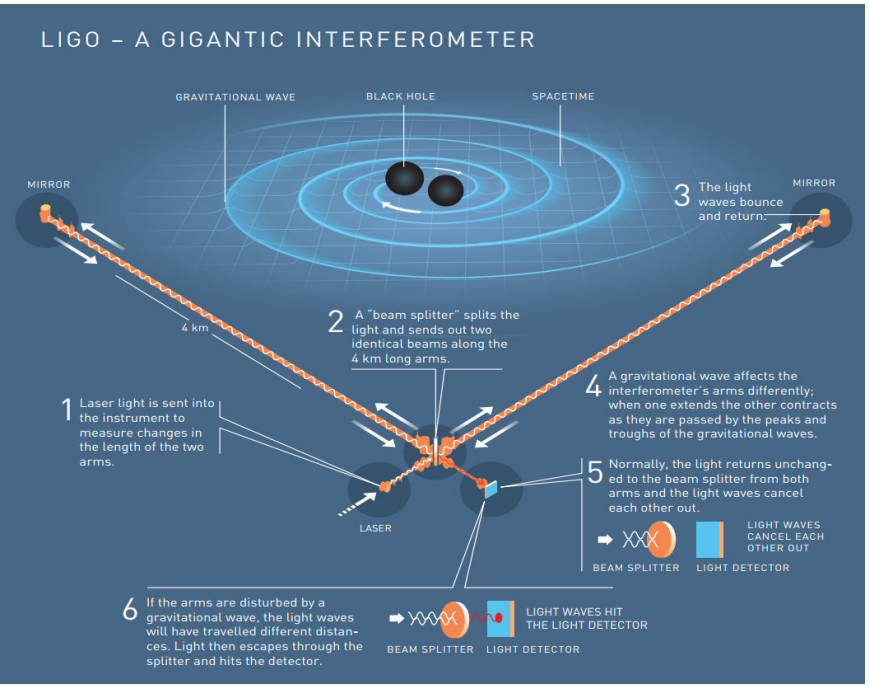
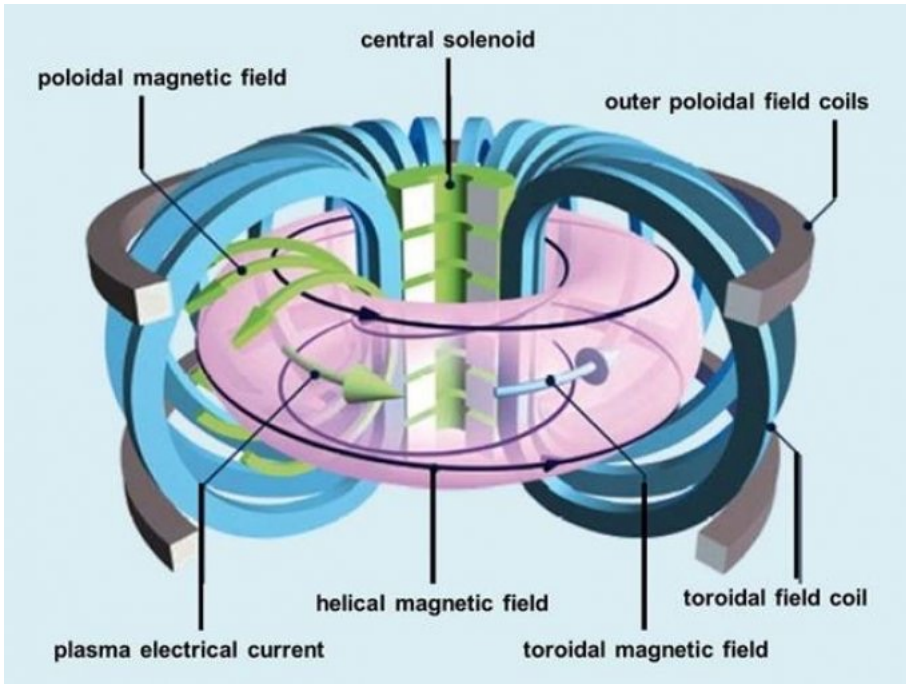


or



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