Quantum Computing and the Shell Model

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Quantum Bits

Can use any two-state system, e.g. the spin of an electron:

$$|\uparrow\rangle \rightarrow |0\rangle$$

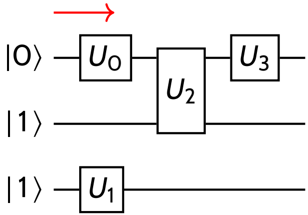
$$|\downarrow\rangle \rightarrow |1\rangle$$

An N-qubit "register" has 2^N "computational-basis" states, e.g.

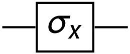
$$|1\rangle\,|1\rangle\,|0\rangle\,|1\rangle\,|0\rangle\,|0\rangle\,|0\rangle\,\ldots$$

Circuit Model

Computer acts on qubits or sets of qubits ("wires") with sequence of unitary transformations ("gates"), e.g.:



Some common gates:

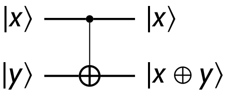


Not

$$\sigma_x\,|0\rangle = |1\rangle$$
$$\sigma_x\,|1\rangle = |0\rangle$$

Hadamard

$$H\,|0\rangle = \frac{1}{\sqrt{2}}\left(|0\rangle + |1\rangle\right)$$



Controlled not

Flips bottom bit if top bit is 1

Mapping States

Any simulation requires a mapping of qubits onto physical states. Qubits are two-state systems, just like spins, so the mapping to spins is straightforward.

Fermions orbitals — full or empty — are similar, but a little more complicated because of the Pauli exclusion principle.

Basic idea: $|0\rangle$ represents an empty orbital, $|1\rangle$ an occupied one.

$$a_i^\dagger \approx \sigma_-^{(i)}$$

To incorporate antisymmetry, need something more complicated, e.g., Jordan-Wigner mapping:

$$a_i^\dagger = \sigma_z^{(1)} \sigma_z^{(2)} \ldots \sigma_z^{(i-1)} \sigma_-^{(i)}$$

Hybrid Algorithms

One idea for reducing depth of circuits — the "Variational Quantum Eigensolver" (VQE) — is to offload some of the computation onto a classical computer.

Variational Method

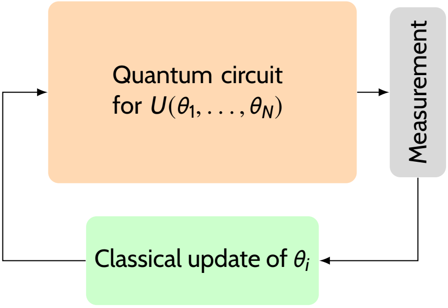
- Construct ground-state ansatz

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

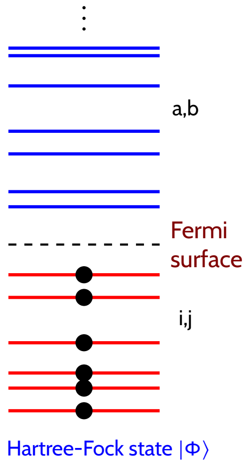
  that depends on parameters θ_i. $|\Psi_0\rangle$ is some simple "reference" state.

- Vary parameters to minimize $\langle\Psi|H|\Psi\rangle$.

Hybrid Implementation



Ansätze for Many-Body Problem



Fall into two categories:

- What the hardware is best at doing
- Good guesses according to many-body physics

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.)

Unfortunately, the first kind is limited by hardware, and the second, often, 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: $|\Psi\rangle = e^{-i\theta_1 A_1} |\Psi_0\rangle$

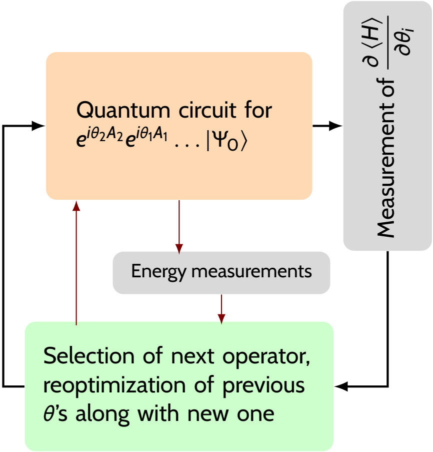
Iteration 2: $|\Psi\rangle = e^{-i\theta_2 A_2} e^{-i\theta_1 A_1} |\Psi_0\rangle$

$\vdots \qquad \vdots$

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

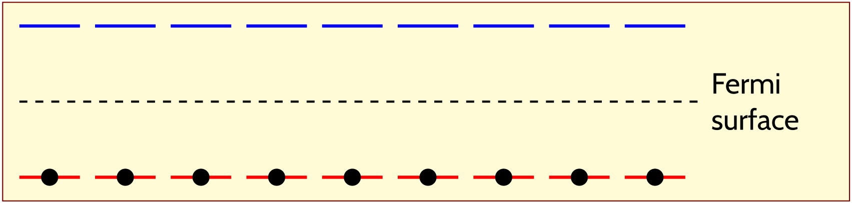
$|\Psi_0\rangle$ is a "reference state," e.g. the Hartree-Fock state $|\Phi\rangle$.

At each iteration select operator A_i that produces largest $\frac{\partial\langle H\rangle}{\partial\theta_i}$ to add to set.



Likpin model

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



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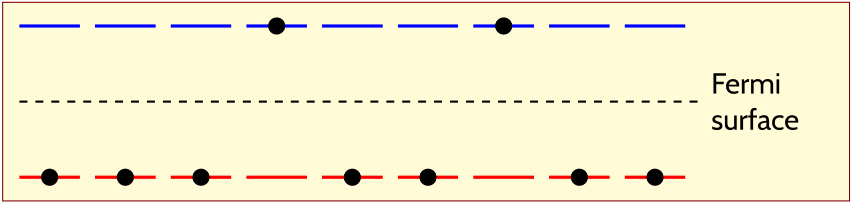

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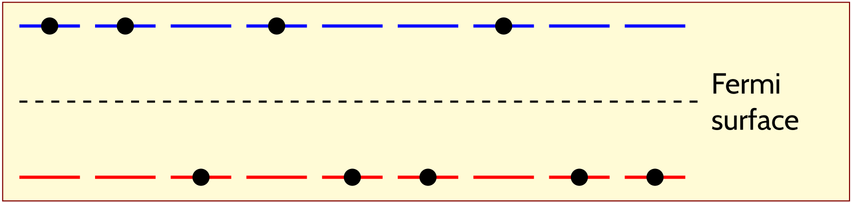

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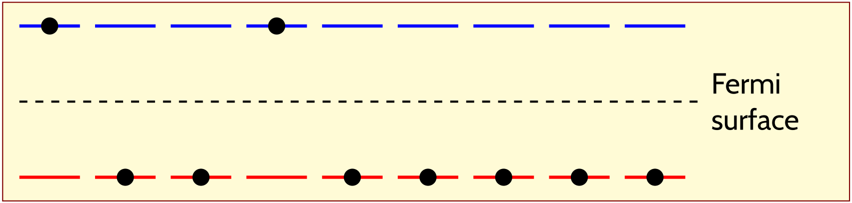

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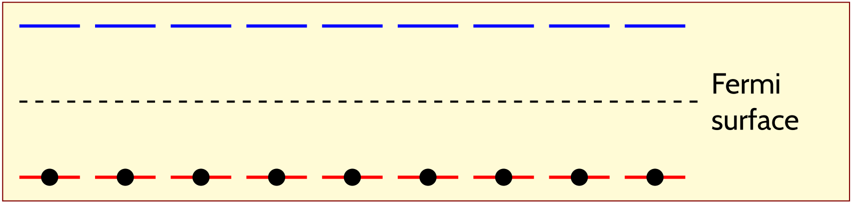


Equivalent to a set of spins with Hamiltonian:

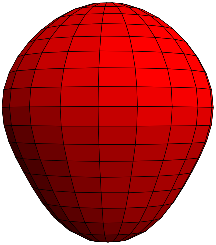
$$H = \varepsilon J_z - \frac{1}{2} V \left(J_+^2 + J_-^2 \right)$$

$$= \frac{\varepsilon}{2} \sum_{i=1}^{N} \sigma_{i,z} - \frac{1}{8} V \sum_{i,j=1}^{N} \left(\sigma_{i,+} \sigma_{j,+} + \sigma_{i,-} \sigma_{j,-} \right)$$

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

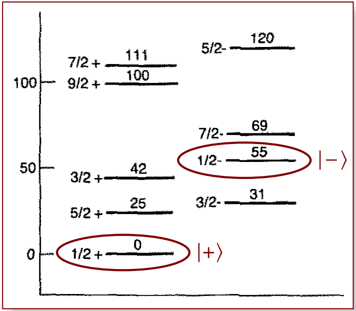
When intrinsic state |⟩ is asymmetric, it breaks parity.

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

$|\pm\rangle = \frac{1}{\sqrt{2}}\Big($ |⟩ ± |⟩ $\Big)$

Symmetric state $|+\rangle$ gains binding energy when symmetry is restored.

Parity Doublet in ^{225}Ra



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

$$\text{“Number Parity”} = (-1)^{\#\text{ excited particles}}$$
$$= (-1)^{\#\text{ up spins}} \quad \text{in spin interpretation}$$

is conserved.

But for large enough *V*, Hartree-Fock state breaks the symmetry: each single-particle state contains both spin-up and spin-down.

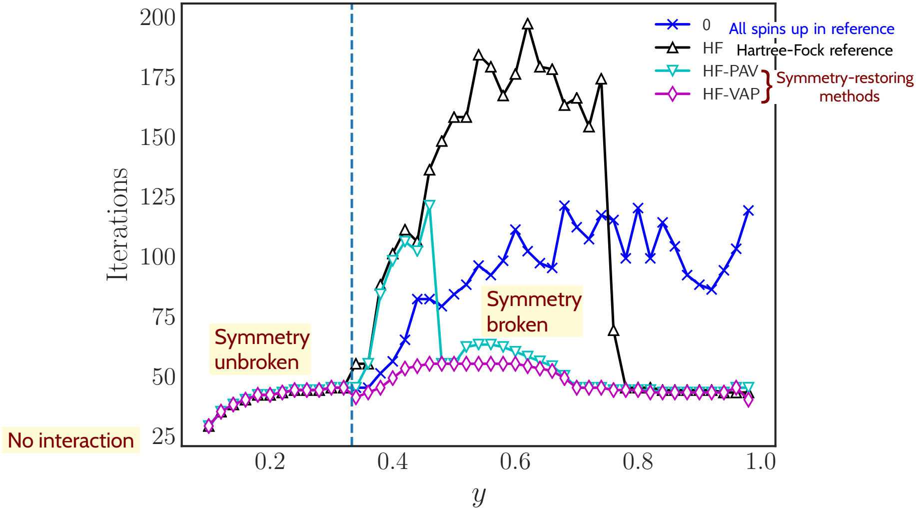
Transition occurs when $V = \varepsilon/(N-1)$.

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

Does it help to restore the symmetry explicitly?

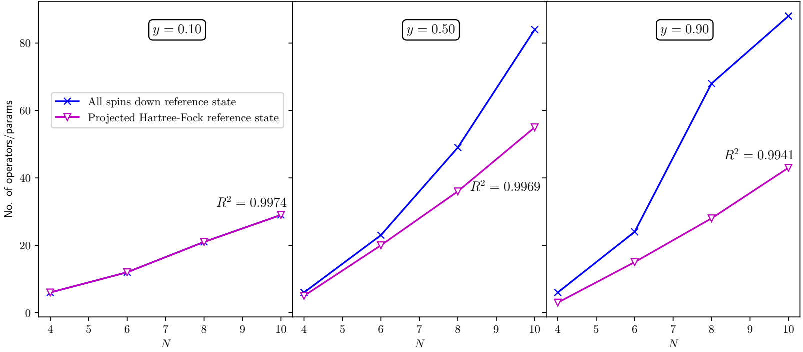
Results on Symmetry Breaking

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



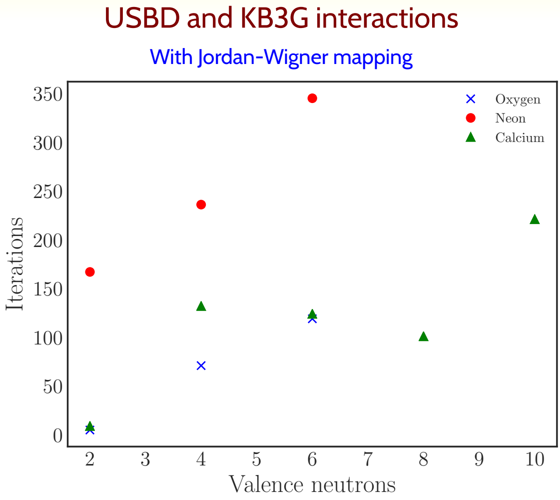
Symmetry-breaking reference state and symmetry restoration help.

Results on Scaling



Best method scales linearly in N

Scaling in the Shell Model



Not as orderly, but still quite mild.

Haven’t yet tried breaking symmetries.

Finally …

- Projection helps.
- Scaling is mild.

After this work, Antonio, Javier, and collaborators investigated shell-model calculations in more detail, designed explicit circuits to implement ADAPT-VQE.

Results are promising, but to get a fixed, nucleus-independent accuracy, need the number of CNOT gates to be roughly proportional to basis size. So no quantum advantage yet.

Still a lot of possible improvements, though.

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Thanks for listening!

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