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Quantum Computation - A sign of quantum supremacy

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Quantum computation as the name suggests is the use of quantum phenomena to perform computational tasks. As predicted by Richard Feynman, an extraordinarily brilliant physicist of the 20th century, quantum computers can do many tasks that an ordinary computer cannot. In this paper, an attempt is made to obtain the electronic energy levels of hydrogen molecule and lithium hydride by employing quantum algorithm based on variational principle. An introduction to basic ideas of quantum computation and qubit Hamiltonian for these molecules are summarized. It is a common misconception that the term 'quantum' is associated with 'complicated', and complex mathematical equations and hence cannot be learnt easily. The objective of this paper is to eliminate this misconception and that any quantum phenomenon can be understood with very little mathematics and very few equations.

Keywords: Qubits; Electronic structure; Quantum gates; Algorithms; Open Fermion

"When we get to the very, very small world—say circuits of a few atoms—we have a lot of new things that would happen that represent completely new opportunities for design. Atoms on a small scale behave like nothing on a large scale, for they satisfy the laws of quantum mechanics. So, as we go down and fiddle around with the atoms down there, we are working with different laws, and we can expect to do different things. We can manufacture in different ways. We can use, not just circuits, but some system involving the quantized energy levels, or the interactions of quantized spins."
– Richard P. Feynman

1. Introduction and basic ideas

Quantum computing was proposed almost four decades back by Yuri Manin and Richard Feynman but surprisingly, the progress is not swift as that happened in classical computing.

What is the difference between classical and quantum computing?

Like '*bits'* in classical computing, the fundamental unit in quantum computing is a '*qubit'*. The difference between a qubit and a bit is that while a bit can be either 0 or 1, a qubit can be either 0,1, or a mixture of 0 AND 1 at the same instant. A classical approach would consider the system as a classical 'physical' model while a quantum chemical method, broadly, would be based on the Schrödinger's equation and computation can be used whenever necessary. Classical computation is based on two states, 0 and 1, i.e. a binary system. Quantum computation is based on more than two states, 0, 1 and arbitrary superposition of the two States. In quantum computation, a qubit is a two-state system where the linear superposition are also allowed states. For example, spin of electron has two possible states – up-spin (represented as$|0\rangle$) and down-spin (represented as$|1\rangle$). Apart from the two, we also consider an arbitrary linear combination of the two states, i.e. $a|0\rangle + b|1\rangle$.

This difference arises due to two major attributes – superposition and entanglement, which are inherent outcome of quantum mechanics itself, which set a qubit different from a classical bit. Superposition is a linear combination of distinct quantum states, which in turn form a new and valid quantum state. The famous double slit experiment of Thomas Young is a 'classical example of quantum mechanical superposition. Entanglement on the other hand is a quantum mechanical state in which a particle cannot be described explicitly. An entanglement will become disentangled from the results of measurements. It is to be noted here that the outcome of the

measurements on individual qubits could be either 0 or 1. However, the outcome of the measurement on one qubit will always be associated with the measurement on the other qubit.

This makes a quantum computer to accommodate a large number of logical *gates* simultaneously; so this leads to a further question –

What are logical gates and how do they differ in classical computers and quantum computers? As we all know, in an electrical circuit, logic gates will make choices based on a combination of digital signals coming from the inputs. Most of the logic gates have two inputs and one output. Some of the common logic gates are AND (the output is true when only both the inputs are true, or else false), OR (output is true if either or both the inputs are true) XOR (exclusively or – implying that the output is true only when one of the inputs is true) and many more. Like classical logic gates quantum logic gates are the building blocks for quantum computers and they work by the combination of qubits. However, due to the superposition phenomenon, quantum logic gates exist simultaneously. Not only that, quantum gates are reversible due to unitarity of quantum mechanics. For example, classically, addition of 5 and 2 gives 7. Using quantum algorithms, addition is supposed to be reversible, so in this example, from 7, we should know which two numbers were added, 5 and 2, or 6 and 1, and so on. Similar to the gates used in classical computation, there are quantum gates in quantum computing.

This reversibility is an extraordinary advantage because quantum gates never lose information. Qubits that are entangled on their way into a quantum gate remain entangled in the way out, keeping the information safely intact throughout the transition. Many of the classical gates found in conventional computers, on the other hand, *do* lose information, and hence cannot retrace their steps. It should also be noted here that the number of qubits in the input and output however must be equal.

How does a quantum computer work?

Unlike digital computing, vectors and matrices are integral parts of quantum computing. In a quantum computer, elemental particles such as electrons and photons or ions are involved. Their charge or polarization are represented in qubits. The nature and behavior of these particles form the basis of quantum computing.

A quantum gate is implemented physically as the quantum mechanical evolution of an isolated quantum system. The transformation the system undergoes is governed by the famous Schrödinger's equation

$$i\hbar\partial|\psi\rangle/\partial t = \mathcal{H}|\psi\rangle$$

$$U = \exp(-i\mathcal{H}t/\hbar)$$

Where 'H' is the Hamiltonian, which specifies the physical fields, forces and energy and 'U' is a special kind of matrix, known as unitary matrix.

In quantum computing, size of this matrix is decided by the number of qubits. For 'n' number of qubits, the representation will be a square matrix of 2^n x 2^n elements. The concepts of vectors, phases and matrix representations make the understanding of quantum computing different, but not difficult.

For example, let a system of two particles exist in such a way that the total spin of the system is zero. If the spin of one of the particles is measured on a particular axis and found to be anticlockwise, a measurement of the spin of the other particle (of course, along the same axis) will depict a spin state to be clockwise. It appears as though the other entangled particle has somehow "felt" that a measurement is performed on the other and "knows" what the outcome should be. But, in reality, this response happens without any 'dialogue' between the entangled particles.

The superposition can be shown as a two matrix representation - either as a row matrix, ('bra') or a column matrix ('ket') as given below,

$$\langle 1| = [0 \quad 1] \quad ; \quad \langle 0| = [1 \quad 0] \text{ (bra)}$$

$$|1\rangle = \begin{bmatrix}0\\1\end{bmatrix} \quad ; \quad |0\rangle = \begin{bmatrix}1\\0\end{bmatrix} \text{ (ket)}$$

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In terms of accuracy and time, quantum computation surpasses the classical computation methods. Some of the problems which have taken a very long time on a classical computer, only take polynomial time on a quantum computer. The classic example is a search in a database – for instance if it requires 2^n -1 steps to solve a problem classically, it only takes a square root of 2^n steps by a quantum algorithm called Grover's algorithm [1].

Quantum gates are defined using Pauli matrices, which are defined as,

$$X = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix};\ Y = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix};\ Z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}.$$

The most important measurement in quantum computation is the phase, as the NOT, EXOR quantum gates will work only on the basis of change in phase. The measurement of phase is done by the use of a phase gate, also known as T-gate (U). Control-NOT gate (U_π) has a target and a control. If control is 1, the target value is changed, similar to XOR gate ($1 \oplus 1 = 0\ or\ 1 \oplus 0 = 1$) and if the control is 0, there is no change in the value of target. Hadamard gate (H or $U_{-\pi/2}$) forms a superposition of the two qubits.

$$U = \begin{bmatrix} 1 & 0 \\ 0 & e^{i\pi/4} \end{bmatrix},\ \mathrm{U}_\pi \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

$$\mathrm{U}_{-\pi/2} \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ -1 & 1 \end{pmatrix} \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix}$$

$$= \frac{1}{\sqrt{2}} (|0\rangle + |1\rangle)$$

An algorithm is a specific procedure to solve a defined problem. A quantum algorithm uses quantum gates; sometimes, hybrid algorithms are constructed, like variational quantum eigensolver (VQE) to reduce the complexity of using more gates.

2. Quantum mechanics to quantum computing

A molecule is characterized by its ground-state and excited state energies, defining its electronic structure [2].

The first step in solving a quantum mechanical problem is to write the corresponding expression of Hamiltonian – in simple terms, describing a dynamic system in terms of coordinates in space and time. Hence the first task in quantum computing is to encode a Hamiltonian of a quantum particle such as an electron, which is a fermion (fermion is a subatomic particle that has a half-integral spin and follows the statistical description given by Fermi and Dirac) into a qubit Hamiltonian. For example, the fermionic Hamiltonian of the hydrogen molecule, in atomic units can be written as given below

$$H_{H_2} = -\sum_i \frac{\nabla_i^2}{2} - \sum_{i,I} \frac{Z_I}{|\bar{r}_i - \bar{R}_I|} + \frac{1}{2} \sum_{i \neq j} \frac{1}{|\bar{r}_i - \bar{r}_j|}$$

Here,

$-\sum_{\mathrm{i}} \frac{\nabla_{\mathrm{i}}^2}{2}$ is the kinetic energy term,

$+\frac{1}{2} \sum_{\mathrm{i} \neq \mathrm{j}} \frac{1}{|\bar{\mathrm{r}}_{\mathrm{i}} - \bar{\mathrm{r}}_{\mathrm{j}}|}$ is for electron $-$ electron repulsion,

$-\sum_{i,I} \frac{Z_I}{|\bar{r}_i - \bar{R}_I|}$ is nucleus $-$ electron attraction term.

The first quantization, and the wave function have to be projected in the form of Slater determinants of Basis sets to compress the exponentially increased terms. Here, we use the basis set Slater-Type Orbitals – 3 Gaussian orbitals (abbreviated as STO-3G, a linear combination of atomic orbitals). To further compress the terms, we resort to creation and annihilation operators $a^\dagger$ and a. In simple terms, they increase/decrease the number of particles by one in a particular energy state/orbital, and can be interpreted as excitation/de-excitation to higher/lower levels... We write a Slater determinant indicating which spin orbitals are occupied by electrons in terms of occupation number vector, $|f\rangle$ in Fock space.

$$\psi(x_0, \ldots, x_{N-1}) = |f_{M-1}, \ldots, f_p, \ldots, f_0\rangle = |f\rangle$$

$$f_p = \begin{cases} 1, when\ \phi_p\ is\ occupied \\ 0, when\ \phi_p\ is\ unoccupied \end{cases}$$

The action of creation and annihilation operators can be written as:

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$$a_p|f_{M-1}, f_{M-2} \dots f_0\rangle = \delta_{f_p,1}(-1)^{\sum_{i=0}^{p-1} f_i}|f_{M-1}, f_{M-2}, \dots, f_p \oplus 1, \dots, f_0\rangle$$

$$a_p^\dagger|f_{M-1}, f_{M-2} \dots f_0\rangle = \delta_{f_p,0}(-1)^{\sum_{i=0}^{p-1} f_i}|f_{M-1}, f_{M-2}, \dots, f_p \oplus 1, \dots, f_0\rangle$$

Here, $(-1)^{\sum_{i=0}^{p-1} f_i}$ enforces exchange in antisymmetric fermions and δ is Kronecker symbol. $a^\dagger$ and 'a' operators use XOR gate (which is equivalent to CNOT quantum gate)
where$0 \oplus 1 = 1\ and\ 1 \oplus 1 = 0$.

The Hamiltonian has to be expressed in a form that the computer can understand. Hence, we need to encode the Hamiltonian in a computer-friendly language. Here, we use a special type of encoding, the Jordan-Wigner encoding, which is a transformation that maps spin operators on fermionic creation and annihilation operators. We store the occupation number of a spin orbital in $|0\rangle$ and $|1\rangle$ state of a qubit:

$$|f_{M-1}, f_{M-2}, \dots f_0\rangle \rightarrow |q_{M-1}, q_{M-2}, \dots q_0\rangle \ ; \ q_p = f_p \in \{0,1\}.$$

The number operator $n_i = a_i^\dagger a_i$ counts number of electrons in the ith orbital:$n_i|f\rangle = f_i|f\rangle$. We need to express the creation and annihilation operators in terms of gates.

The annihilation operator is casted in terms of Pauli matrices:

$$a_p = Q_p \otimes Z_{p-1} \otimes \dots Z_0$$

Where $Z_{p-1} \otimes \dots Z_0$ computes the parity of the state, and Q_p changes the occupation number of pth spin orbital. Q is defined as

$$Q = |0\rangle\langle 1| = \begin{bmatrix}1\\0\end{bmatrix}[0 \quad 1] = \frac{1}{2}(X + iY),$$

$$Q^\dagger = |1\rangle\langle 0| = \begin{bmatrix}0\\1\end{bmatrix}[1 \quad 0] = \frac{1}{2}(X - iY).$$

Finally, the Hamiltonian can be expressed as a linear combination of Pauli operators

$$H = \sum_j h_j P_j = \sum_j h_j \prod_i (Pauli\ matrices)$$

Here, we have successfully converted a fermionic Hamiltonian into a qubit Hamiltonian.

3. Variational Algorithm

Quantum computation is unitary. The unitary method is a technique for solving a problem by first finding the value of a single unit, and then finding the necessary value by multiplying the single unit value [3]. Hence, the evolution of an initial state Ψ(t0) to a final state Ψ(t) is affected by a unitary operator $\hat{U} = e^{-i\hat{H}t}$, where $\hat{H}$ is the Hamiltonian operator of the quantum system [4]. As $\hat{U}$ acts on an energy eigenstate, $|E_n\rangle$ of $\hat{H}$, a phase factor $e^{-iE_nt/\hbar}$ is multiplied to the initial state. Thus, to find the lowest energy eigenstate $|E_0\rangle$ we have to make a phase estimation.

Rayleigh-Ritz variational principle states that for a trial wavefunction $|\psi(r_1, r_2 \dots)\rangle$ with parameters $\{r_i\}$, the expectation value of Hamiltonian in this total state is greater than or equal to the ground state energy:

$$\langle\psi|H|\psi\rangle \geq E_0$$

Thus, we can find a good approximation to the ground state energy by minimizing with respect to parameters $\{r_i\}$[5]. The algorithm is as given below:

Step1: Preparation, storage and measurement of the wave function on a quantum computer. This involves mapping of the problem Hamiltonian using a collection of qubits that were discussed above. This is followed by building a quantum circuit.

Step2: We now use classical computer to update the parameters using an optimized algorithm. The Hamiltonian is evaluated with respect to initial quantum state parametrized in terms of variables that are classically optimized to minimize the Hamiltonian [6].

4. Quantum simulation with quantum algorithms

Open Fermion is an open-source software developed for quantum simulation of in chemistry and materials science using quantum algorithms. The first step in this simulation is to specify the molecular properties. For this purpose, we need to specify the coordinates, bond length, spin and charge. We also need to specify the basis set in which we hope to expand the wave function to solve the Schrödinger equation. In the present study, simulations for hydrogen molecule and LiH were attempted and an STO-3G basis set was used. In second-quantized form, the Hamiltonian for hydrogen molecule has one-electron and two-electron integrals. These integrals are evaluated by classical algorithm using Psi4, an open source program. Here, only four spin orbitals are required – two each for an atom with up and down spin. The Jordan-Wigner encoded Hamiltonian was solved by another open source software, Open Fermion.

5. Inspiration from classical methods

We briefly sketch the chain of arguments through the classical methods which eventually lead to the quantum algorithm.

First of all, the Hartree-Fock (HF) method gives a Slater determinant wave function after optimization of the spatial form of spin orbitals in order to minimize the energy. As a first approximation, the Coulomb repulsion among the electrons were neglected. The function was modified by considering the motion of each electron in the mean field of other charges. For N electrons, one solves N coupled equations, first calculating position of each electron, then updating the potential, iteratively, until convergence is achieved. In the second quantized form, the Fock operator is diagonalized to arrive at a self-consistent field (SCF).

We would like to illustrate the construction of state of H_2 on a quantum computer using UCC (*Unitary Coupled Cluster Operator)* with single and double excitations (UCCSD).

In H_2, each atom (A, B) contributes one orbital and there are two possible Z-components of spins for each orbital (up (u) and down (d)). So, the orbitals are:$|1s_{Au}\rangle$, $|1s_{Ad}\rangle$, $|1s_{Bu}\rangle$, $|1s_{Bd}\rangle$. The overlap of the orbitals gives rise to molecular orbital basis with single electron orbitals with four possibilities:

$$|\sigma_{bu}\rangle = \frac{1}{\sqrt{N_b}}(|1s_{Au}\rangle + |1s_{Bu}\rangle$$

$$|\sigma_{bs}\rangle = \frac{1}{\sqrt{N_b}}(|1s_{Ad}\rangle + |1s_{Bd}\rangle$$

$$|\sigma_{au}\rangle = \frac{1}{\sqrt{N_a}}(|1s_{Au}\rangle - |1s_{Bu}\rangle$$

$$|\sigma_{ad}\rangle = \frac{1}{\sqrt{N_a}}(|1s_{Ad}\rangle - |1s_{Bd}\rangle$$

Where, 'b', 'a' denote bonding and antibonding orbitals respectively, N_b and N_a are the normalized constants. The Slater determinants in occupation number basis is:

$$|\psi\rangle = |f_{\sigma_{ad}}, f_{\sigma_{au}}, f_{\sigma_{bd}}, f_{\sigma_{bu}}\rangle.$$

Now, with Jordan-Wigner coding, a quantum circuit can be made as given below:

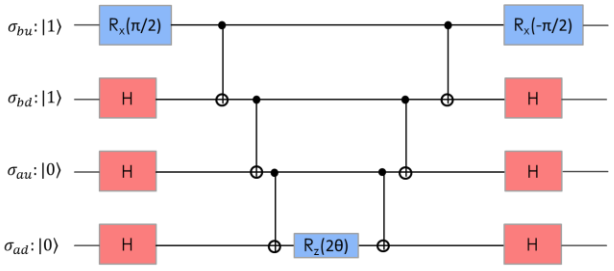

Fig. 1: Quantum circuit corresponding to the Unitary Coupled Cluster Operator with single and double excitations (UCCSD) acting on the Hartree-Fock wave function to yield the optimized ground state of hydrogen atom [7].

The results for the ground state of both H_2 and LiF obtained by quantum computing are given in Figure 2 and 3. The graph is plotted by varying the bond length

of the molecule, obtaining a minimum ground state energy.

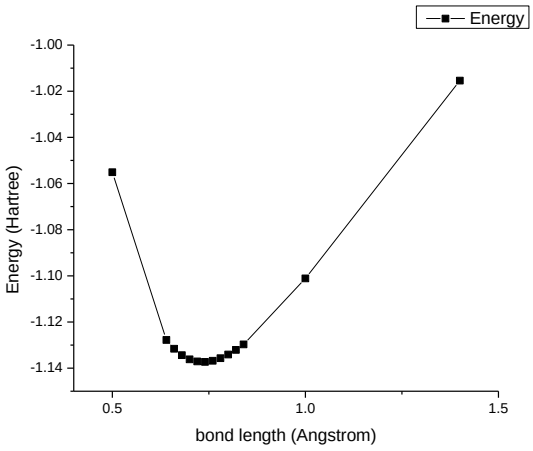

Fig. 2: Energy of the hydrogen molecule as a function of inter-atomic distance. At a distance of 0.74 Angstroms, the minimum here corresponds to the ground state. This is in agreement with the experimentally measured value.

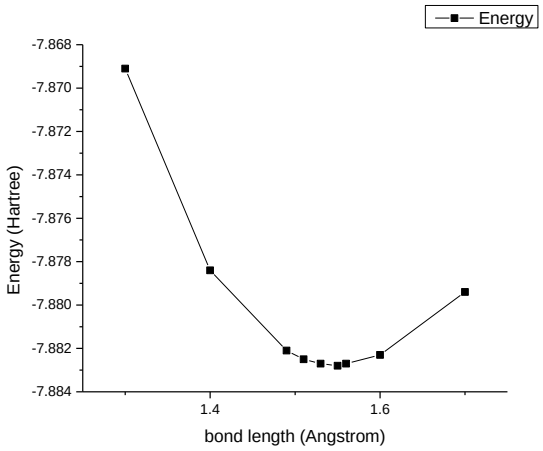

Fig. 3: Energy of the Lithium hydride molecule as a function of inter-atomic distance. At a distance of 1.55 Angstroms, the minimum here corresponds to the ground state. This also is in agreement with the experimentally measured value.

6. Conclusion

Here we have presented an introduction to the subject of quantum computing applied to the understanding of simple molecules like hydrogen and lithium hydride. Once understood, the method can be extended to more complex molecules. It is believed that by 2035, all computational chemistry will have essential subroutines based on quantum algorithms [8]. It is indeed going to be a 'quantum leap' in science and technology.

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