Quantum Computing of the Deuteron Binding Energy

Improving on arXiv:1801.03897

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Contents Overview

What is Quantum Computing?

Quantum Computing is the application of **Quantum Information Science (QIS)** to the development of *machines* capable of performing operations and calculations based on quantum logic instead of the usual classical logic.

The usefulness of this kind of computation lays not only on the ability to engineer exponentially faster machines, but also on things such as being able to **efficiently simulate nature at the quantum level**, or creating encryption systems which are fundamentally secure.

CLASSICAL LOGIC
Set Theory (Boolean algebra)

- **AND** $\Rightarrow$ $A \cup B$
- **OR** $\Rightarrow$ $A \cap B$
- **NOT** $\Rightarrow$ $\overline{A}$
- **XOR** $\Rightarrow$ $A \cap B - A \cup B$

QUANTUM LOGIC
Quantum Theory (Non-Commutative)

- **Probabilistic measurement**
- **Measurement causes disturbance**
- **Superposition**
- **Entanglement**
- **Uncertainty principle**

The Abacus Effect

To try to understand the power of Quantum Computing in abstract, we can resort to what might be called **"The Abacus Effect"**.

Before the abacus was invented, the only way of counting was through a "thermometer-like" scale, which was highly inefficient as it meant adding one physical bead per unit. The abacus did something great: it introduced the concept of **digits**, which was later put into an even more concise notation by the Arabs through the introduction of **numerals**.

This means that, instead of counting up to N using N raw elements, we can count using only $\log_b(N)$ abacus elements —where b is the base of our number system (i.e. the amount of beads per row in the abacus). Therefore, for $b \geq 2$, the abacus introduced an **exponential decrease in resource requirements** to represent the exact same thing.

Quantum computers do something analogous. To represent the quantum state of a system made out of N subsystems —each of which with b degrees of freedom— we would usually need b^N classical elements (i.e. numbers). By using quantum systems for this representation, we would only need N quantum elements (i.e. each subsystem). Again, an exponential decrease in resource requirements.

Quantum Software: IBM's Qiskit

Working with quantum systems is extremely difficult, and in many cases very expensive, this makes quantum computing research unavailable to many groups and institutions. In order to solve this problem, IBM has developed **Qiskit**, a python framework for quantum computation and quantum information.

This framework allows the construction of quantum circuits —today's most common way of representing quantum computation— for running using different backends. These backends range from simulators to actual quantum devices accessible on the cloud through the IBMQ API included in Qiskit. It also includes tools for handling noise and error correction, developing quantum based applications and tools, or making use of well known, pre-programmed algorithms. It also allows work through different levels of abstraction, from microwave pulses on hardware to high level algorithm implementation.

Case Study

As a starting point we decided to reproduce the paper **Cloud Quantum Computing of an Atomic Nucleus** (arXiv:1801.03897) by Dumitrescu *et al.*

In this paper, IBM's QX5 quantum computer was used to simulate the **deuteron binding energy**, through a Hamiltonian from pionless effective field theory:

$$H_N = \sum_{n,n'=0}^{N-1} \langle n' | (T+V) | n \rangle \, a_{n'}^{\dagger} a_n$$

Where N is the basis dimension for a discrete variable representation in the harmonic oscillator basis.

Hamiltonian Mapping onto qubits

In order to simulate a quantum system on a quantum computer, we need to map its Hamiltonian onto the qubits of the device. To do so, in this case, we can use the **Jordan-Wigner transformations** which map the creation/annihilation operators onto Pauli matrices. This is necesarry as no direct measurement of a general quantum operator can be performed in a quanutm computer. However, it is possible to perform Pauli measurements with ease.

$$a_n^\dagger \to \frac{1}{2}\left[\prod_{j=0}^{n-1} -Z_j\right](X_n - iY_n) \qquad a_n \to \frac{1}{2}\left[\prod_{j=0}^{n-1} -Z_j\right](X_n + iY_n)$$

Where a spin up $|\uparrow\rangle$ on qubit n represents zero deuteron in state $|n\rangle$, and a spin down $|\downarrow\rangle$ one deuteron. For different values of N, this returns:

$$\begin{aligned}
H_1 &= 0.218291(Z_0 - I) \quad \Rightarrow \quad E_1 = \langle\downarrow|H_1|\downarrow\rangle \simeq -0.436\text{MeV} \\
H_2 &= 5.906709I + 0.218291Z_0 - 6.125Z_1 - 2.143304(X_0X_1 + Y_0Y_1) \\
H_3 &= H_2 + 9.625(I - Z_2) - 3.913119(X_1X_2 + Y_1Y_2) \\
&\cdots
\end{aligned}$$

Unitary Coupled Cluster

To determine ground-state energy we first need to know the region of Hilbert-space representing valid states of our quantum system. Then, we can use the **Unitary Coupled Cluster ansatz**. For this, we define unitary operators entangling two and three orbitals:

$$U_2(\theta) = \exp\left[\theta(a_0^\dagger a_1 - a_1^\dagger a_0)\right] = \exp\left[i\frac{\theta}{2}(X_0 Y_1 - X_1 Y_0)\right]$$

$$U_3(\eta,\theta) = \exp\left[\eta(a_0^\dagger a_1 - a_1^\dagger a_0) + \theta(a_0^\dagger a_2 - a_2^\dagger a_0)\right]$$

$$\simeq \exp\left[i\frac{\eta}{2}(X_0 Y_1 - X_1 Y_0)\right] \exp\left[i\frac{\theta}{2}(X_0 Z_1 Y_2 - X_2 Z_1 Y_0)\right]$$

These operators will transform our initial quantum state into some other state in the region of interest according to their parameters.

References

"The only thing demonstrated by an impossibility proof is a lack of imagination."
– John Stewart Bell –

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