# Solving Nuclear Structure Problems with the Adaptive Variational Quantum Algorithm

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With A. Romero Marquez, S. Economou, H.L. Tang

September 13, 2022

# Quantum Computing in the NISQ[1] Era

Quantum computers perform unitary transformations on qubits, so given an initial state $|\Psi(0)\rangle$ and a mapping, they can evaluate the unitary transformation

$$|\Psi(t)\rangle = e^{-iHt} |\Psi(0)\rangle \ .$$

They can also find eigenvalues through a unitary "phase estimation" circuit. The problem? Need to implement the transformation in hardware.

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Though time evolution and phase estimation can be implemented with few qubit gates, you need a lot of them chained together, a deep circuit that maintains coherence.

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## Variational Method

- Construct ground-state ansatz

  $$|\Psi\rangle = U(\theta_1, \theta_2, \ldots, \theta_N)\,|\Psi_0\rangle \ ,$$

  that depends on parameters $\theta_i$.
  $|\Psi_0\rangle$ is some simple state.

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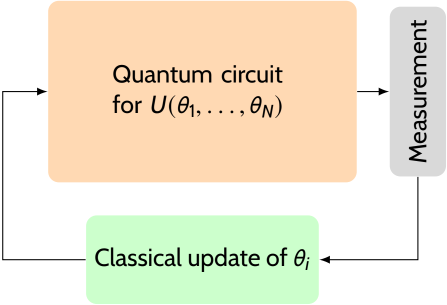
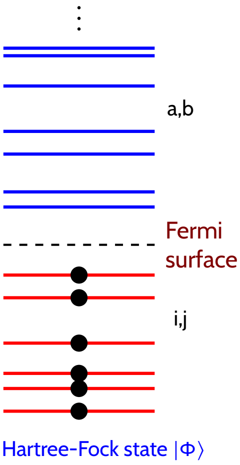
## Hybrid Implementation



# Ansätze for Many-Body Problem

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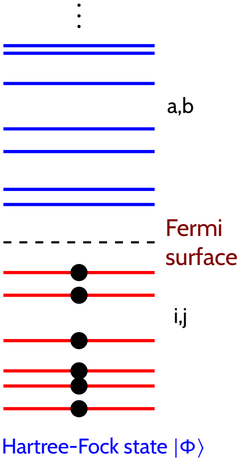


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Typical of the latter is "unitary coupled clusters."

$$|\Psi\rangle = e^{T-T^\dagger}\,|\Phi\rangle$$

$$T = \sum_{ia} t_i^a a_a^\dagger a_i + \sum_{iajb} t_{ij}^{ab} a_a^\dagger a_b^\dagger a_j a_i + \ldots .$$

(Series for $T$ but has to be truncated somewhere.)

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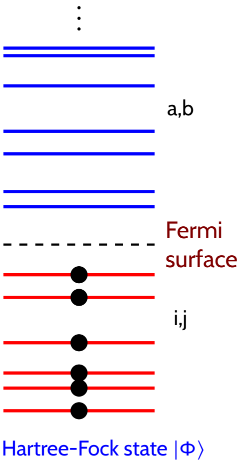


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Unfortunately, the first kind is limited by hardware, and the second, usually, to systems that aren't too strongly correlated.

# ADAPT-VQE

Grimsley, Economou, Barns, and MayHall, Nature Comm. 10:3007 (2019)

Want a procedure capable of producing the exact ground state.

Ansatz:

Iteration 1: $|\Psi\rangle = e^{-i\theta_1 A_1} |\Psi_0\rangle$

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$A_1, A_2 \ldots$ are all operators of the form $a_\alpha^\dagger a_\beta$ and $a_\alpha^\dagger a_\beta^\dagger a_\gamma a_\delta$.

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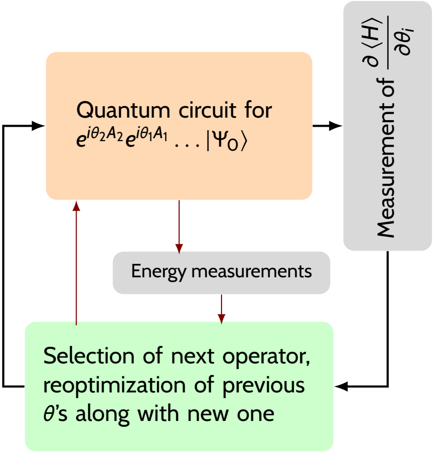

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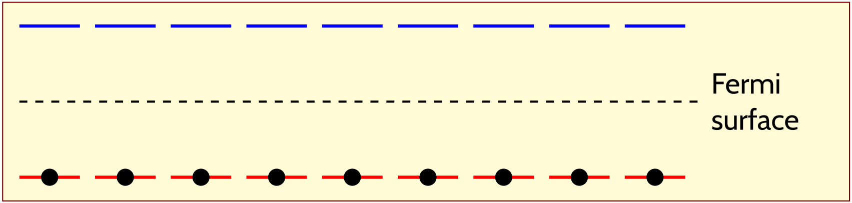
Want to understand, how efficiency of ADAPT-VQE scales with $N$.
Investigate with simple solvable model of nuclear interactions.



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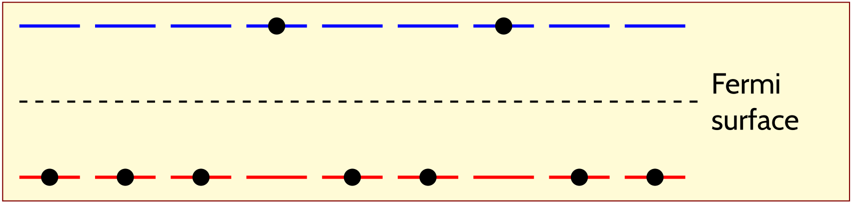

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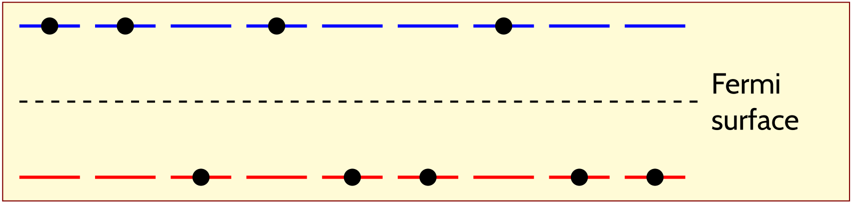

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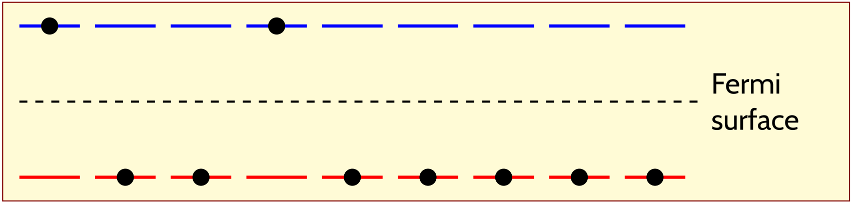

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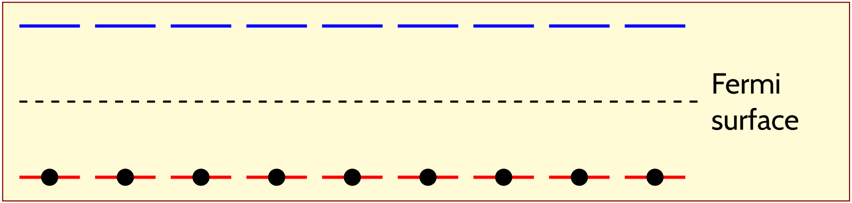


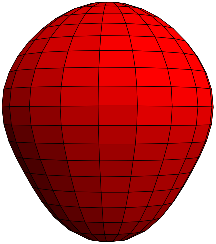

Equivalent to a set of spins with Hamiltonian:

$$\begin{aligned} H &= \varepsilon J_z - \frac{1}{2} V \left( J_+^2 + J_-^2 \right) \\ &= \frac{\varepsilon}{2} \sum_{i=1}^{N} \sigma_{i,z} - \frac{1}{8} V \sum_{i,j=1}^{N} \left( \sigma_{i,+}\sigma_{j,+} + \sigma_{i,-}\sigma_{j,-} \right) \end{aligned}$$

All spins interact with the same strength.

# Spontaneous Symmetry Breaking in Nuclear Structure

Example: Parity in octupole-deformed systems



Calculated $^{225}$Ra density

Parity is broken spontaneously in mean-field theory, which gives good description of "intrinsic state," but contains only a single orientation for that shape.

To work with this wave function you have to first "restore" reflection symmetry.

# Symmetry Restoration

When intrinsic state $|$$\rangle$ is asymmetric, it breaks parity.

To get states with good parity, we superpose the intrinsic state and its reflection:

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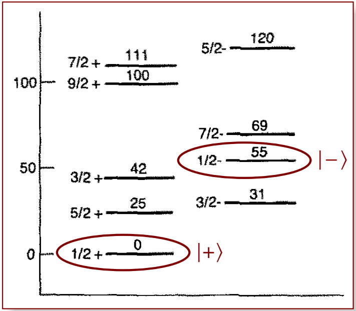

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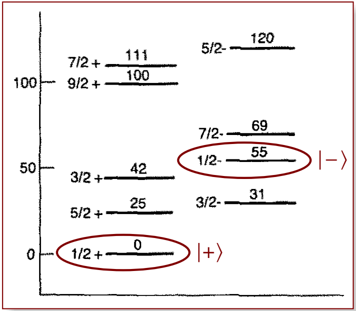


In a variational calculation you can restore symmetry — also called “projecting” onto states with good quantum numbers — after energy minimization (PAV) or before the variation, in the ansatz itself (VAP).

The second method harder but gives better results.

# Symmetry Breaking in Lipkin Model

*H* excites particles in pairs, so

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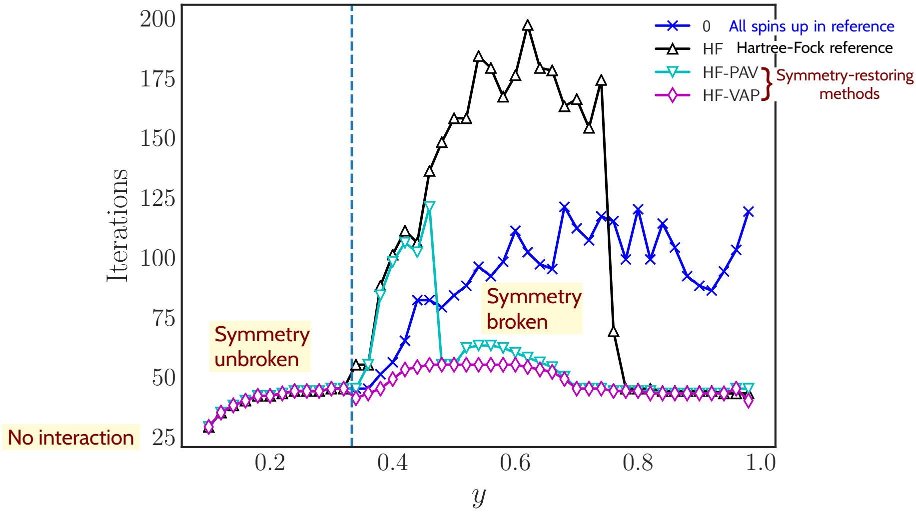
How does the transition affect ADAPT-VQE's efficiency?

Does it help to restore the symmetry explicitly?

# Results on Symmetry Breaking

From Antonio Marquéz Romero

$$y = \left(1 + \frac{\varepsilon}{(N-1)V}\right)^{-1}, \quad N = 10$$



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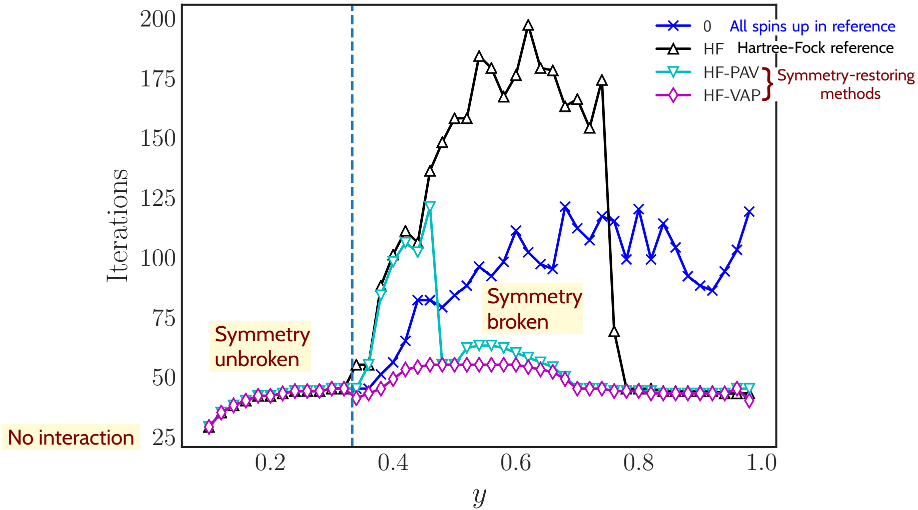
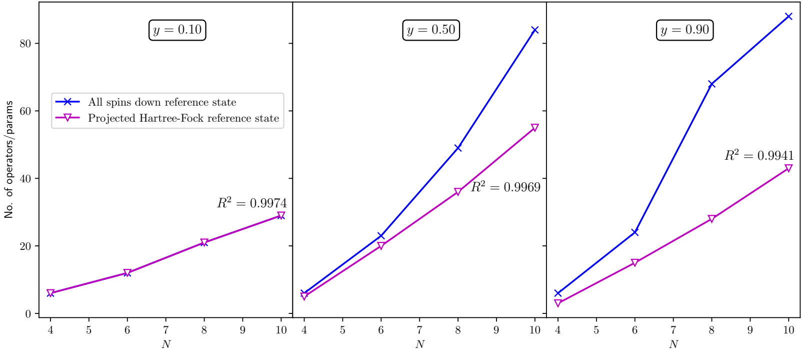



Symmetry-breaking reference state and symmetry restoration help!

# Results on Scaling



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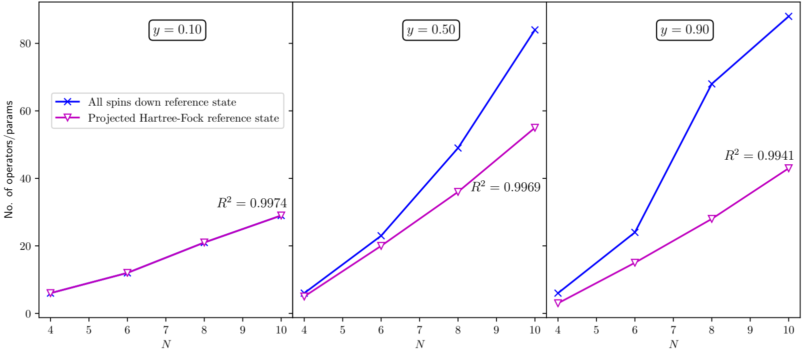


Our best method scales linearly in *N*!

That's promising. What about the effects of noise?

# Effects of Noise

Qiskit custom noise models:

Weak: 10% depolarizing gate-error rate, plus shot noise

Strong: 20% depolarizing gate-error rate, plus shot noise

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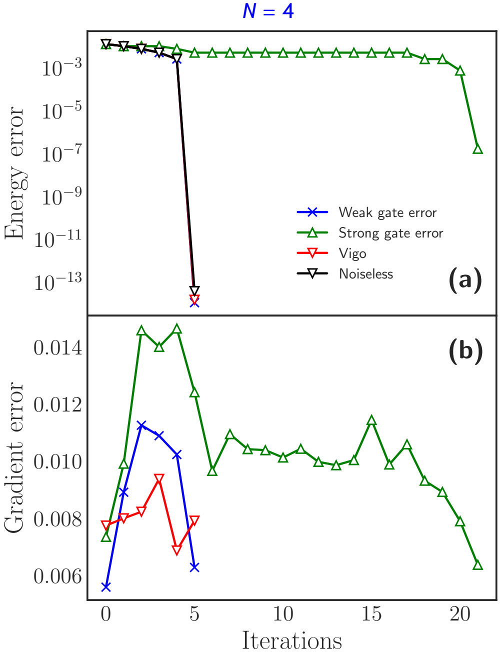
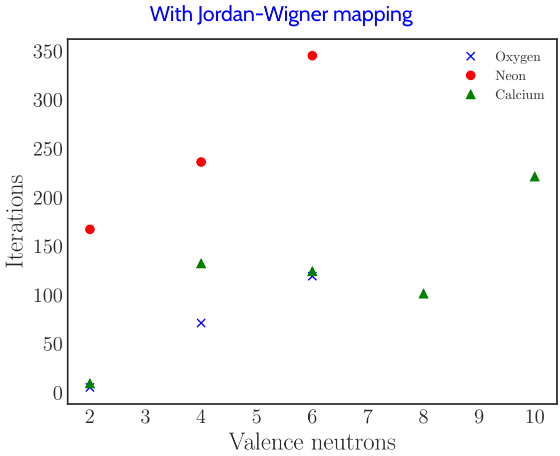
Qiskit Vigo: Noise from actual device, includes measurement error.



# Scaling in the Shell Model




Not as orderly, but still quite mild.

We haven't yet tried breaking symmetries or looking at noise.

# Finally …

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Thanks for listening!