Quantum Computation of Heavy Quarkonium Masses

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Project Overview

- Quantum Simulator
  - Ideal (noiseless) simulation of quantum computer
  - Computed $1S$ and $2S$ masses of $c\bar{c}$
  - Variational quantum eigensolver (VQE)
  - Unitary couple cluster (UCC) ansatz
- Quantum Computer
  - Real (noisy) quantum processor
  - Computed the $1S$ mass of $c\bar{c}$
  - VQE w/ UCC ansatz
  - Zero-noise extrapolation

Challenges of Low-Energy QCD

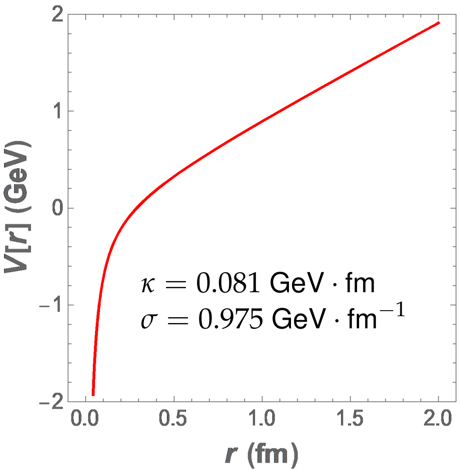
$$\mathcal{L}_{\text{QCD}} = \sum_{q=1}^{N_f} \overline{\psi}_q (i\not{D} - m_q)\psi_q - \frac{1}{2}\text{tr}\{F_{\mu\nu}F^{\mu\nu}\}$$

- Nonperturbative at energy scales relevant to hadron formation
- Gluon self-interactions confine color-charged quarks and gluons
- Only colorless quark combinations such as mesons ($q\bar{q}$) and baryons (qqq) can freely propagate

The Cornell Potential

$$V(r) = -\frac{\kappa}{r} + \sigma r$$

- Nonrelativistic $Q\bar{Q}$ effective potential
- Coulombic at short distances
- Confining at long distances
- No string-breaking



The Quantum Advantage

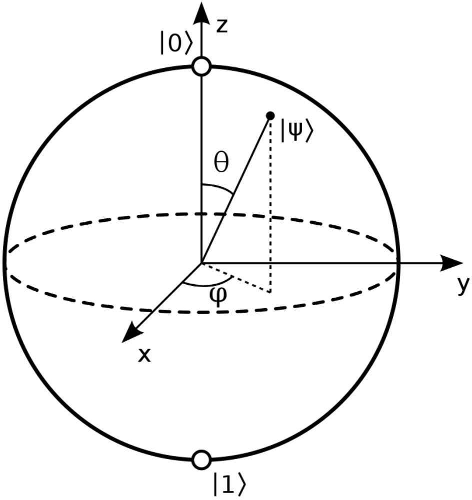
> *Nature isn't classical, dammit, and if you want to make a simulation of nature, you'd better make it quantum mechanical.*
>
> *—Feynman, 1981*

- Superposition and entanglement expand the number of ways information is stored and manipulated
- Arbitrary state may be prepared using a circuit that is (at most) polynomial in the dimension of the Hilbert space
- Modern quantum computers subject to noise (decoherence)
- Requires error mitigation

What is a Qubit?

- A quantum system with two orthogonal basis states $\{|0\rangle, |1\rangle\}$
- Each normalized superposition corresponds to a Bloch vector
- To rotate the Bloch vector, act with a unitary operator/quantum gate
- Multi-qubit basis is

$$\{|q_{N-1} \cdots q_0\rangle\}, \quad q_i \in \{0, 1\}$$



Mapping a Hamiltonian onto a Quantum Circuit

$$H_N = \sum_{m,n=0}^{N-1} \langle m| (T+V) |n\rangle a_m^\dagger a_n$$

- Expand Hamiltonian in the reference basis $\{|n\rangle\}$
- Keep only the first few terms since these are most important for determining the ground state
- Map the nth basis state to the computational state

$$|0\rangle^{\otimes(N-n-1)} |1\rangle |0\rangle^{\otimes n}$$

- Use Jordan-Wigner transformation to map creation/annihilation operators to Pauli operators

Variational Method

Principle

For any ansatz $|\psi(\vec{\theta})\rangle$ and Hamiltonian H bounded below,

$$\langle\psi(\vec{\theta})|\, H \,|\psi(\vec{\theta})\rangle \geq \varepsilon,$$

where ε is the ground state energy of H.

Objective

Estimate ε by minimizing $\langle H\rangle$ with respect to $\vec{\theta}$.

UCC Ansatz

- General form:

$$U(\vec{\theta}) = e^{T(\vec{\theta}) - T^\dagger(\vec{\theta})}$$

- Single-particle 3-orbital ansatz:

$$U(\theta, \varphi) = \exp\left\{\theta(a_1^\dagger a_0 - a_0^\dagger a_1) + \varphi(a_2^\dagger a_0 - a_0^\dagger a_2)\right\}$$

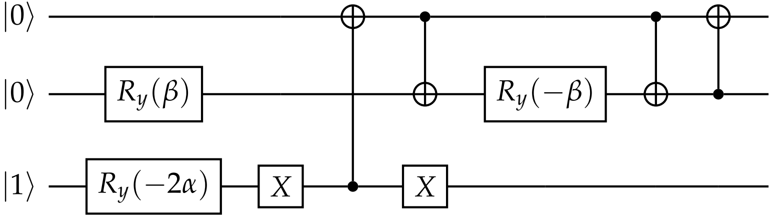
- Acting on the ground state of the reference basis gives

$$U(\alpha, \beta)\,|001\rangle = \cos\alpha\,|001\rangle + \sin\alpha\sin\beta\,|010\rangle + \sin\alpha\cos\beta\,|100\rangle$$

- Gate representation:

$$U(\alpha, \beta) = X_{12}X_{21}R_{y1}(-\beta)X_{21}R_{y1}(\beta)X_0X_{02}X_0R_{y0}(-2\alpha)$$

3-Qubit Ansatz Circuit Diagram



Noiseless Calculation

- Ran noiseless quantum circuit on IBMQ QASM Simulator
- Ground state of H_3 from exact diagonalization is 492.6 MeV
- Measured ground state using simulator to be 493 ± 1 MeV
- First excited state of H_3 from exact diagonalization is 1210.8 MeV
- Measured first excited state using simulator to be 1212 ± 2 MeV
- Bare mass of charm quark is known to be 1275 ± 35 MeV

Noise Scaling

- Given a circuit U, construct the circuit

$$U_\lambda \equiv U(U^\dagger U)^n$$

- Define a noise scaling parameter λ to be the ratio of the noise in U_λ to the noise in U
- Assuming the prevalence of noise is approximately proportional to circuit depth,

$$\lambda = 2n + 1, \quad n \text{ a nonnegative integer}$$

Zero-Noise Extrapolation

- Assuming a global depolarization channel,

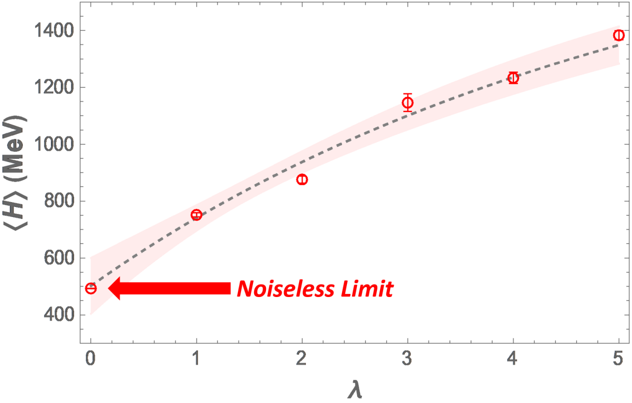
$$\rho \to r^{\lambda}\hat{U}\rho\hat{U}^{\dagger} + \frac{1}{N}(1 - r^{\lambda})I$$

- If $\mathcal{O}$ is a traceless unitary operator,

$$\langle\mathcal{O}\rangle_{\lambda} = \text{tr}(\rho\mathcal{O}) = r^{\lambda}\,\langle\widetilde{0}|\,\hat{U}^{\dagger}\mathcal{O}\hat{U}\,|\widetilde{0}\rangle$$

- $\langle\mathcal{O}\rangle_0$ corresponds to noiseless expectation value

Noise Scaling of $\langle H \rangle$



$\langle H \rangle$ vs. λ with 95% confidence mean prediction bands. Noiseless extrapolation gives 502 ± 98 MeV, which is in good agreement with the 493 ± 1 MeV calculated using the noiseless quantum simulator.

Summary & Extensions

- Demonstrated a variational method of estimating the eigenvalues of a Hamiltonian on a quantum computer
- Implemented a zero-noise extrapolation technique for mitigating errors due to a global depolarizing channel
- Spin dependent corrections to static potential necessary to accurately simulate J/ψ and η_c
- Quantum computing techniques discussed here may be extended to simulate more complex quark states like the X(6900)

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