A First Application of Quantum Computing in QCD

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Content

Introduction to Quantum Computing

Why Quantum Computers?

- Let us say we want to simulate an N particle quantum system (2 level, for simplicity). The state is described as

$$
\begin{aligned}
\Psi_1 &= a_0 |0\rangle + a_1 |1\rangle \\
\Psi_2 &= a_0 |00\rangle + a_1 |01\rangle + a_2 |10\rangle + a_3 |11\rangle \\
&\vdots \\
\Psi_N &= \sum_k^{2^N} a_k |\epsilon_k \cdots \epsilon_k\rangle
\end{aligned}
$$

How can we represent this state in a computer?

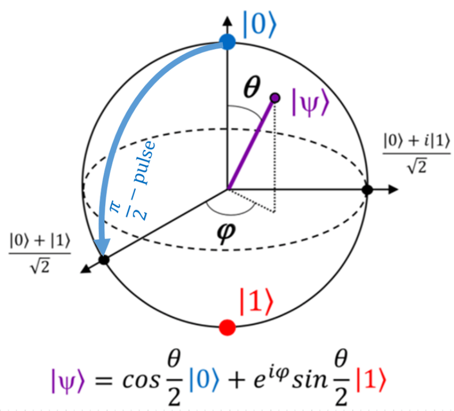
Classical Computers

- Regular computers use bits $\{0, 1\}$
  - Real number $\rightarrow$ 64bits
- N particles 2-level quantum system $\rightarrow 2^N \cdot 2 \cdot 64$ bits
- We need exponential memory to a general quantum system: $\mathcal{O}(2^N)$
  - 128gb of RAM $\rightarrow$ 30 qubits

Quantum Computers

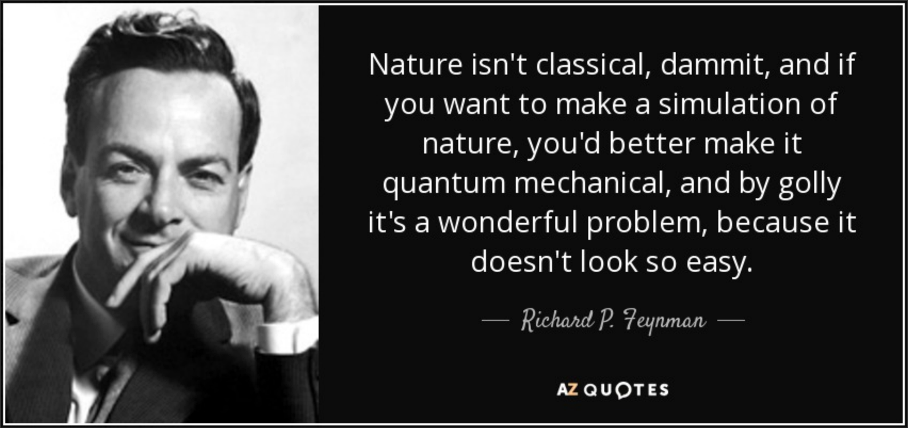
- Quantum computing (QC) uses qubits, which are two level quantum systems:

$$|\Psi\rangle = a\,|0\rangle + b\,|1\rangle\,, \quad |a|^2 + |b|^2 = 1 \tag{1}$$



Quantum Computers

- Qubits can represent a 2-level quantum system of N particles with N qubits
- For a general quantum system, we need polynomial qubits
- This is the motivation to use QC to simulate quantum systems as suggested by Feynman


Nature isn't classical, dammit, and if you want to make a simulation of nature, you'd better make it quantum mechanical, and by golly it's a wonderful problem, because it doesn't look so easy.
— Richard P. Feynman —
AZ QUOTES

How to use Quantum Computers

- We can operate qubits by applying "gates" (unitary operators)
- Some examples are the pauli operators ($\sigma_x \equiv X$, $\sigma_y \equiv Y$ and $\sigma_z \equiv Z$). One of the most useful is the Hadamard:

$$H = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \quad (2)$$

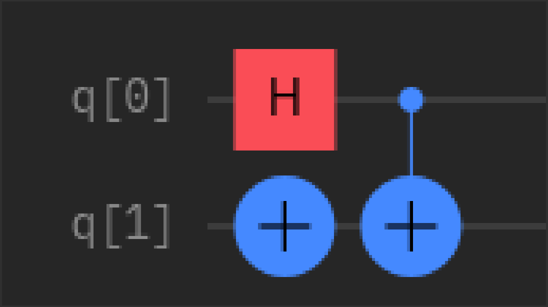
because it takes a state $|0\rangle$ or $|1\rangle$ and turns it into a superposition

More Quantum Gates

Operator	Gate(s)		Matrix
Pauli-X (X)	X	⊕	$\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$
Pauli-Y (Y)	Y		$\begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}$
Pauli-Z (Z)	Z		$\begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$
Hadamard (H)	H		$\frac{1}{\sqrt{2}}\begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}$
Phase (S, P)	S		$\begin{bmatrix} 1 & 0 \\ 0 & i \end{bmatrix}$
$\pi/8$ (T)	T		$\begin{bmatrix} 1 & 0 \\ 0 & e^{i\pi/4} \end{bmatrix}$
Controlled Not (CNOT, CX)	● / ⊕		$\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix}$
Controlled Z (CZ)	● / Z	● / ●	$\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \end{bmatrix}$

Circuits

- For example, a Bell state can be created by the following:



$$|00\rangle \implies \frac{|01\rangle - |10\rangle}{\sqrt{2}} \tag{3}$$

Application to QCD

Simulating Effective Potentials: step-by-step

1. Choose a quark model, *i.e.*, fix the form of the potential and the model parameters.
2. Calculate the matrix elements of the model Hamiltonian in a finite set of basis states. Typically Harmonic oscillator states are used.
3. Rewrite the Hamiltonian matrix in terms of Pauli operators acting on a set of qubits.
4. Determine the ground state using an quantum-classical algorihm.

Choosing a quark model

- We will consider the effective potential:

$$V(r) = -\frac{\kappa}{r} + \sigma r \tag{4}$$

with[1]

$$\begin{aligned} \kappa &= 0.4063 \text{ MeV} \\ \sqrt{\sigma} &= 441.6 \text{ MeV} \end{aligned}$$

- This leads to the hamiltonian (in harmonic oscillator basis)

$$H = \sum_{m,n=0}^{N-1} \langle m|T + V|n\rangle \, a_m^\dagger a_n \tag{5}$$

[1] https://doi.org/10.31349/SuplRevMexFis.3.0308068

Representing using Pauli Gates

- QC only operate a limited set of gates
- We can use the so called Jordan-Wigner transformation

$$
\begin{aligned}
a_n^\dagger &= \frac{1}{2}\left(\prod_{j=0}^{n-1} Z_j\right)(X_n - iY_n) \\
a_n &= \frac{1}{2}\left(\prod_{j=0}^{n-1} Z_j\right)(X_n + iY_n)
\end{aligned}
$$

This allows us to rewrite the hamiltonian

- We use $N = 3$ (easier, but low precision)

The Hamiltonian

$$
\begin{aligned}
H_0 &= \frac{1}{2}\left(\frac{21\omega}{4} + V_{00} + V_{11} + V_{22}\right) \\
H_1 &= -\frac{1}{2}\left(\frac{3\omega}{4} + V_{00}\right) Z_0 \\
&\vdots \\
H_5 &= \frac{1}{4}\left(-\sqrt{5}\omega + 2V_{12}\right) X_1 X_2 \\
&\vdots \\
H_9 &= \frac{1}{2} V_{02} Y_0 Z_1 Y_2 \\
H &= \sum_{k=0}^{9} H_k
\end{aligned}
$$

Variational Quantum Eigensolver

- Given H, how can we find the energies?
- We use the variational principle that says

$$\langle\Psi|H|\Psi\rangle \geq E_0 \tag{6}$$

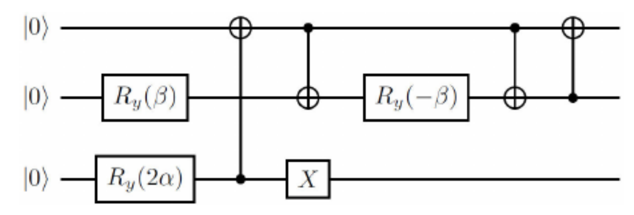
  where E_0 is the ground state energy and $|\Psi\rangle$ is an ansatz
- We can get higher excited states by picking a $|\Phi\rangle$ orthogonal to $|\Psi\rangle$; in this case

$$\langle\Phi|H|\Phi\rangle \geq E_1 > E_0 \tag{7}$$

Variational Quantum Eigensolver

- We use the UCC ansatz

$$|\psi(\alpha,\beta)\rangle = \cos\alpha\,|001\rangle + \sin\alpha\sin\beta\,|010\rangle + \sin\alpha\cos\beta\,|100\rangle \quad (8)$$



- We, then, find the parameters α, β that minimize the energy
- We need some method to reduce noise (not discussed here)

VQE Simulation Results

- Results from: D. Gallimore and J. Liao, DOI: https://doi.org/10.31349/SuplRevMexFis.3.0308068
- The ground state energy:

$$\langle H \rangle_0 = 493 \pm 1 \text{ MeV} \tag{9}$$

- The first excited state energy:

$$\langle H \rangle_1 = 1212 \pm 2 \text{ MeV} \tag{10}$$

- Actually, $E_0 \sim 3800$ MeV

Limitation and the future

Quantum Computers and QCD

- We are in the Noise-intermediate scale quantum (NISQ), which means QCs are still very noisy and decohere "fast"
- Current QCs can only do some small tasks that can also be done by HPC much more easily
- The point of QCs is the promise of overcoming (some) classical limitations in the future - IBM says they will have 100k qubits by 2033
- Mix of HPC with QC - hybrid quantum-classical
- Quantum Lattice?

Thank you!

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