Original Article

Quantum computers based on nuclear magnetic resonance (NMR)

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ABSTRACT

One of the available methods for building a quantum computer involves the use of the concept of NMR. This concept is based on the molecules' nuclei spin states considered as qubits, and this technology utilizes a group of atoms, molecules, or even macromolecules. It is noted MRI and NMR have applications in the fields of chemistry, physics, molecular biology, and medicine. Moreover, quantum computers similar NMR utilizes molecules in which some of the atoms have nuclei behaving like spin systems. In addition, each nucleus has various energy levels, indicating different qubits. In this computational method, logical gates, including the CNOT, will play an integral role. The nanoscale NMR device is capable of demonstrating the characteristics of molecules, macromolecules, and cells in a non-invasive fashion, i.e., it can indicate the position of atoms without destroying them. This will significantly contribute to our understanding of molecules, macromolecules, and living cells. On the other hand, qubits are quantum sensors with a high sensitivity in order to be used for imaging a biomolecule. Hence, identifying the building of biological molecules can be highly important.

Keywords: Quantum computers, Qubit, Quantum algorithms, Biomolecules, Nuclear magnetic resonance

Introduction

The current study aims at exploring the relationship between the concept of quantum computers and nuclear magnetic resonance (NMR). The theory of quantum computers argues that such computers can utilize quantum mechanical characteristics to present and process information. Moreover, such computers can be utilized for searching huge databases in a very fast way; in comparison, conventional computers may take a long time to perform the same search [1].

Quantum mechanics describe the behavior of electrons, protons, atoms, and molecules. In addition, a quantum computer works based on controlling the superposition of states and a qubit is carrying out a large number of parallel operations [1,17].

Recently, a quantum computer was developed by IBM researchers. These qubits are programmed using RF (radio frequency) pulses, and they can be detected by NMR devices similar to those employed in hospitals. Moreover, researchers utilized NMR to manipulate particles inside the nuclei of the atoms in a number of molecules. In addition, scientists proposed a number of algorithms to be used with quantum computers. These algorithms provide various benefits differentiated to their usual counterparts. For instance, Grover's quantum algorithm provides a square root advantage over conventional algorithms.

Moreover, quantum computers use an exponential advantage over conventional ones since they are exponentially better in, for example, factoring numbers. If conventional computers were used for performing the same operation, they would need to be extremely huge can reach the same results [1-3].

Magnetic resonance imaging (MRI) is a non-invasive imaging method and it can only detect a small range of fields near the resonance frequency of the sensor. Resonance refers to the

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tendency of an object to oscillate with a higher energy at a particular frequency [4, 5].

Nanoscale MRI can display the characteristics of cells and macromolecules in a non-invasive manner, i.e., it can show the location of the atoms without destroying them [4, 5].

In order to recognize important and relevant problems and customize hardware and software to these particular cases, there is cooperation between quantum computing researchers and computational chemists and biochemists. The important point for a quantum computer relates to the fact that it can perform operations on all its possible inputs simultaneously. The result of a measurement can be extracted based on the wave function reduction, while such an expectation value for the observable is non-deterministic [1, 6, 7]. Using NMR on macroscopic ensembles of quantum spins, such as macromolecules or bio-macromolecules can provide a promising method for realizing a computational model to a certain extent. It is possible to program an NMR computer similar to a quantum computer; however, nuclear magnetic resonance computers limited over 50 bits [1, 4, 5].

In the NMR quantum computer, the molecule spins of a liquid specimen will be separated from the spins in all the other molecules. Each molecule is an independent quantum computer. The NMR spectrum is the sum of a certain number of observables over all the molecules in the specimen, and it is proportional to the average ensemble assumption value of the observable. Therefore, it can be said that an NMR quantum computer utilizes quantum mechanics at the molecular level to perform computations, followed by Using a form of classical parallelism to amplify the results to the macroscopic level [1, 4, 5].

Explanation

Quantum computing is still a highly theoretical concept, and quantum computers are not yet available for practical applications. Nonetheless, if quantum computers can be made, they will be perform calculations that take a lot of time by conventional computers in a very quick and easy fashion. Recently, there have been a number of developments in the field of quantum computing [1, 8, 9].

The modern world is a digital one, which is based on binary digits or bits. The value of a bit is either 0 or 1, indicating the electric charge state in a transistor or a chip. In the quantum realm, there are quantum bits, a.k.a. qubits. In contrast to bits, qubits can have states of 0 and 1 at the same time, along with any other state between these two. In 1995, Erwin Schrodinger proposed a paradox where a cat is put inside a closed box which also contains a radioactive substance. Since radioactive decompose is a random process, it cannot be said with certainty whether the cat inside the box is alive or not at any point in time. Similarly, an atom is in a state called the 'superposition state' where the atom is both decomposed and not at the same time. Following the above paradox, it is only when the box is extend that the cat will assume a certain state, i.e., being alive or dead. This paradox was developed by Schrodinger as an illustration for the superposition state in the quantum theory. Without performing the act of observation, we cannot be certain about the behavior of elements in any system [1, 2, 8, 9].

Under superposition conditions, two quantum systems are correlated with their states provided that their state is not observed or determined.

Similar to the cat paradox, the cat-state is recreated here in which two or more particles have the possibility of being in two distinct states. This is the first step for producing a logical operation between two qubits. Qubits that are in the cat state are highly significant and sensitive. These cat states will be decoupled as soon as there is even the smallest interference originated from outside the system [1, 8, 9].

Qubits can have many states concurrently, and they can perform a much larger number of mathematical computations compared to conventional bits. However, the quantum entanglement between the qubits must work properly. Qubits constitute the core components in quantum computing. An exponential volume of information can be encoded using superposition when the spin of a particle in the superposition is a linear combination of the up spin and down spin [1, 8, 9].

Among various quantum methods utilized for constructing small quantum computers, NMR can be considered unique. The liquid-state NMR is old and successful technology for constructing quantum computers [1, 10-12].

As it is widely known, magnetic resonance imaging (MRI) and nuclear magnetic resonance (NMR) are significant methods with important applications in medicine as well as biology. Peter Williston Shor proposed a method for utilizing entanglement and superposition to identify the prime factors on an integer in 1994. Quantum computer solve this problem in a much shorter runtime compared to the best available conventional computers [1, 11, 12].

Once researchers evaluated the discovery made by Shor, they realized that constructing an effective quantum computer would be immensely difficult. This is while any interaction between a system and its environment (e.g., the colliding between atoms) is a measurement. Once this happens, the superposition of quantum states collapses into a certain state which can be identified and measured by an observer. This is known as 'de coherence', further rendering quantum computation difficult. In order to mitigate this issue, quantum computers must carefully be isolated. For instance, using magnetic fields, a limited number of charged particles can be trapped, followed by cooling them into pure quantum states. However, even these difficult experiments are just basic and rudimentary quantum operations since these computers only have a small number of bits and they will lose their coherence very rapidly as energy levels vary. The parallel spin corresponds to 1, and the anti-parallel spin corresponds to 0. In any fluid, the number of opposing spins is equal. Once a field is applied, the generation of parallel spins is facilitated, resulting in a slight imbalance between the two states [1, 2, 8, 9].

Accordingly, the NMR methods apply different electromagnetic fields. In this method, in order to make some spins flip between the states, it is essential to apply an oscillating field with a suitable frequency. This will make it possible to redirect nuclear spins as necessary. As an example, a radio frequency of the magnetic field can be applied to protons placed in a fixed magnetic field, e.g., LOT, to change their direction [1, 8, 13-15].

Such radio waves will make the nuclear spins rotate about the direction of the oscillating field, which is configured in a way to have a right angle with the fixed field. In case the pulses of the oscillating radio frequency can be maintained for a sufficient time as to rotate the spins by 180 degrees, the additional magnetic nuclei Which were previously parallel to the fixed field will point in the opposite direction, i.e., the anti-parallel direction [1, 8, 14-16].

When a pulse with half the above duration is applied, the probability of the particles being aligned in parallel or anti-parallel will be equal. In other words, the spins will be in both states, i.e., 0 and 1. The classical representation of such conditions shows the spin axis of the particle with a 90-degree angle to the fixed magnetic field. Consequently, the spin axis of the particle will rotate about the magnetic field, which is looping around with a specific frequency. As a consequence, it will emit a small weak radio signal which can be detected by the NMR device. Each nucleus in an NMR experiment is capable of impacting its neighboring magnetic field. In liquids, the constant movement of molecules relatively will neutralize the majority of these local magnetic disturbances. Nonetheless, a magnetic nucleus can impact another magnetic nucleus in the same molecule since it interferes with the electrons that are orbiting around both of them [1, 8, 13-15].

A logic gate (e.g., a controlled NOT gate) can be generated using two nuclear spins due to the above-mentioned interaction inside the molecule.

The rotations applied to the spins and the controlled NOT gate (C-NOT gate) can be utilized for performing quantum computations. In a quantum logic gate, the underlying spins can be in superposition of up spin and down spin. Hence, quantum computation can be applied to a combination of apparently incompatible inputs [1, 8, 9].

Considering the NMR devices available at the moment, the quantum computers that can be constructed can only have approximately 10 qubits.

The lowest rate at which the spins flip around will be the measure for determining the effective cycle time of a quantum computer. However, increasing the size of quantum computers to a level that can enable them to compete with the fastest conventional computers is highly difficult. However, if this is done, the quantum computers will be the best natural laboratories to investigate the principles of the quantum theory [1, 4, 5, 8, 9].

Moreover, quantum computers can be useful for solving problems raised when trying to design traditional microchips with significantly small transistors. When these microchips is reduced to the possible limit, they will act similar to quantum mechanical phenomena [1, 2, 4, 8, 9].

Scientists have come up with algorithms that can be run on quantum computers in order to increase the accuracy and speed of medical imaging. Of course such computers have not yet been constructed. These developments might be able to contribute to the treatment of various types of diseases, including different types of cancers. Interestingly, scientists have developed quantum algorithms in order to enhance the process of running computations on available hardware. Quantum computing can provide various applications, including the MRI of the body or groups of cells or molecules inside the cells. When working with such small sizes, conventional MRI methods cannot provide good performance. Therefore, it is essential to construct a new apparatus to perform such works that require immense precision [1, 2, 5, 6, 8, 9].

When trying to construct such a device, one of the significant challenges was the measure a magnetic field in a sufficiently accurate way using the resonance of single electrons inside a molecule [1, 2, 8, 13-15].

With regards to MRI, only a narrow range of fields generated by molecules adjacent to the resonance frequency of the sensor can be detected, which makes the imaging process very difficult. In order to mitigate this issue, it is necessary for highly advanced image processing methods to fully understand the subject of the imaging. However, such methods require using various software applications to deal with the limitations of the hardware, making the required time for scans much longer, while also making the interpretation process very difficult [1, 2, 8, 14-16].

Quantum computing provides a much better way to master the hardware restrictions and to obtain an image of the entire magnetic field. The researchers were able to improve the ratio of maximum detectable field strength to the field precision by expanding the field, reaching twice the ratio obtained by the conventional method. In a nanoscale MRI device, atoms are configured in a way that the atoms are not destroyed, while in the currently available methods, some samples are destroyed [6, 7, 14, 15].

It is also worth mentioning that quantum computers process power and speed levels not seen before. For instance, physicians can utilize quantum computers to find diagnoses or treatment methods they would never be able to find on their own. With regards to precision medicine, quantum computers can allow physicians to completely understand the disease of a patient. Having access to such information will allow physicians to produce the most effective treatments customized based on the characteristics of individual patients, such as their gender, age, genetic makeup, race, and so on. Quantum computers will be utilize a database of molecule structures with amazing speeds, study each cell or tissue, and significantly enhance the speed of treatment and medicine design. Moreover, physicians will be employ quantum computers to simulate clinical trials with remarkable efficiency [1, 8, 9, 11, 14, 15].

By visualizing individual macromolecules, quantum computers will be produce significantly accurate imaging results, which can then be utilized for training algorithms to pinpoint changes and anomalies in the quickest way possible. Moreover, such computers can facilitate high-speed drug design, in-silico clinical trials simulated using virtual humans, quick sequencing and analysis of the whole genome, transferring hospitals to the cloud, creating predictive healthcare mechanisms, and securing medical data using quantum uncertainty [1, 2, 8, 9].

Quantum computers can evaluate all possible molecules in a significantly short time, and drug tests can be performed based on any potential cell model or simulated human tissue [1, 2, 8, 9].

It should be mentioned that in-silico clinical trials can be performed without using human subjects or even real human cells to evaluate a potential treatment or drug, while it will provide a precise description of the impact of the selected treatment or drug. In this method, a simulation will be used to evaluate the impacts of a medical drug, device, or treatment [14-16].

However, the current available technology and the current understanding of molecular biology do not allow completely-simulated clinical trials. However, such trials will have amazing benefits and advantages over in-vivo trials. Quantum computers can contribute significantly to the achievement of simulating virtual humans, which will include equations and variables such as body fluids, hormones, electrolytes, metabolism, and even skin temperature. Quantum computers will allow an unlimited number of clinical trials using virtual human subjects, significantly reducing the time needed for such trials, while also maximizing their quality and comprehensiveness [1, 8, 9, 12, 14, 15].

Conclusion

The environment has a significant impact on superposition states, so these states use as highly accurate and sensitive sensors in order to reduce the cost and minimize the size of components such as lasers [1-4].

In order to measure very small magnetic fields, solid-state quantum sensors can be utilized, which will have several applications in the fields of biosensors, MRI, and so on [1-4].

Quantum imaging devices will use entangled light to obtain more information from light during the imaging process, which will hugely contribute to the improvement of imaging technologies. Moreover, various quantum computers have been proposed based on different platforms. Many of these platforms and architectures illustrate the underlying principles of quantum computing based on solid-state systems and atomic systems. Nuclear spins in solids are an example of the former, while nuclear spins in macromolecules and molecules are an example of the latter [1, 2, 13-15].

In addition, the distinguishing characteristic of NMR or MRI compared to other quantum methods is the fact that these have already been utilized to construct small quantum computers. For instance, NMR facilitated the first complete application of a quantum algorithm. Moreover, the liquid-state NMR is the most successful and one of the oldest quantum technologies [1, 2, 10, 14, 15].

Considering this success, it may be surprising that some previous studies have argued that NMR would be limited to quantum computers with only about 10 qubits. However, many new estimates are around 10 to 20 qubits. This shows that compared to the majority of other potential quantum technologies, the limitations of NMR are clear and understood [1, 2, 10, 14, 15].

Quantum computers have amazing contributions to the field of medical science, and algorithms based on quantum computing can provide better ways for diagnosing various diseases [1, 13, 15, 16].

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