

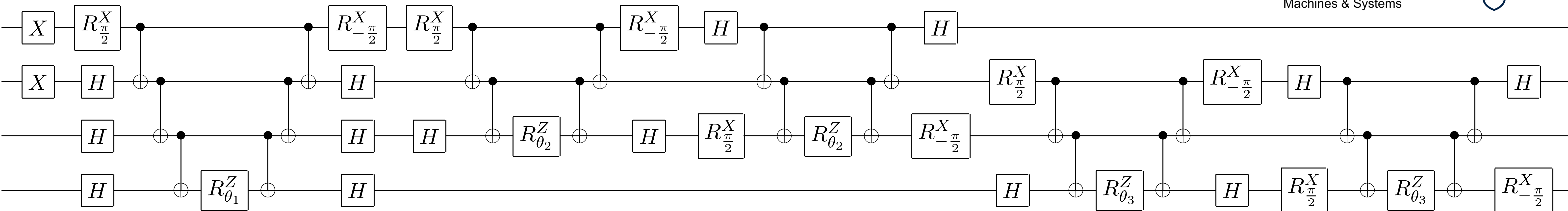
Bayesian optimisation for variational quantum eigensolvers

| Ben Moseley – Michael Osborne – Simon Benjamin

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MOTIVATION

Quantum computers could potentially simulate molecules exponentially faster than classical computers.

But **finding the ground state energy of molecules can be challenging** and current quantum computers are noisy.

How does **Bayesian optimisation** perform?

METHOD

Variational quantum eigensolvers

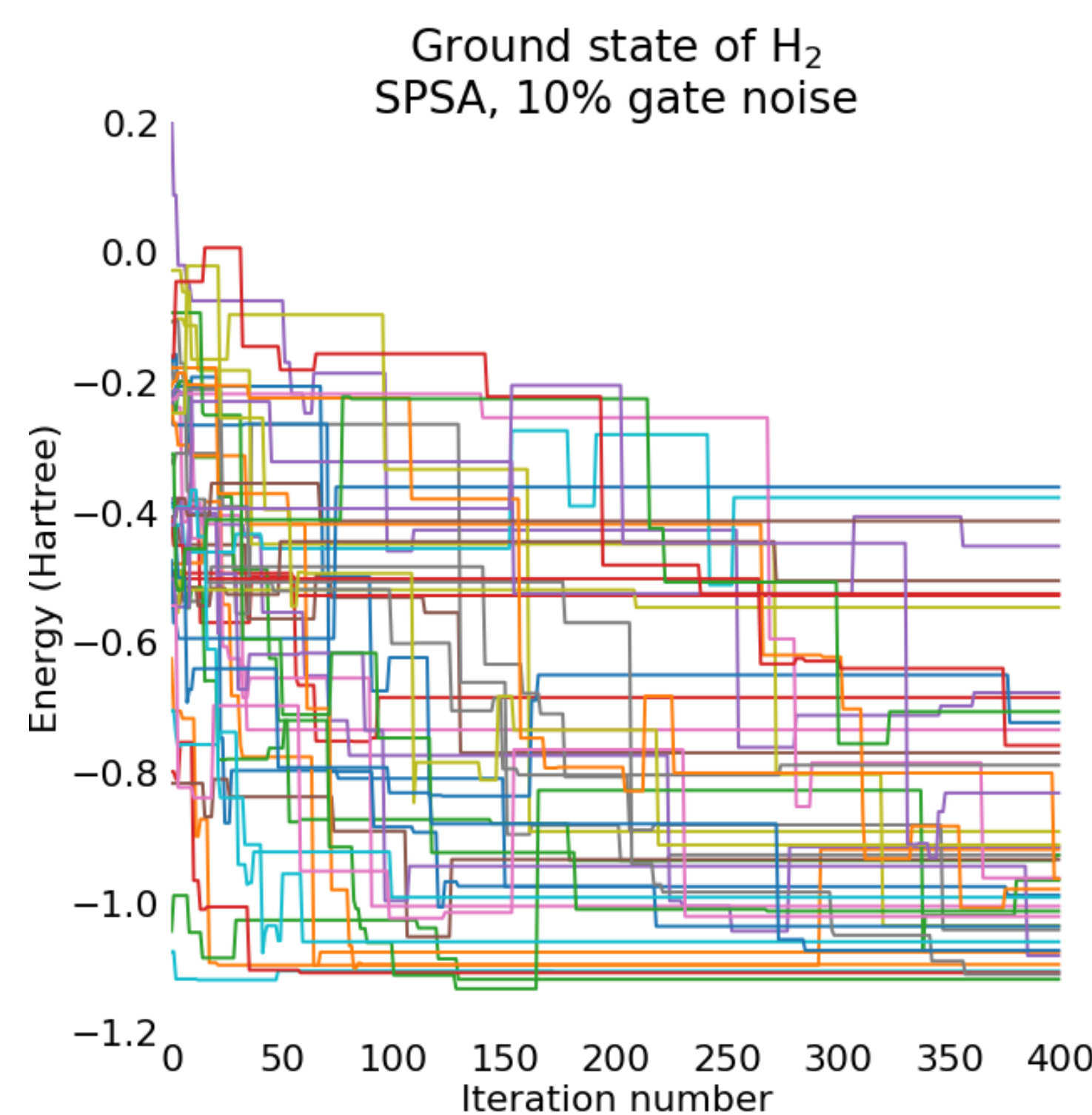
Simulating large molecules on a classical computer is intractable. We use a quantum computer to calculate the expected energy of molecules efficiently and classical optimisation to search for the ground state energy.

THEORY

VQEs rely on the variational principle for quantum mechanics, which states for any parameterised trial wavefunction $|\psi(\theta)\rangle$

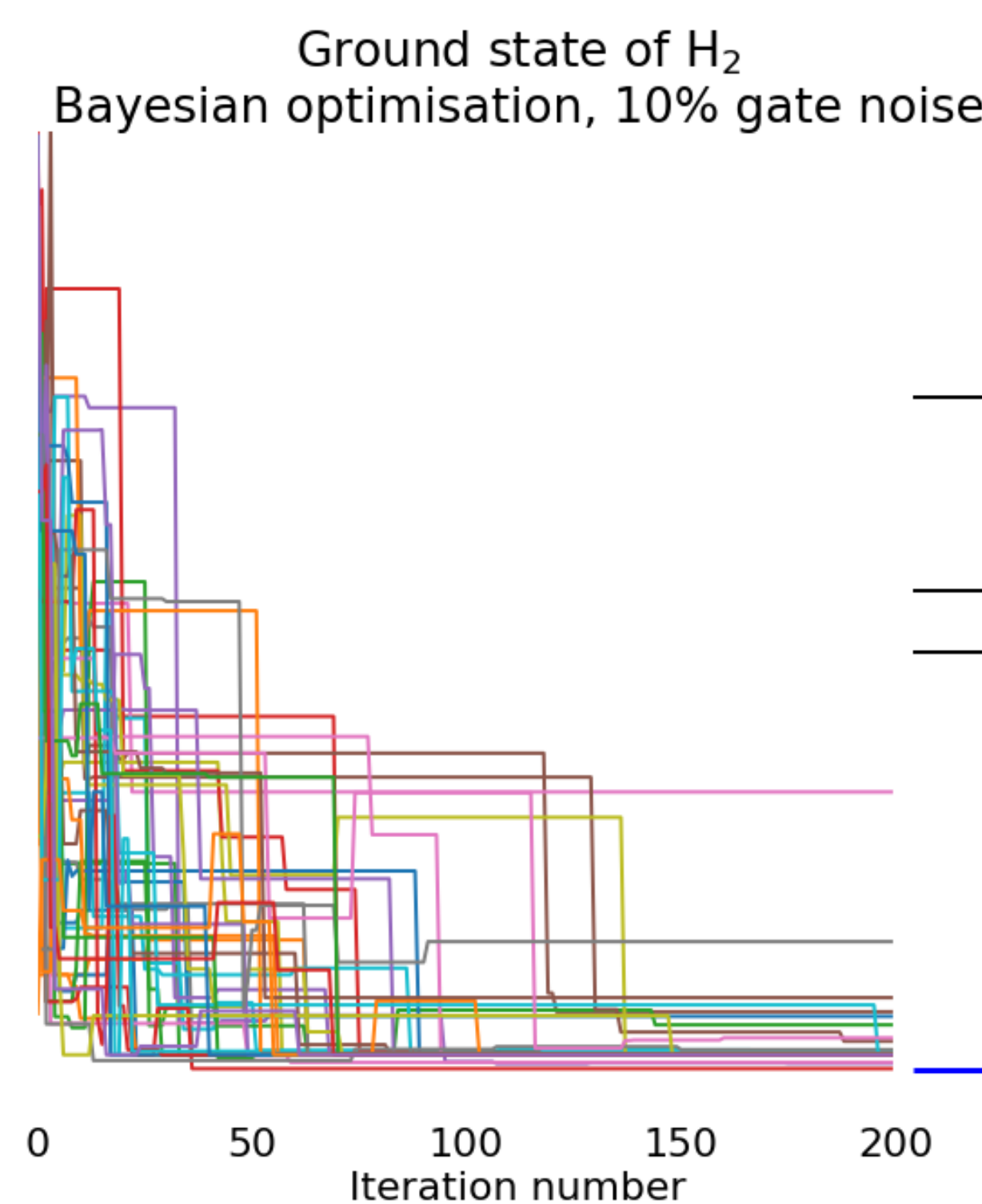
$$\langle \psi(\theta) | H | \psi(\theta) \rangle \geq E_0$$

where H is the Hamiltonian of the system and E_0 is the ground state



energy. Molecular Hamiltonians are mapped onto qubits using the second quantised form.

This optimisation problem is in general non-linear and stochastic.



RESULTS

When simulating molecular hydrogen with 10% gate noise in our quantum computer simulation, **Bayesian optimisation** with expected improvement and Gaussian process regression converges to within 0.06 Hartree of the ground state **83%** of the time, compared to **18%** for **simultaneous perturbation stochastic approximation (SPSA)**.

