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Benchmarking quantum computers with robust phase estimation of molecular hydrogen

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Quantum Simulation to Benchmark Quantum Hardware

A long-held promise of quantum computers is the efficient simulation of physical systems. While large systems are out of the reach of extant hardware, can smaller test systems provide useful benchmarks?

Here, we perform a simulation of molecular hydrogen on hardware provided by the IBM Quantum Experience, in particular calculating the eigenenergies of the system by estimating the *phase* of the time evolution operator. We examine the use of **robust** phase estimation to assess potential advantages on noisy hardware.

Basics of Quantum Simulation

To perform time evolution $U = e^{-itH}$, we Trotterize.

To perfom the preparation and measurements, we precompute the required quantum circuits (by exact diagonalization of the Hamiltonian).

Extensibility to larger chemicals will require another technique, e.g., adiabatic state preparation or VQE.

We have circuits to (a) prepare (and measure) a linear superposition of energy eigenstates and (b) evolve a state for some time t.
Run these per the Robust Phase Estimation algorithm.

Robust Phase Estimation (RPE)

What is RPE?

- Determines the *relative* phase θ induced by a unitary U between eigenvectors $|E_i\rangle$ and $|E_j\rangle$.

$$\theta \propto E_j - E_i$$

- Uses *no* controlled-U gates
- Naturally robust to errors
- Exhibits Heisenberg scaling

How does it work?

Linear combinations of the eigenstates $|E_i\rangle$ and $|E_j\rangle$:

$$|{\pm x}\rangle = |E_i\rangle \pm |E_j\rangle \quad \text{and} \quad |{\pm y}\rangle = |E_i\rangle \pm i\,|E_j\rangle$$

And perform two kinds of experiments:

$$P_{N,x} = \left|\langle +x|U^N|+x\rangle\right|^2 = \frac{1}{2}\left(1+\cos N\theta\right)$$

$$P_{N,y} = \left|\langle +y|U^N|+x\rangle\right|^2 = \frac{1}{2}\left(1+\sin N\theta\right)$$

Estimate θ

If $P_{1,x}$ and $P_{1,y}$ were known exactly, we would get an exact value for θ. But statistical error scales as $\nu^{-1/2}$, where ν is the number of trials.

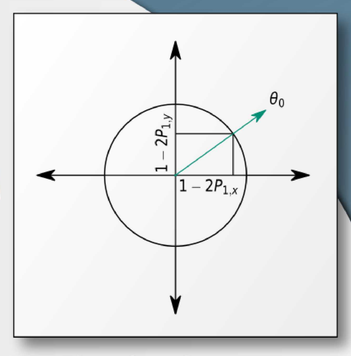
Can we do better?

By increasing N, the effect of uncertainty in P affects the estimates of θ less.

However, there are multiple θ consistent for any observed $P_{N,x}$ and $P_{N,y}$ for $N > 1$.

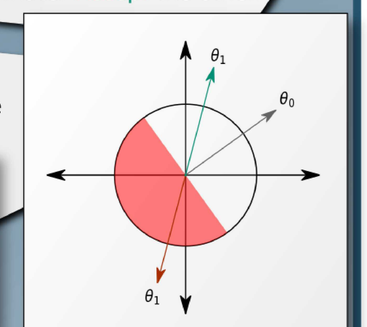
Robust Phase Estimation uses *iterative* estimates for various values of N to find θ. (We choose $N_k = 2^k$.)

Careful choice at each generation k of the number of trials performed, ν_k, and the number of applications of U, N_k, will acheive Heisenberg scaling.

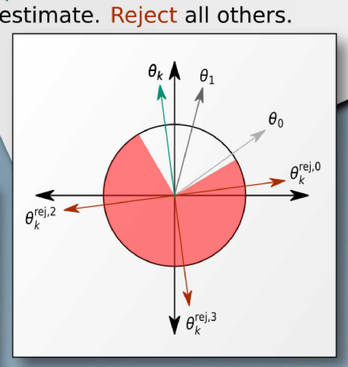


First θ estimate:
Just solve for θ.

Second θ estimate:
Solve for the *two* θ's consistent with $P_{2,x}$ and $P_{2,y}$.
One is rejected because it is very different from the first estimate. Accept the other.



Subsequent θ:
Solve for the N_k θ's consistent with $P_{N_k,x}$ and $P_{N_k,y}$.
Optionally, check if all previous estimates are consistent with the new estimate.
Accept the new value closest to the last estimate. Reject all others.



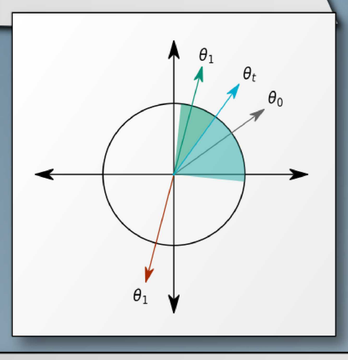
Robustness to noise

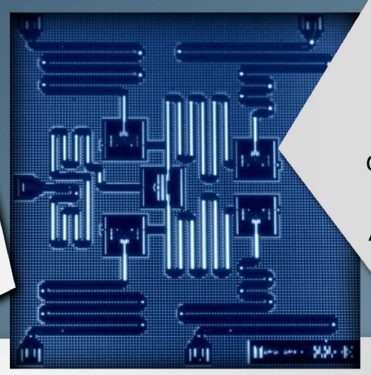
Of the N_k consistent solutions at generation k, RPE chooses θ_k closest to θ_{k-1}. Is this the same as $\theta_k^{\text{correct}}$, the estimate closest to the *true angle* $\theta^{(t)}$?

In other words:

Q: **How much noise can RPE tolerate?**

A: **Errors in P_N can be as large as $\left(1+\left(\tan\frac{\pi}{4}\right)^{-1}\right)^{-1}/2 \approx 31.6\%$.**





Even for a virtual H_2 molecule that uses only 2 qubits, implementing U uses 3 controlled-X gates. This precludes $N \gtrsim 30$ because of hardware fidelities.

Can anything be done?

In order to extrapolate to better results that will ostensibly become available, we have pre-compiled U^{N_k} to 3 CX gates.

Run on IBM Q "Vigo"

What do we get?

Using this pre-compiling, we find all energy gaps for H_2 at various separations. By using our knowledge of $\mathrm{Tr}[H]$, we can get the absolute energy scale (see future work: this doesn't scale).

Can we explain the error?

The following are equivalent:

- The error of the measured $\theta_k^{\text{correct}}$ is small enough:

$$|\theta_k^{\text{correct}} - \theta^{(t)}| < \frac{\pi}{3N_k} \qquad (\star)$$

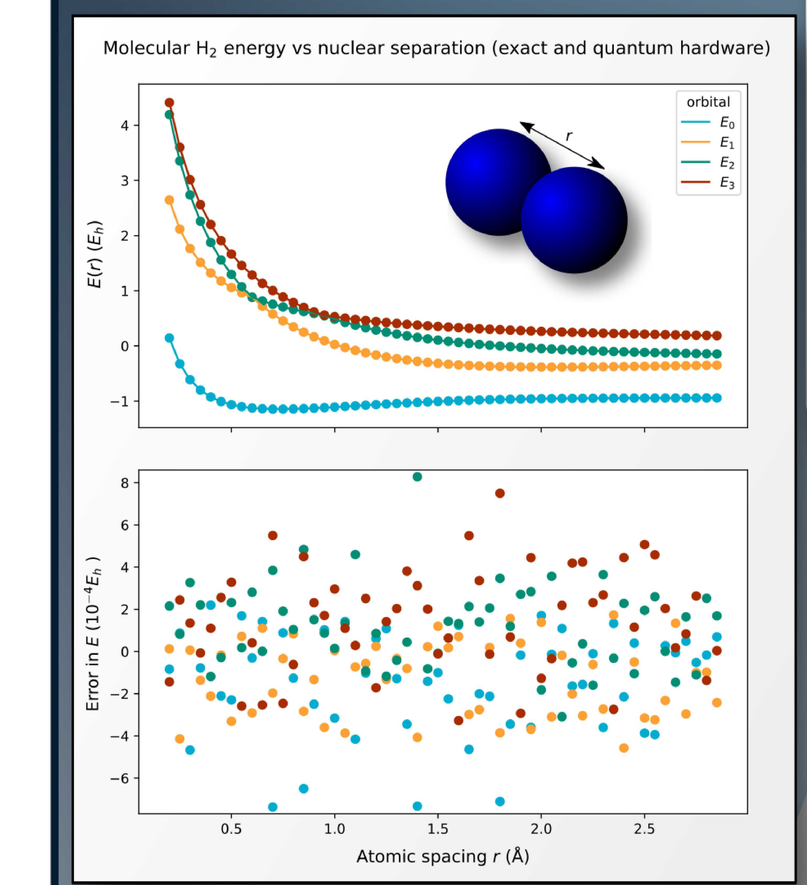
- θ_k "strongly converges" to $\theta^{(t)}$:

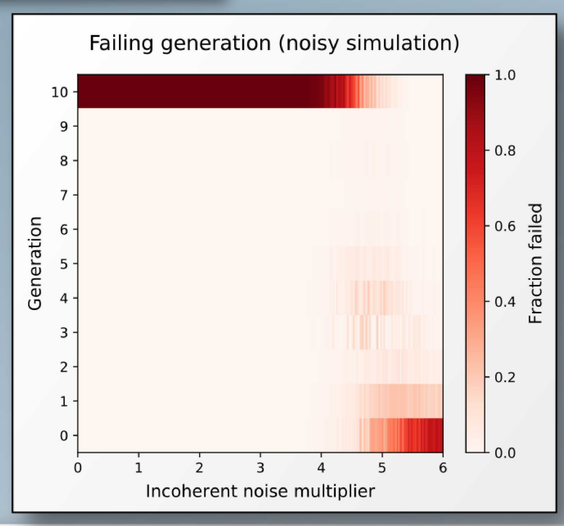
$$|\theta_k - \theta^{(t)}| < \frac{\pi}{3N_k}$$

- The θ_k estimates are "consistent:"

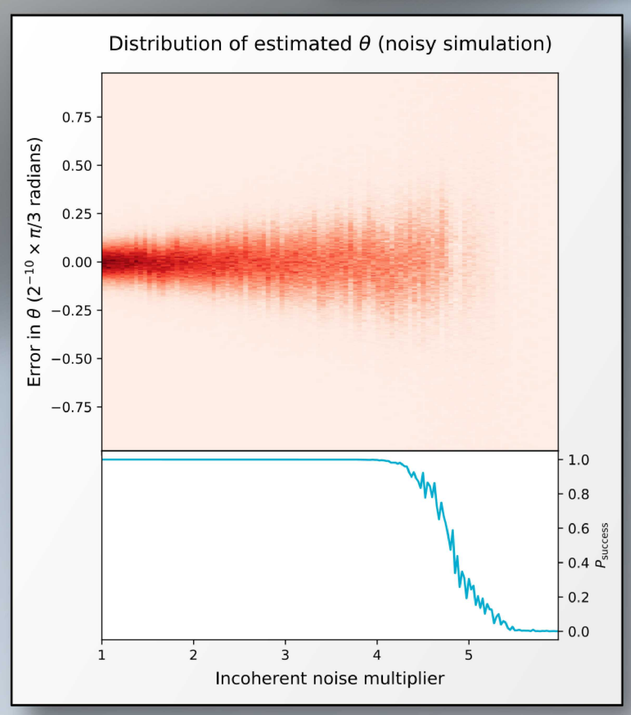
$$|\theta_{k'} - \theta_k| < \frac{\pi}{3N_{k'}} + \frac{\pi}{3N_k} \qquad (\diamond)$$

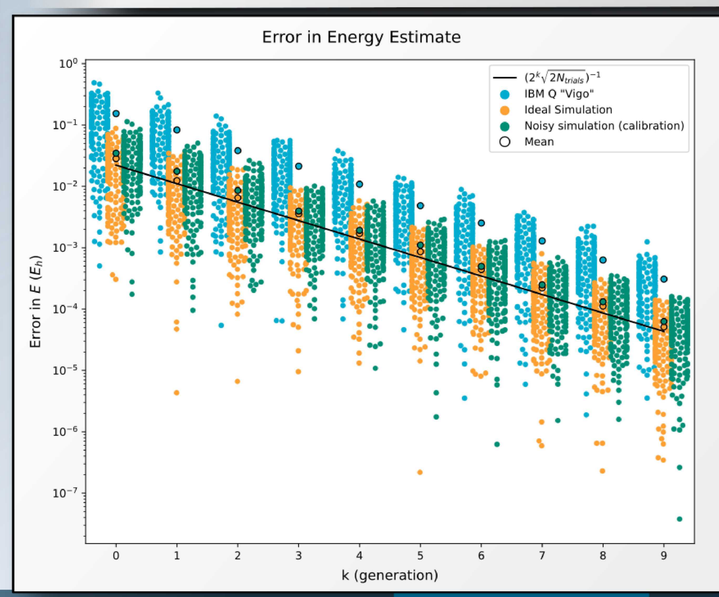
Eq. ($\diamond$) depends only on experimental data! It tells you if you can trust your phase estimate.





The constituent error models provided by IBM for their quantum hardware (Qiskit `basic_device_noise_model`) incoporates gate durations, thermal relaxation and SPAM errors, from calibration data. For the tested platforms, (Vigo, Yorktown, Tenerife, Ourense) this model is inadequate to describe the observed spreads in energy estimates (spread for Vigo is shown below). Moreover, merely increasing the decoherence rate (upward from the observed $T_1 = 124.9\,\mu s$ and $T_2 = 45.2\,\mu s$) in the system inadequately describes the performance of the protocol: there are no observed consistency check failures (see Eq. ($\diamond$)) from the hardware, but producing qualitatively equivalent error distributions with only decoherent noise necessitates such failures.





Future Work

This same approach can in principle be generalized. The next simplest case to consider would be H_3, which (as a function of atomic separations) has a conical intersection of the ground state energy and first excited energy. However, generically implementing the time evolution $U = e^{-itH}$ requires order 10^2 CNOT gates [5], leaving such a calculation in the realm of simulation.
Given the techniques developed here, requirements on qubit gate fidelities and cross-talk can be made. More generally, we plan to develop generalized requirements as chemical size scales up, generically providing minimum requirements for particular applications.
The code that implements the RPE and analysis is being released as part of the `pyGSTi` Python package.

References

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