# Enhancing quantum computers for quantum chemistry

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# Main challenge

Noise effects are particularly detrimental in quantum chemistry calculations

Small changes in parameters can significantly change the result

Therefore, current quantum computers are not very suitable for simulating quantum chemistry

Optimal noise control is obviously the answer, but still far from reach

What can we do in meantime?

Reduce the number of qubits to solve a quantum chemistry problem!

# But can we reduce qubits?

Recently, Dupont et al presented a remarkable proposal to HALVE the number of qubits

**Doubling the size of quantum simulators by entanglement forging**

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Quantum computers are promising for simulations of chemical and physical systems, but the limited capabilities of today's quantum processors permit only small, and often approximate, simulations. Here we present a method, classical entanglement forging, that harnesses classical resources to capture quantum correlations and double the size of the system that can be simulated on quantum hardware. Shifting some of the computation to classical post-processing allows us to represent ten spin-orbitals on five qubits of an IBM Quantum processor to compute the ground state energy of the water molecule in the most accurate simulation to date. We discuss conditions for applicability of classical entanglement forging and present a roadmap for scaling to larger problems.

# What is entanglement forging?

Consider the problem of computing expectation values in a pure quantum state of $2N$ qubits

This problem is at the heart of quantum variational algorithms e.g. Energy minimization for finding ground states.

Start with random state → compute energy → make variations that lower energy → repeat

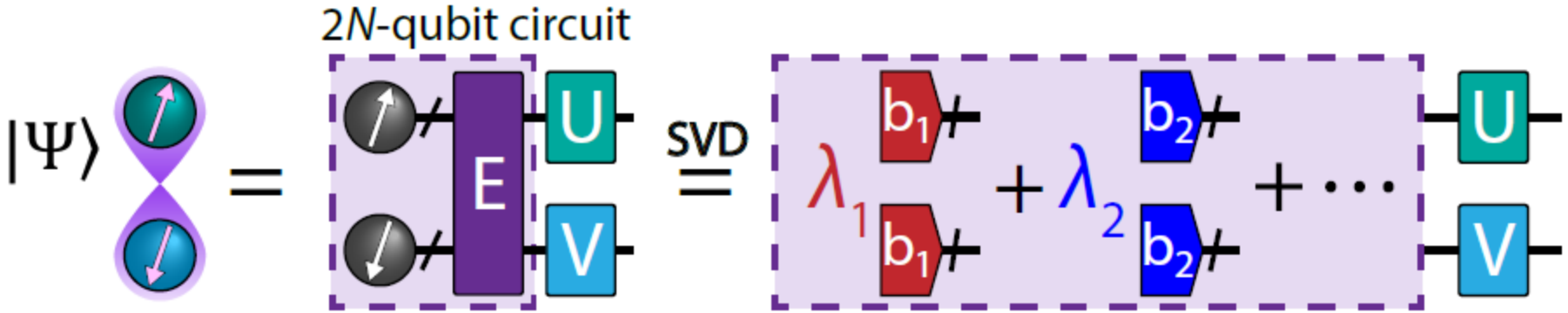
Say, we are interested only in the expectation value of strings of Pauli operators e.g. many interesting Hamiltonians (Ising, Heisenberg)

# What is entanglement forging?

**Key result of the paper:** If the state of **2N** qubits has small entanglement between half the qubits the then expectation value of Pauli string operators = sum of products of only **N-site** expectation values

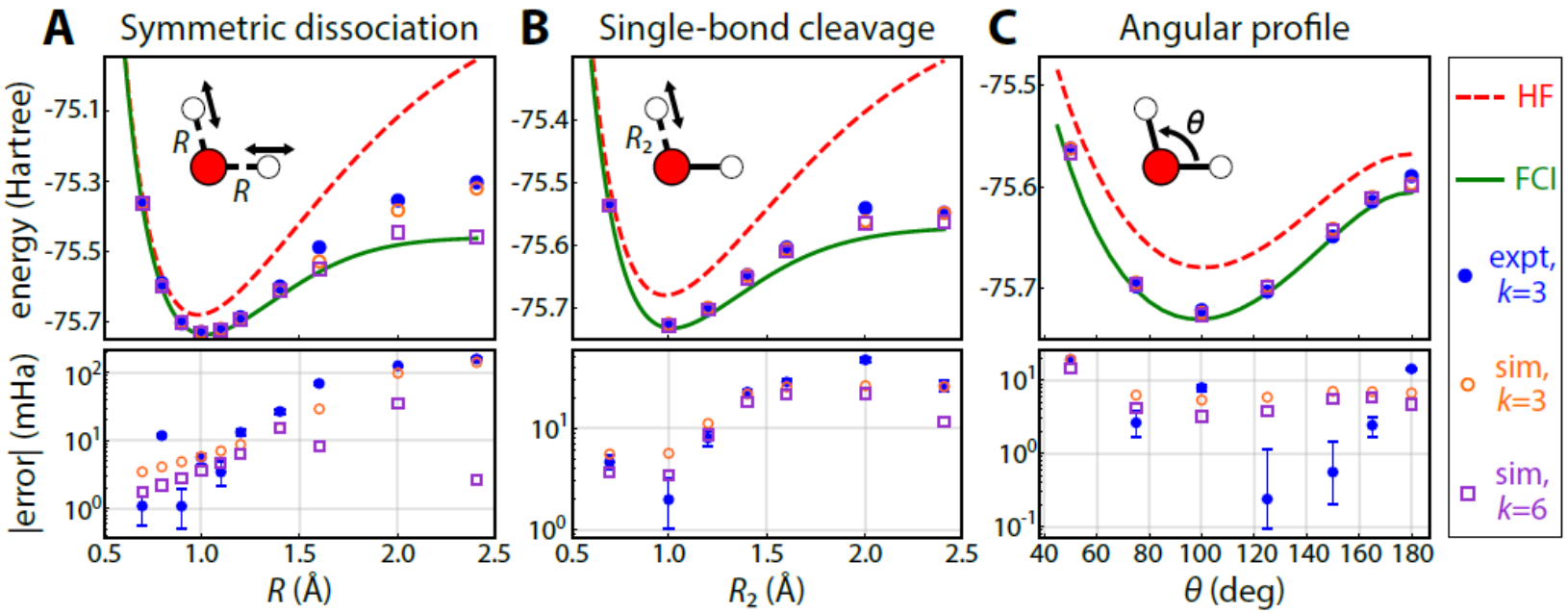
This can increase the accuracy of the variational optimization

Main mathematical tool to derive this result: **Schmidt decomposition**



# Benchmarking results

The authors report the most accurate to-date ground state simulation of the water molecule



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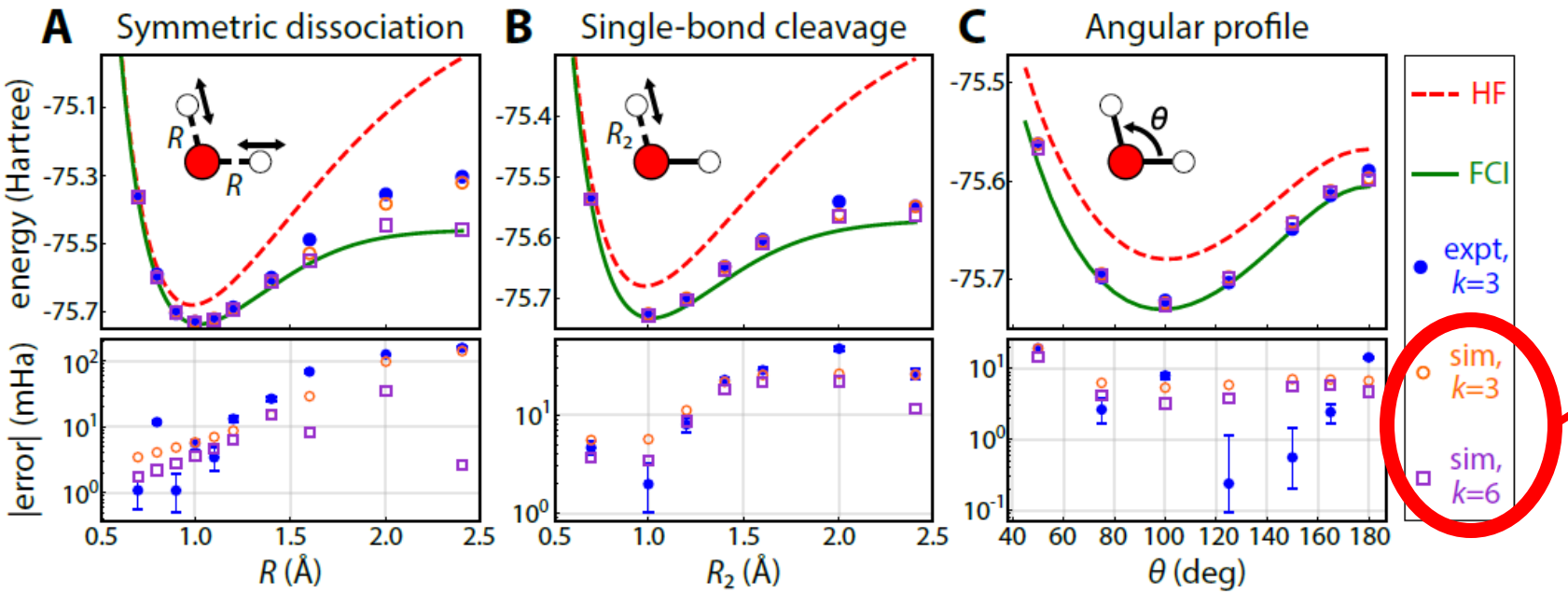



An important parameter is k: the number of Schmidt states to keep in the ground state

# Our project

The authors make a very non-trivial assumption: not only do they fix the number of Schmidt vectors, but also the Schmidt vectors themselves.

This requires solid intuition about the molecular structure of the water at low energies (e.g. which orbitals are likely to the filled, occupations ruled out by symmetries)

In this project, we tried to improve their algorithm by additionally optimizing the Schmidt vectors (i.e. we only fixed the number of Schmidt states to retain in the ground state)

# Approach

We had to address questions such as:

How do you set up the Schmidt vectors for a variational optimization?

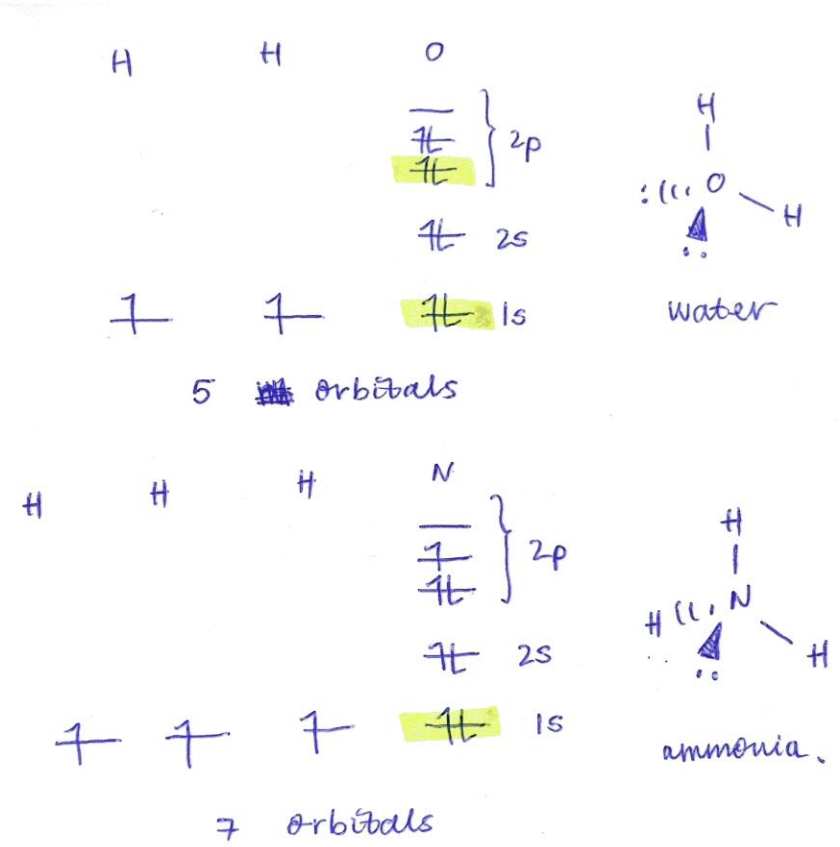
What is the optimal direction in the space of Schmidt vectors?

We tried a few different strategies:

-- Random selection of Schmidt vectors

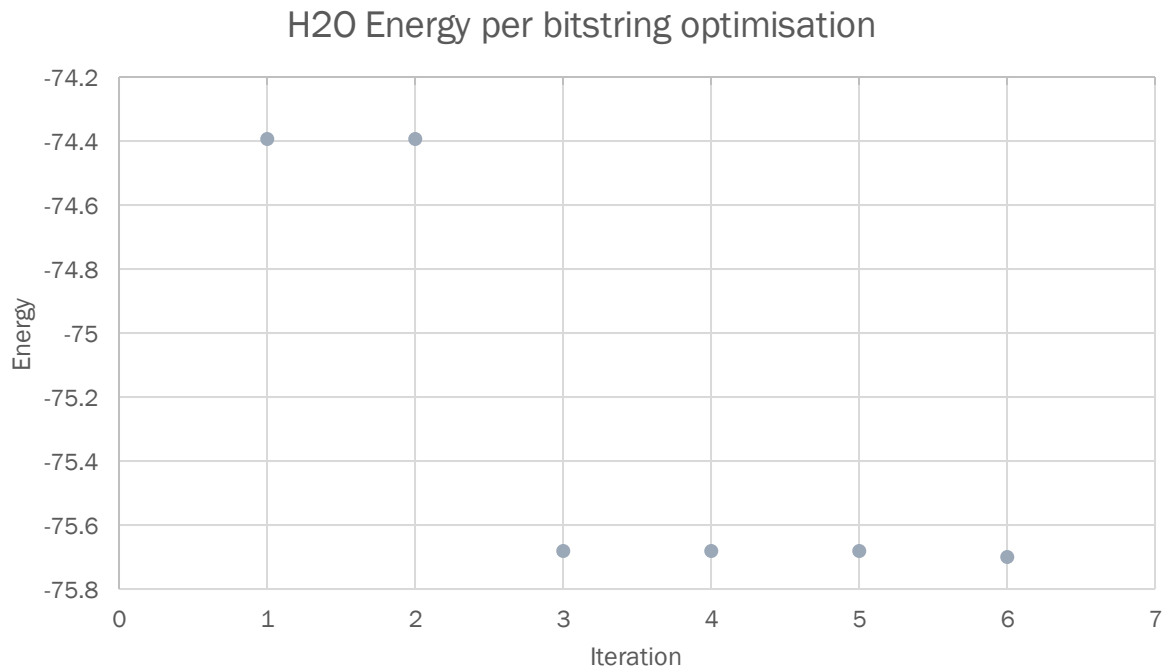
-- Descent in the direction of filling nearest orbitals

# Some Background Chemistry



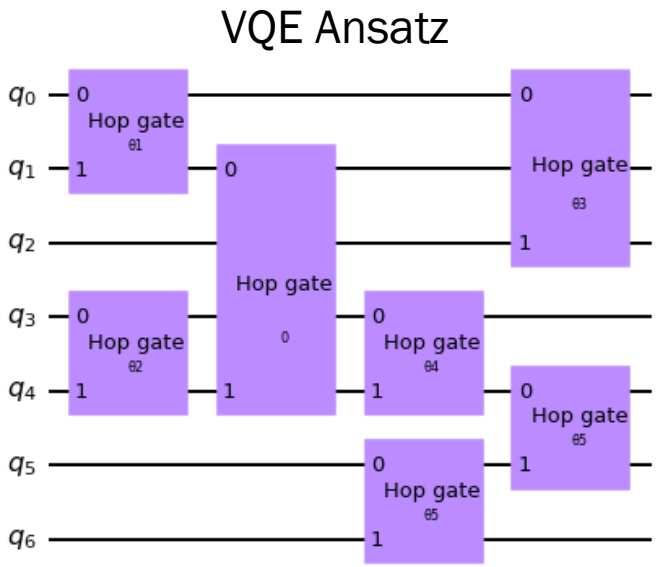
# Results - Water

Classically Determined Ground State= -75.7289



# Results - Ammonia

Classically Determined Ground State = 56.04931106499788
Energy determined via VQE/Entanglement Forging = 55.9999
Bitstrings = [[0, 1, 1, 1, 1, 0, 0], [0, 1, 1, 1, 0, 1, 0], [1, 1, 1, 1, 0, 0, 0]]



# Other ideas (that didn't work)

We also tried to extend the entanglement forging protocol to multiple partitions

We considered states of qN qubits that had limited entanglement across q bipartitions.

Our goal was to show that the expectation value of Pauli string operators for qN qubits reduces to a sum of products of only N-site expectation values

Recall that this way the key in the original protocol

For this generalization, we replaced the Schmidt decomposition (for a single bipartition) with a q-sites **Matrix Product State** decomposition.

While we believe this is a fruitful approach to follow, and could potentially improve the original protocol, we were not able to show that this setup could generalize the existing construction.