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Quantum Mechanical Mechanism of DNA Forming and Replicating

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Abstract

DNA, deoxyribonucleic acid, carrying encoded genetic information at molecular level, is the most significant discovery in the history of genetics. Previous researches on DNA included topics of bases, base-pairing, hydrogen bonds, structure, base sequence, dynamics, replication and mutation. DNA must duplicate itself, and so DNA structure and DNA replication are the fundamental problems. Watson and Crick described the structure and the mechanism for replication of DNA. Other authors focused their studies on DNA replication. DNA molecules are micro-entities ruled by laws of quantum mechanics, but the mechanisms, found previously of DNA forming and replicating, were not explored by applying quantum mechanics. Here we show that controlled by quantum mechanics, the quantum state of DNA is a bio-quantum-entangled state, the mechanism of DNA forming and replicating is a process of bio-quantum entangling, de-entangling and re-entangling. This bio-quantum mechanical result is different from the conventional biochemical descriptions of DNA structure and replication. DNA genetics is bio-quantum genetics in nature. With this deep understanding, reform and progress should be expected for further development of genetics.

Keywords

Quantum State of DNA, Bio-Quantum Genetic Mechanism of DNA Forming and Replicating, Process of Bio-Quantum Entangling, De-Entangling and Re-Entangling, Quantum Mechanics, Quantum Computation, Quantum-Genes or Soft-Genes

1. Introduction

The post-World War Two discovery brought about a revolution in genetics. Watson, Crick, Wilkins and Franklin established the three-dimensional structure of

DNA [1]-[7]. DNA, carrying encoded genetic information at molecular level, is the most important discovery in the history of genetics. Authors published research works related to DNA.

Authors studied the relative importance of hydrogen bonding and base-pair stacking to the structure, stability, and functions of DNA [8]; reconciliation of theory and experiment of hydrogen bonding in DNA base pairs [9]; the nature and role of hydrogen bonds in DNA base pairs [10] [11]; the strength of individual hydrogen bonds in DNA base pairs [12]; the theory of the electronic structure of four periodic B-DNA models [13]; the theoretical analysis of the structural and thermodynamic parameters of complementary adenine-thymine, adenine-uracil, and guanine-cytosine base pairs with hydrogen bonds by density functional methods [14].

A number of researches discussed dynamics of DNA [15]-[32].

Bashar Ibrahim suggested modeling of DNA segregation mechanism [33].

Watson and Crick described a mechanism for DNA replication [3] [4]. Kang Cheng and Chang Hua Zou proposed a 3-D physical model to explain how a complete functional DNA polymerase traps a deoxyribonucleoside triphosphate, and how it moves along a DNA template strand in DNA replication [34]. They suggested a model of the separation of nucleotide sequences and the unwinding of a double helix in DNA replication process [35]. They developed their informatics and physics models for natural DNA replication, beyond lengths of chemical bounds; half quantitatively elucidate a probability of the wrong paring [36]. Based on experimental findings, Anneke Bruemmer, Carlos Salazar, Vittoria Zinzalla, Lilia Alberghina and Thomas Hoefer suggested a mathematical model of the molecular network leading to the activation of replication origins [37]. Ahmad A. Rushdi published a mathematical model of DNA replication, denoting the genetic replication channel. A novel formula for the capacity of this channel is derived, and an example of a symmetric replication channel is studied. Rigorous deduction of the channel flow capacity in DNA replication secures accurate understanding of the behavior of different DNA segments from various organisms [38]. Olivier Hyrien & Arach Goldar studied eukaryotic DNA replication by mathematical modelling [39].

Application of quantum mechanics to life science leads to development of quantum biology. Schrodinger's publication "What Is Life" is considered as the origin of quantum biology [1] [40]. In relation to DNA, Bernard Pullman reviewed developments in the quantum mechanical studies on the electrical structure of the nucleic acids [41]. Richard H. Steele introduced quantum physics into biology in an intuitive way, discussed the quantization of simple systems in quantum theory. Theoretical calculations for a helical DNA system gave a conduction resistance in agreement with a experimentally determined parameter [42]. Lian-Ao Wu, Stephen S. Wu, and Dvira Segal used an approximate method in quantum mechanics to demonstrate a universal DNA breathing dynamics [43]. Yi-Fang Chang studied extensive quantum theory of DNA [44].

Previously, I proposed the System of Bio-Quantum Genetics, suggested the Bio-Quantum Genetic Model of Plant Heredity and the Bio-Quantum Genetic Model of Human Genetics [45]. DNA molecules are micro-entities, ruled by laws of quantum mechanics. DNA genetic information is quantum information in nature. In the present paper, I discuss DNA forming and replicating process within the theoretical framework of the System of Bio-Quantum Genetics [45], obtaining a bio-quantum mechanical result theoretically.

The conventional theory of DNA established by Watson and Crick is biochemical [3]. In this paper I develop a bio-quantum mechanical theory of DNA. I establish the bio-quantum states of the bases with the orthonormality by means of Dirac Notation, the bio-quantum states of the base pairs by bio-quantum pairing. I construct the normalized bio-quantum-entangled state of DNA by bio-quantum entangling of the DNA bio-quantum subsystems. The bio-quantum-entangled state of DNA is separated by bio-quantum de-entangling into two templates for replication. Then two replication partners are found by means of quantum computation. Finally, two duplicates of the original DNA are formed by bio-quantum re-entangling of the templates and the partners for replication.

In terms of quantum genetic information, DNA is a bio-quantum-entangled state, DNA forming and replicating is a process of bio-quantum entangling, de-entangling and re-entangling. DNA genetics is bio-quantum genetics in nature.

I understand that quantum mechanics and quantum computation control the DNA forming and replicating process. On the other hand, every generation of DNA obeys the fundamental principles of quantum mechanics. In other words, the fundamental principles of quantum mechanics are inherited by every generation of DNA. Therefore, I define, logically and biologically, the “software”, the fundamental principles of quantum mechanics: superposition, uncertainty and entanglement (and de-entanglement), the rules of mathematical inference in quantum mechanics and Grover’s fast quantum mechanical algorithm for database search as the quantum-genes or soft-genes of DNA forming and replicating [45].

The bio-quantum DNA is different from the classical or biochemical DNA. The key differences between the classical and quantum aspects of DNA are:

A. The two chains of classical DNA are held together by hydrogen bonds between the bases [3], while the quantum DNA is formed by bio-quantum entangling of the quantum states of the bases.

B. The classical DNA chains separate by breaking of hydrogen bonds [3], while the quantum state of DNA separates by quantum de-entangling, during the DNA replication process.

C. The free nucleotides (strictly poly-nucleotide precursors) attach themselves, by forming hydrogen bonds, onto the moulds, the separated DNA chains, to create the DNA duplicates, in the classical biochemical DNA model [3], while the bio-quantum states of templates and the bio-quantum states of partners are entangled to create the bio-quantum states of DNA duplicates in the bio-quantum DNA model.

2. Bio-Quantum Genetic DNA

The conventional biochemical DNA of Watson and Crick was constructed by the two chains held together by hydrogen bonds [3]. Now our bio-quantum genetic DNA is a bio-quantum system, formed by its two bio-quantum subsystems entangled.

3. The Bio-Quantum States of the Bases

The bases, adenine, thymine, guanine and cytosine, are a complete set of independent basic genetic information elements of DNA, in terms of biological chemistry. Translated into quantum mechanics, their quantum states are a complete set of "basic vectors" for construction of DNA quantum state or vector in Dirac representation. Therefore, we define their bio-quantum states, by means of Dirac Notation [46] [47], as

$$\begin{gathered} |A\rangle \equiv |b_1\rangle \\ |T\rangle \equiv |b_2\rangle \\ |G\rangle \equiv |b_3\rangle \\ |C\rangle \equiv |b_4\rangle \end{gathered} \tag{1}$$

with the orthonormality

$$\langle b_i | b_j \rangle = \delta_{ij} \qquad (i, j = 1,2,3,4) \tag{2}$$

4. The Bio-Quantum States of Base Pairs

Pairing bases leads to bio-quantum states of base pairs. Then the bio-quantum states of adenine-thymine (A-T) pair, thymine-adenine (T-A) pair, guanine-cytosine (G-C) pair and cytosine-guanine (C-G) pair, are

$$\begin{gathered} |A\rangle|T\rangle = |b_1\rangle|b_2\rangle \equiv |p_{12}\rangle \\ |T\rangle|A\rangle = |b_2\rangle|b_1\rangle \equiv |p_{21}\rangle \\ |G\rangle|C\rangle = |b_3\rangle|b_4\rangle \equiv |p_{34}\rangle \\ |C\rangle|G\rangle = |b_4\rangle|b_3\rangle \equiv |p_{43}\rangle \end{gathered} \tag{3}$$

with the orthonormality

$$\begin{aligned} \langle p_{ik} | p_{jl} \rangle &= \langle b_k | \langle b_i | b_j \rangle | b_l \rangle \\ &= \langle b_k | \delta_{ij} | b_l \rangle = \delta_{ij} \langle b_k | b_l \rangle \\ &= \delta_{ij}\delta_{kl} \qquad (i, j, k, l = 1,2,3,4) \end{aligned} \tag{4}$$

Equation (4) is the normalizing condition of the bio-quantum state of DNA.

5. Forming DNA by Bio-Quantum Entangling

Suppose that the DNA system consists of s base pairs. Then the bio-quantum states of its two subsystems are

$$c_1 \sum_{r=1}^{s} |b_i\rangle_r \tag{5}$$

and

$$c_2\sum_{r=1}^{s}\left|b_j\right\rangle_r \tag{6}$$

respectively.

Obeying the purine-pyrimidine pairing regulation, entangling the two subsystems forms the DNA. Then the bio-quantum state of the DNA is

$$\left|DNA\right\rangle = c_1c_2\sum_{r=1}^{s}\left(\left|b_i\right\rangle_r\left|b_j\right\rangle_r\right) = c_1c_2\sum_{r=1}^{s}\left|p_{ij}\right\rangle_r \tag{7}$$

If the DNA system consists of g A-T pairs, h T-A pairs, m G-C pairs and n C-G pairs, then the bio-quantum state of the DNA is

$$\begin{aligned}&\left|DNA\right\rangle = c_1c_2\left(g\left|p_{12}\right\rangle + h\left|p_{21}\right\rangle + m\left|p_{34}\right\rangle + n\left|p_{43}\right\rangle\right),\\&g+h+m+n=s.\end{aligned} \tag{8}$$

according to Equation (7).

Under the normalizing condition Equation (4), the normalizing of the bio-quantum state of DNA in Equation (8) is

$$\begin{aligned}&\left\langle DNA\middle|DNA\right\rangle = c_1{}^2c_2{}^2\left(g^2\left\langle p_{12}\middle|p_{12}\right\rangle + h^2\left\langle p_{21}\middle|p_{21}\right\rangle\right.\\&\left.+m^2\left\langle p_{34}\middle|p_{34}\right\rangle + n^2\left\langle p_{43}\middle|p_{43}\right\rangle\right)\\&=c_1{}^2c_2{}^2\left(g^2+h^2+m^2+n^2\right)\\&=1\end{aligned} \tag{9}$$

It is from Equation (9) that

$$\begin{aligned}&c_1c_2 = \frac{1}{\sqrt{M}},\\&M = g^2+h^2+m^2+n^2.\end{aligned} \tag{10}$$

The normalized bio-quantum-entangled state of DNA

$$\begin{aligned}&\left|DNA\right\rangle = \frac{1}{\sqrt{M}}\sum_{r=1}^{s}\left|p_{ij}\right\rangle_r = \frac{1}{\sqrt{M}}\sum_{r=1}^{s}\left(\left|b_i\right\rangle_r\left|b_j\right\rangle_r\right)\\&M = g^2+h^2+m^2+n^2,\\&s = g+h+m+n,\end{aligned} \tag{11}$$

is well established from Equations (7), (8), (9) and (10).

6. Separating DNA by Bio-Quantum De-Entangling

It is from Equation (11) that

$$\begin{aligned}\left|DNA\right\rangle &= \frac{1}{\sqrt{M}}\sum_{r=1}^{s}\left|p_{ij}\right\rangle_r = \frac{1}{\sqrt{M}}\sum_{r=1}^{s}\left(\left|b_i\right\rangle_r\left|b_j\right\rangle_r\right)\\&=\frac{1}{\sqrt{M}}\left[\left|b_i\right\rangle_1,\left|b_i\right\rangle_2\ldots\left|b_i\right\rangle_s\right]\begin{bmatrix}\left|b_j\right\rangle_1\\\left|b_j\right\rangle_2\\.\\.\\.\\\left|b_j\right\rangle_s\end{bmatrix}\end{aligned} \tag{12}$$

From Equation (12), the bio-quantum-entangled state of DNA is de-entangled into

$$\left[\left|b_i\right\rangle_1,\left|b_i\right\rangle_2\ldots\left|b_i\right\rangle_s\right]\equiv\left|Temp_i\right\rangle, \tag{13}$$

and

$$\begin{bmatrix}\left|b_j\right\rangle_1\\ \left|b_j\right\rangle_2\\ \cdot\\ \cdot\\ \cdot\\ \left|b_j\right\rangle_s\end{bmatrix}\equiv\left|Temp_j\right\rangle \tag{14}$$

The DNA system is separated. The bio-quantum states $\left|Temp_i\right\rangle$ and $\left|Temp_j\right\rangle$ are the bio-quantum states of DNA subsystems, and will serve as the templates for DNA replication.

7. Finding the Replication Partner of the First DNA Duplicate

Suppose the bio-quantum state of the resource pool of the bases in the cell to be [3]

$$\left|E_1\right\rangle=\sum_{t=1}^{N}\frac{1}{\sqrt{N}}\left|e_1\right\rangle_t \tag{15}$$

where $N=4^s$ ($s=g+h+m+n$),

$$\left|e_1\right\rangle=\begin{bmatrix}\left|e_j\right\rangle_1\\ \left|e_j\right\rangle_2\\ \cdot\\ \cdot\\ \cdot\\ \left|e_j\right\rangle_s\end{bmatrix},\qquad \left|e_j\right\rangle=\left|A\right\rangle,\left|T\right\rangle,\left|G\right\rangle,\left|C\right\rangle.$$

Each of $\left|e_j\right\rangle_1$ - $\left|e_j\right\rangle_s$ has four possible options, $\left|A\right\rangle,\left|T\right\rangle,\left|G\right\rangle and\left|C\right\rangle$, and so the total number of $\left|e_1\right\rangle$ is 4^s $\left(N=4^s\right)$.

Now, a quantum computation by means of Grover's fast quantum mechanical algorithm for database search proceeds to find, from $\left|E_1\right\rangle$, the replication partner, which is going to equal $\left|Temp_j\right\rangle$ [48]-[50]:

1) Defining a function as

$$f_1\left(e,Temp\right)=\begin{cases}1,if & \left|e_1\right\rangle_t=\left|Temp_j\right\rangle\\ 0,if & \left|e_1\right\rangle_t\neq\left|Temp_j\right\rangle\end{cases} \tag{16}$$

2) Repeating the following operations (a) and (b) for $O\left(\sqrt{N}\right)$ times (Grover Iteration):

(a) Applying the oracle operation:

$$\left|e_1\right\rangle_t\xrightarrow{O}\left(-1\right)^{f_1\left(e,Temp\right)}\left|e_1\right\rangle_t \tag{17}$$

where $f_1(e, Temp)$ is the function defined by Equation (16).

(b) Performing Grover operation

$$D|E_1\rangle, \tag{18}$$

where

$$D = WRW, \tag{19}$$

where W is the Walsh-Hadamard Transform Matrix and R is the phase rotation matrix.

3) Measuring the resulting state of $|E_1\rangle$ results in, with a probability of $O(1)$, the replication partner $|Part_1\rangle$, which is

$$|Part_1\rangle = |Temp_j\rangle = \begin{bmatrix} |b_j\rangle_1 \\ |b_j\rangle_2 \\ . \\ . \\ . \\ |b_j\rangle_s \end{bmatrix} \tag{20}$$

8. Re-Entangling to Create the First DNA Duplicate

Entangling $|Temp_i\rangle$ in Equation (13) and $|Part_1\rangle$ in Equation (20) results in the (normalized) bio-quantum state of the first DNA duplicate, $|DNA\rangle_{dup1}$, identical to $|DNA\rangle$, the bio-quantum-entangled state of the original DNA expressed by Equation (11):

$$\begin{aligned} |DNA\rangle_{dup1} &= \frac{1}{\sqrt{M}}\left[|b_i\rangle_1, |b_i\rangle_2 .. |b_i\rangle_s\right] \begin{bmatrix} |b_j\rangle_1 \\ |b_j\rangle_2 \\ . \\ . \\ . \\ |b_j\rangle_s \end{bmatrix} \\ &= \frac{1}{\sqrt{M}}\left(|b_i\rangle_1 |b_j\rangle_1 + |b_i\rangle_2 |b_j\rangle_2 + \dots + |b_i\rangle_s |b_j\rangle_s\right) \\ &= \frac{1}{\sqrt{M}}\sum_{r=1}^{s}\left(|b_i\rangle_r |b_j\rangle_r\right) = \frac{1}{\sqrt{M}}\sum_{r=1}^{s}|p_{ij}\rangle_r \end{aligned} \tag{21}$$

The first DNA replication procedure is completed.

9. Finding the Replication Partner of the Second DNA Duplicate

Suppose the bio-quantum state of the resource pool of the bases in the cell to be [3]

$$|E_2\rangle = \sum_{t=1}^{N}\frac{1}{\sqrt{N}}|e_2\rangle_t \tag{22}$$

where $N = 4^s$ ($s = g + h + m + n$),

$|e_2\rangle = \left[|e_i\rangle_1, |e_i\rangle_2 \dots |e_i\rangle_s \right]$. $|e_i\rangle = |A\rangle, |T\rangle, |G\rangle, |C\rangle$.

Each of $|e_i\rangle_1$ - $|e_i\rangle_s$ has four possible options, $|A\rangle, |T\rangle, |G\rangle and |C\rangle$, and so the total number of $|e_2\rangle$ is 4^s $\left(N = 4^s\right)$.

Now, a quantum computation by means of Grover's fast quantum mechanical algorithm for database search proceeds to find, from $|E_2\rangle$, the replication partner, which is going to equal $|Temp_i\rangle$ [48]-[50]:

1) Defining a function as

$$f_2\left(e, Temp\right) = \begin{cases} 1, if & |e_2\rangle_t = |Temp_i\rangle \\ 0, if & |e_2\rangle_t \neq |Temp_i\rangle \end{cases} \tag{23}$$

2) Repeating the following operations (a) and (b) for $O\left(\sqrt{N}\right)$ times (Grover Iteration):

(a) Applying the oracle operation:

$$|e_2\rangle_t \xrightarrow{O} (-1)^{f_2(e, Temp)} |e_2\rangle_t \tag{24}$$

where $f_2(e, Temp)$ is the function defined by Equation (23).

(b) Performing Grover operation

$$D|E_2\rangle, \tag{25}$$

where

$$D = WRW, \tag{26}$$

where W is the Walsh-Hadamard Transform Matrix and R is the phase rotation matrix.

3) Measuring the resulting state of $|E_2\rangle$ results in, with a probability of $O(1)$, the replication partner $|Part_2\rangle$, which is

$$|Part_2\rangle = |Temp_i\rangle = \left[|b_i\rangle_1, |b_i\rangle_2 \dots |b_i\rangle_s \right] \tag{27}$$

10. Re-Entangling to Create the Second DNA Duplicate

Entangling $|Part_2\rangle$ in Equation (27) and $|Temp_j\rangle$ in Equation (14) results in the (normalized) bio-quantum state of the second DNA duplicate, $|DNA\rangle_{dup2}$, identical to $|DNA\rangle$, the bio-quantum-entangled state of the original DNA expressed by Equation (11):

$$\begin{aligned} |DNA\rangle_{dup2} &= \frac{1}{\sqrt{M}} \left[|b_i\rangle_1, |b_i\rangle_2 \dots |b_i\rangle_s \right] \begin{bmatrix} |b_j\rangle_1 \\ |b_j\rangle_2 \\ \cdot \\ \cdot \\ \cdot \\ |b_j\rangle_s \end{bmatrix} \\ &= \frac{1}{\sqrt{M}} \left(|b_i\rangle_1 |b_j\rangle_1 + |b_i\rangle_2 |b_j\rangle_2 + \dots + |b_i\rangle_s |b_j\rangle_s \right) \\ &= \frac{1}{\sqrt{M}} \sum_{r=1}^{s} \left(|b_i\rangle_r |b_j\rangle_r \right) = \frac{1}{\sqrt{M}} \sum_{r=1}^{s} |p_{ij}\rangle_r \end{aligned} \tag{28}$$

The second DNA replication procedure is completed.

11. Conclusion

DNA molecules are micro-entities, obeying the fundamental laws of quantum mechanics. Bio-quantum state of DNA is formed by quantum entangling of bio-quantum states of bases. Mechanism of DNA forming and replicating is a process of bio-quantum entangling, de-entangling and re-entangling. Soft-genes control the bio-quantum genetic process of DNA forming and replicating.

Conflicts of Interest

The author declares no conflicts of interest.

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