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The simulation of virus life cycle with quantum gates

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ABSTRACT

Quantum physics and molecular biology are two disciplines that have evolved relatively independently. However, recently a wealth of evidence has demonstrated the importance of quantum mechanics for biological systems and thus a new field of quantum biology is emerging. There are many claims that quantum mechanics plays a key role in the origin and/or operation of biological organisms. We consider the nucleonic acid of virus as a quantum system in this paper and discuss virus life cycle from the view-point of quantum and simulate it using quantum gates for the first time. The maximally entangled states show infected cell can change to entire cell, the virus can switch from the lysogenic to the lytic and the prophages can remain latent in the bacterial chromosome for many generations.

1. Introduction

Erwin Schrödinger believed that quantum mechanics, or some variant of it, would soon solve the riddle of life. His insight has inspired many researchers to investigate the molecular basis of a living organism, so quantum mechanics might play a key role in biology [1]. Davies has discussed that quantum theory fills a missing link in existing models of the origins of life, of which there are many. His astrobiology research has focused on the origin of life [2]. Very exciting work on microtubules and consciousness has been presented by Hameroff and Penrose [3]. They have brought together fundamental physics and biology and have developed the "Orch OR" (orchestrated objective reduction) model of consciousness based on quantum computation in brain microtubules. Nanopoulos has made several contributions to particle physics and cosmology working on string unified theories, fundamentals of quantum theory, astroparticle physics and quantum-inspired models of brain function [4]. Popp's research group has coined the term biophotons to express the biological origins and the quantum character of this radiation [5]. In addition, there is evidence to support the idea that biophotons are responsible for triggering some biochemical reactions in and between cells. Quantum effects can be related to many biological processes. There are electromagnetic field effects involving for example water, biomolecules, cells, and living organisms [6]. Fraser has amassed evidence for how a quantum electrodynamics field, which he calls the human body-field, underlies and controls the biochemical activities of the body [7]. McFadden has worked controversial areas the origin of life and consciousness; his quantum evolution's book has hypothesis that genetic mutation can be adaptive, or directed through quantum effects [8]. To be sure, biology systems are quintessential information processors. Pati has researched in quantum information, quantum computation and quantum mechanics of bio-systems [9]. Matsuno has argued that actomyosin functions as a heat engine (a device that converts heat energy into mechanical energy) is able to maintain a constant velocity due to quantum mechanical coherence and entanglement [10]. Cope has produced pivotal work linking physics and biology, and developed a solid-state theory of biological processes. He has deduced that the activity in the cell is not just electrochemical, and looked at the cell function as if the organelles were three-dimensional semiconductors [11].

DNA is what makes up your genes and stores all the information about you inside your cells; it is also "Ariadnes magic ball of thread" for understanding point of departure of information physics. Replication of DNA and synthesis of proteins have been studied from the view-point of quantum database search [12]. The structure of DNA and protein reveals that life has indeed taken the route of digitizing its information. DNA and RNA chains use an alphabet of 4 nucleotide base, while proteins use an alphabet of 20 amino acids. The molecular structure of DNA has been studied by Patel. He has worked on quantum algorithms, and has used concepts from information theory to understand the structure of genetic languages [13]. DNA has been studied from the view-point of computer science [14]. DNA computing is an alternative method of performing computations. It is based on the observation that in general it is possible to design a series of biochemical experiments involving DNA molecules which is equivalent to processing information encoded in these molecules. Nagland et al. established fundamental theories about biophotons and cell growth and differentiation, essential differences between a tumor tissue and a normal one, some experimental evidence of

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DNA as source of biophotons and theoretical models like the exciplex model [15]. They hypothesized that the scattering patterns of photons of cells contained information about viral (or bacterial) infections. The virologist Lipkind found the first indications of assessing virus infections by biophotons.

Thus there are many claims that quantum mechanics plays a key role in the origin and/or operation of biological organisms and we can consider the DNA molecule as a quantum system. Purpose of this paper is relation between quantum mechanics and biology. It means the mechanism of living systems can be explained by quantum. Thus we have studied the mechanism of infected cell by virus from a quantum point of view. We have simulated virus life cycle by quantum gates for the first time. This simulation produces superposition of two maximally entangled states and shows infected cell can change to entire cell with probability 25 percent, the virus can switch from the lysogenic to the lytic with probability 25 percent and the prophages can remain latent in the bacterial chromosome for many generations with probability 50 percent.

2. Virus and its life cycle

Viruses can cause the death of their host cells by eliminating, through many systems, the host cells potential to perform the proton motile force, which at last of all is the main characteristic of the quantum energy state of life, be by synthesizing viral proteins, or by destroying the liposome's membranes, the chloroplasts' membranes, the mitochondria's membranes, or the whole cell membrane. Viruses are extremely small and cannot be viewed with a light microscope, ranging in size 20–1400 nm in length and burst time ranges from 20 to 40 min. Furthermore today DNA is regarded not as magic matter but as a computer—an information-processing and replicating system of astonishing precision. Anton Zeillinger's group in Vienna has demonstrated that the fullerene molecule, composed of 60 carbon atoms (the famous "buckyball"), can pass through two slits simultaneously [16]. Few physicists doubt that as the technology advances, bigger and more complex systems will be shown to inhabit the quantum world. Fullerene molecules are spheres with a diameter similar to that of the DNA double helix. If fullerene can enter the quantum multiverse then DNA may do the same so we can consider virus genetic matter or even virus as a quantum system.

There are many variations of life cycle of a virus depending on the type of virus and the host, but in general this cycle can be described by: (1) recognition of host, (2) genetic material enters host, (3) replication using host nucleotides, (4) protein synthesis using host enzymes, ribosomes, tRNA, ATP, (5) self-assembly of capsids and packaging of genome, (6) release from host.

We first investigate bacteriophage (or phage which is a virus that infects bacteria) life cycle because there are many similarities between bacteriophages and animal cell viruses, thus bacteriophage can be viewed as model systems for animal cell viruses. In addition knowledge of the life cycle of bacteriophage is necessary to understand one of the mechanisms by which bacterial genes can be transferred from one bacterium to another. Then, we have tried modeling phage life cycle from the view-point of quantum.

There are two primary types of bacteriophages: lytic bacteriophages and temperate (latent) bacteriophages. Bacteriophages that replicate through the lytic life cycle are called lytic bacteriophage. During a lytic cycle, the bacteriophage uses the replication machinery of the bacterial cell to make many copies of its viral genome and to produce structural proteins of the phage head and tail. After phage DNA genomes are packaged into phage particles, the cell lyses (ruptures), releasing progeny phage capable of infecting other bacteria. Bacteriophages capable of a lysogenic life cycle are termed temperate phages. During a lysogenic life cycle, the phage's DNA is inserted into the circular bacterial chromosome. The viral genome remains dormant in the bacterial chromosome, being replicated and passed to progeny bacteria along with host DNA sequences. When an appropriate signal (e.g. environmental stress, UV light) impacts the bacterium, the viral plasmid genome is excised from the bacterial chromosome, and the phage initiates a typical lytic cycle.

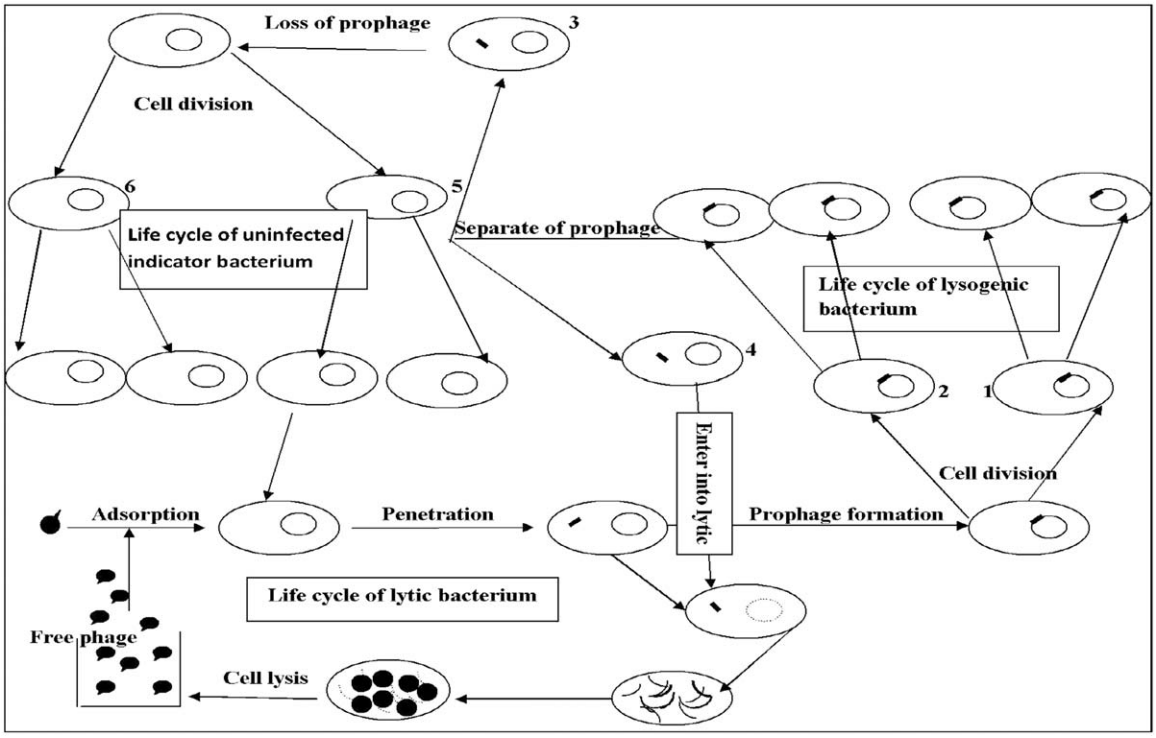

Fig. 1. The virus life cycle (lytic and lysogenic cycles).

We have designed virus life cycle (lytic and lysogenic cycles) in Fig. 1 that can be described as follows:

(a) Adsorption or attachment: In this step, the phage attaches to the wall of the bacterial cell. This is a highly specific interaction dependent upon the binding of the phage to specific receptors on the cell surface.
(b) Penetration: In this step, the phage genome passes through the bacterial cell wall and enters the cytoplasm. This occurs within seconds of adsorption and in the vast majority of cases, the capsid and additional structural elements remain outside of the bacterial cell. Enzyme such as lysozyme is used to weaken the cell wall so that the genome can pass through.
(c) Prophage formation: In this step, phage inserts its genome into the bacterial nucleotide to become a prophage that is virial DNA incorporated into host chromosome.
(d) Virus replication: Every time the bacterial chromosome is replicated, prophage genetic material is also replicated.
(e) Cell division: Cell divides, and virus chromosomes are transmitted to daughter cells thus both cells have viral DNA. These cells may exhibit new properties.

3. Quantum mechanics, quantum gates and circuits

We have used qubit because the beauty of treating qubits as abstract entities is that it gives us the freedom to construct a general theory of quantum computation and quantum information which does not depend upon a specific system for its realization. Two possible states for a qubit are the states $|0\rangle$ and $|1\rangle$, which as you might guess correspond to the states 0 and 1 for a classical bit. The difference between bits and qubits is that a qubit can be in a state other than $|0\rangle$ or $|1\rangle$. It is also possible to form linear combinations of states, often called superpositions:

$$|\psi\rangle = a|0\rangle + b|1\rangle \tag{1}$$

The numbers a and b are complex numbers, although for many purposes not much is lost by thinking of them as real numbers. Put another way, the state of a qubit is a vector in a two-dimensional complex vector space. The special states $|0\rangle$ and $|1\rangle$ are known as computational basis states, and form an orthonormal basis for this vector space [17]; qubits can store more data than bits too.

We have simulated virus life cycle (lysogenic cycle) with Hadamard and controlled-NOT (CNOT) gates. The quantum circuit has been shown for this cycle in Fig. 2. We have just a two-qubit circuit. The quantum circuits are similar to classical computer circuits in that they consist of wires and logical gates. The wires are used to carry the information, while the gates manipulate it (note that the wires do not correspond to physical wires; they may correspond to a physical particle, a photon, moving from one location to another in space, or even to time-evolution). The state of bacterium (host DNA) and virus (phage genome) genetic material are denoted by $|0\rangle$ and $|1\rangle$, respectively. The initial input state is denoted by $|\psi_0\rangle = |0\rangle|1\rangle = |01\rangle$ that shows

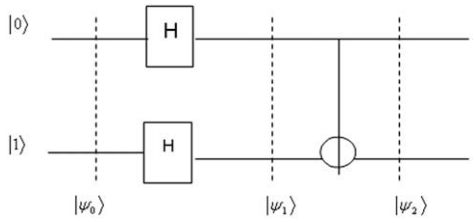

Fig. 2. The quantum circuit of the lysogenic life cycle.

prophage formation during the lysogenic life cycle of a temperate bacteriophage (see Fig. 1).

We have used Hadamard gate for replication of host genetic material and replication of virus genomic nucleic acid. While the bacterium replicates, the prophage replicates as a part of the bacterium's nucleotide and nucleic acid of virus becomes part of the host cells' DNA. The Hadamard operator on the upper line (host DNA) and the lower line (phage genome) of the circuit convert $|0\rangle$and $|1\rangle$ into $1/\sqrt{2}(|0\rangle \pm |1\rangle)$, we can load simultaneously both $|0\rangle$ and $|1\rangle$; thus, the Hadamard gate acts on one qubit, and places it in a superposition of $|0\rangle$ and $|1\rangle$.A quantum gate can be represented as a matrix, which is directly derived from the linearity of quantum gates.The Hadamard operation H and the effect of the Hadamard gate on qubits are defined by

$$H = \frac{\sqrt{2}}{2}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \qquad H|1\rangle = \frac{\sqrt{2}}{2}(|0\rangle + |1\rangle)$$
$$H|0\rangle = \frac{\sqrt{2}}{2}(|0\rangle + |1\rangle) \tag{2}$$

The CNOT gate describes cellular division since the CNOT gate acts on two qubits and this gate is useful for demonstrating one particularly fundamental property of quantum information. The single-qubit operations and the CNOT gate constitute a universal set of gates [18]. The CNOT operation and the effect of the CNOT gate on qubits are as following:

$$CNOT = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix}, \quad \begin{matrix} CNOT|00\rangle = |00\rangle \\ CNOT|01\rangle = |01\rangle \\ CNOT|10\rangle = |11\rangle \\ CNOT|11\rangle = |10\rangle \end{matrix} \tag{3}$$

In Fig. 2, $|\psi_1\rangle$ is the state of the system prior to applying the CNOT gate. It is represented by

$$|\psi_1\rangle = \left[\frac{|0\rangle + |1\rangle}{\sqrt{2}}\right]\left[\frac{|0\rangle - |1\rangle}{\sqrt{2}}\right] = \frac{1}{2}(|00\rangle - |01\rangle + |10\rangle - |11\rangle) \tag{4}$$

In Fig. 2, $|\psi_2\rangle$ is the state of the system after applying the CNOT gate. It is represented by

$$|\psi_2\rangle = \left[\frac{|0\rangle - |1\rangle}{\sqrt{2}}\right]\left[\frac{|0\rangle - |1\rangle}{\sqrt{2}}\right] = \frac{1}{2}(|00\rangle - |01\rangle + |11\rangle - |10\rangle) \tag{5}$$

Thus Fig. 2 has two Hadamard gates followed by a CNOT gate. The Hadamard gates take the input $|\psi_0\rangle$ to $|\psi_1\rangle$, and then the CNOT gate gives $|\psi_2\rangle$ as the output state.

4. Discussion and results

We have shown the virus life cycle (lytic and lysogenic cycles) and the quantum circuit for lysogenic cycle in Figs. 1 and 2, respectively. The quantum circuit has been simulated with the Hadamard and CNOT gates. The replications of host and virus genetic material have been described by Hadamard gates. We have used the CNOT gate to describe cell division. From Fig. 1, it can be seen that the Hadamard gates change the input state ($|\psi_0\rangle$) to $|\psi_1\rangle$ and finally, the CNOT gate takes the input $|\psi_1\rangle$ to $|\psi_2\rangle$. We can generate the linear combination of Bell states with two Hadamard gates and a CNOT gate that has been explained by state $|\psi_2\rangle$. This state is formed after cell division in lysogenic life cycle of a temperate bacteriophage, then, we can write

$$|\psi_2\rangle = \left[\frac{|0\rangle - |1\rangle}{\sqrt{2}}\right]\left[\frac{|0\rangle - |1\rangle}{\sqrt{2}}\right]$$
$$= \frac{1}{\sqrt{2}}\left[\frac{1}{\sqrt{2}}(|00\rangle + |11\rangle) - \frac{1}{\sqrt{2}}(|01\rangle + |10\rangle)\right]. \tag{6}$$

Eq. (6) represents superposition of two maximally entangled states. The state $1/\sqrt{2}(|00\rangle+|11\rangle)$ is maximally entangled state and shows separation of prophage. The state $|00\rangle$ shows step of loss of prophage, that cell is entire and describes life cycle of uninfected indicator bacterium (see Fig. 1). This state is with probability 25 percent. We can conclude infected cell changes to entire cell. State $|11\rangle$ shows the virus can switch from the lysogenic to the lytic. This state usually happens with an environmental trigger, such as radiation or the presence of certain chemicals that is a spontaneous event, and it may cause the virus to break out of its latent state and enter into lytic cycle. This state is with probability 25 percent. An example of a virus that enters the lysogenic cycle is herpes, which first enters the lytic cycle after infecting a human, then the lysogenic cycle before traveling to the nervous system where it resides in the nerve fibers as an episomal element. After a long period of time (months to years) in a latent stage, the herpes virus is often reactivated to the lytic stage during which it causes severe nervous system damage.

The state $1/\sqrt{2}(|01\rangle+|10\rangle)$ is maximally entangled state which $|10\rangle$ and $|01\rangle$ show the prophages can remain latent in the bacterial chromosome for many generations. This state is life cycle of lysogenic bacterium (see Fig. 1). From Eq. (6) it follows that the probability for observing state $1/\sqrt{2}(|01\rangle+|10\rangle)$ is 50 percent and this describes the bacterium reproduces normally, copying the prophage and transmitting it to daughter cells and this produces a colony of bacteria with prophage.

5. Conclusion

The entanglement is one of the strangest phenomena in physics, and it is also a computational resource. If two particles are entangled, measuring one of them will lead to a correlated result when the other is measured. While measurement of the first particle gives a random result, the state of the second particle will be fixed. Ability of particles to be entangled gives rise to many interesting and useful applications, e.g. quantum teleportation.

In the cell division process the cells are evenly divided to two cells in lysogenic cycle, which can be entangled with each other; it means daughter cells are EPR pairs, according to the EPR theory. Entangled states were first investigated in the famous paper of Einstein, Podolsky and Rosen (EPR) [19].

Using quantum gates we are able to stimulate the lysogenic cycle for the first time. In this quantum circuit, the qubits are passed through two Hadamard gates and then both qubits are entangled by a CNOT gate (in Fig. 2). It means that the CNOT gate tangles quantum states of nucleic acids both host and virus into a single bipartite quantum state; such bipartite state stores information within the entanglement. After cell division, the cells of life cycle of lysogenic bacterium (cells 1 and 2 in Fig. 1) can be entangled with each other. Consequently, we believe the life cycle of lysogenic is stopped and prophages cannot remain latent in the bacterial chromosome for many generations when each factor destroys this entanglement. The cells that are separated of phage (cells 3 and 4) are entangled together to prevent from virus entry to lytic cycle. This entanglement has to be destroyed. The cells of life cycle of uninfected indicator bacterium (cells 5 and 6) are entangled together. This entanglement does not have to be destroyed when virus losses prophage and enters into cycle of uninfected.

One of fundamental and characteristic differences between classical and quantum information is the no-cloning theorem. This theorem says that copying of quantum states is prohibited. A number of different versions of the no-cloning theorem have been published [20]. The cell division produces daughter cells that have all the genetic material of the parent cell; according to this theory, information in daughter cells is not same information in parent cell because quantum states cannot be copied. From the no-cloning theorem, it results that information in virus genetic material differs from generation to generation in life cycle of lysogenic. It means that the baby does not have the same virus phage genome of its mother or father but the baby has virus genetic material with new properties and information.

Conflict of interest statement

None declared.

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