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Journal of
Biomedical Research and Reviews

ISSN: 2581-7388
Volume 3: 1
J Biomed Res Rev 2020

Quantum Theory on DNA Structure and Thermal Denaturation

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Abstract

A quantum theory of DNA structure is proposed. DNA quantum model is required for explaining the permanence of the heredity. By introducing the self-consistent harmonic potential in the X-Y plane vertical to helix axis (z-direction) and the periodic potential along the z-axis we obtain the wave function for the single nucleotide and the many-nucleotide system. The helix distribution of bases is deduced from the solution of wave function under the self-consistent potential. The variation of DNA structure (polymorphism) is related to the periodicity of the potential in Z-axis, the quantum state occurring in harmonic potential and the interaction between helix strands. As Watson-Crick (W-C) interaction is introduced between double helices, the quasi-particle transformation is utilized to solve the interacting many-body problem for DNA. It is proved that the phase-transition (thermal denaturation) temperature is related to the frequency ω of harmonic potential. Through comparison with experimental data a simple relation $\omega = \frac{VN}{4\hbar}$ (N means number of base pairs and V the W-C coupling) is deduced. For a DNA sequence of 1000 bp ω is predicted about $(0.9\text{-}1.2)\times10^{17}$/sec. Such a high frequency is necessary for nucleotides of each strand located on a narrow tube. The large temperature fluctuation experimentally observed during DNA thermal denaturation is interpreted by the collective motion of nucleotides.

Keywords: DNA Structure, Thermal Denaturation, DNA Quantum Model, Helix Strands.

Introduction

Since the birth of molecular biology the quantum biochemistry has developed to treat the electronic motion in biological macro-molecules. However, the quantum dynamics was commonly ignored in studying problems such as biomolecular function and conformational change. Only in the latest years the quantum biology re-attracts again the attention of scientists. New progresses have achieved that include the non-trivial quantum effects in photosynthetic light harvesting [1,2], in avian magnetoreception [3] and in conformational transition of proteins [4,5]. However, to our knowledge, the quantum theory of DNA structure as an important part of quantum biology has not been found in literature. The motivation of the present studies is to filling up the gap and to constructing a quantum model of the DNA structure.

Life and non-life should have a unifying microscopic picture. The cornerstone of life -- atoms and molecules -- should obey unifying quantum rules. Although the QM/MM (quantum mechanics / molecular mechanics) multi-scale algorithm has achieved great successes in simulating the biological macro-molecule [6], the classical molecular

Article Information

Article Type: Research
Article Number: JBRR-132
Received Date: 18 November, 2019
Accepted Date: 27 January, 2020
Published Date: 03 February, 2020

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Citation: Luo L, Yang G (2020) Quantum Theory on DNA Structure and Thermal Denaturation. J Biomed Res Rev Vol: 3, Issu: 1 (11-17).

mechanics (MM) is only an approximation in discussing the problems such as DNA structure. More rigorous studies based on quantum mechanics are necessary.

The miracle of heredity stability can only be explained by quantum mechanics. The point was indicated firstly by Schrodinger [7]. He told such a story: Several members of the Habsburg dynasty have a peculiar disfigurement of the lower lip. Its inheritance has been studied carefully and published, complete with historical portraits. Fixing our attention on the portraits of a member of the family in the sixteen century and of his descendant living in the nineteenth, one may conclude that the gene structure responsible for the Habsburger Lippe has been carried on from generation to generation through several centuries. How to understand the permanence of the heredity? Schrodinger indicated that the discrete states and energies in quantum theory provide a clue to solving the problem. In quantum mechanics the time of expectation (lifetime, denoted as t) depends on the ratio ΔE/kT, namely $t=\tau \exp(\Delta E/kT)$ (ΔE means the typical spacing between discrete energy levels). Since ΔE is much larger than kT at room temperature, the quantum state is stable against the thermal disturbance. In other words, as the energy level spacing of molecules participating DNA replication is larger than the thermal and other disturbances, the replication process will be stable. Nowadays, the epigenetic inheritance attracts the attentions of biologists [8]. Epigenetic inheritance describes different phenotypic consequences to be inherited without any change in DNA sequence. The basic cause of this phenomenon is the existence of a self-perpetuating structure in an individual that does not depend on DNA sequence. For example, a proteinaceous structure that assembles on DNA has the ability to sustain the epigenetic effects. We notice that the stability of the epigenetic inheritance can still be explained following above demonstrations. Recently, the role of quantum decoherence was recognized by physicists and it is argued that the decoherence possibly makes the quantum picture ceasing to be effective for some macromolecular system. However, the nucleic acid molecule is a topologically ordered state with complicated non-local quantum entanglement. The non-locality means that the quantum entanglement is distributed among many different components of the molecule. As a result, the pattern of quantum entanglements cannot be destroyed by local perturbations. This significantly reduces the effect of decoherence and makes the quantum theory still effective in treating the genetic stability problems [9]. In his famous book «What is Life?» Schrodinger summarized that we must be prepared to find a new type of physical law prevailing in the living matter and the new principle is not a non-physical but "a genuinely physical one : it is nothing else than the principle of quantum theory over again."[7] This point of view is very visionary. From the points of the existence of several unifying principles between life and non-life and the deep integration of physics and biology we learned about the importance of quantum.

On the other hand, the study on the polymorphism of DNA structure has made great progresses in recent years. As is well known, even in DNA molecules of double helix, there are many structural types. Apart from double helix, it has been observed that the single-stranded DNA is generated for replication in phage, the triple helix and quadruple helix with couplings different from Watson-Crick types are also observed in experiments [10]. More interestingly, the transition of DNA conformational polymorphism was experimentally studied and detected on carbon nanotubes [11]. The polymorphism of DNA structure requires a unifying theory to interpret the mechanism for its formation. We suppose that the theory should be a quantum one, e.g. the nucleic acid had better be looked as a quantum complex system composed of many nucleotides.

The materials are organized as follows. In section 2 a model of nucleotide self-consistent-field is proposed and the solution of nucleotides in the field is obtained. Then in section 3 the interaction between double helices is introduced. The second-quantization method and the quasi-particle transformation are used to solve the many-body interaction problem. In the subsequent section 4 the thermal denaturation of DNA double-helix is studied and it is found that the transition temperature is related to the self-consistent field frequency. The observed temperature fluctuation during denaturation is explained. In section 5 the polymorphism of DNA structure is discussed from the solution of nucleotides in the self-consistent field. Finally in the last section, main results are summarized and several points related to the development of the model are discussed briefly.

Model: Nucleotide-Self-Consistent-Field (NSCF) and the Solution of Nucleotides in NSCF

Nucleic acid is a system of multi-nucleotides. Although the quantum mechanical calculation for oligo-atom reactions was worked out and the rate constant was deduced in recent years [12], the generalization of the quantum calculation to the multi-atom system is still a difficult task. As a primary step to solve the problem we shall use self-consistent-field method. We model the single chain nucleotides as the independent fermions in a self-consistent- field of cylinder shape [13]. The self-consistent- field can be deduced in principle through Hartree-Fock approximation if the interactions between these particles are known. However, we shall assume the self-consistent-field as a 2D harmonic potential or its shape- invariance set in XY plane and a periodic potential in Z-direction. That is, the single particle Hamiltonian written in cylinder coordinate is assumed as

$$H = H_1 + H_2 \tag{1}$$

$$H_1 = -\frac{\hbar^2}{2M\rho}\frac{\partial}{\partial\rho}(\rho\frac{\partial}{\partial\rho}) - \frac{\hbar^2}{2M\rho^2}\frac{\partial^2}{\partial\varphi^2} + \frac{1}{2}M\omega^2\rho^2 \tag{2}$$

$$H_2 = \frac{-\hbar^2}{2M}\frac{\partial^2}{\partial z^2} + V_{sym}(z) \quad (V_{sym}(z) = V_{sym}(z+h)) \tag{3}$$

where V_{sym} is periodic potential with period h.

The solution for Schrodinger Equation

$$H\psi(\rho,\varphi,z) = E\psi(\rho,\varphi,z) \tag{4}$$

is

$$\psi_{n,m,K}(\rho,\varphi,z) = R_{n,m}(\rho)\Phi_m(\varphi)\chi_K(z)$$

$$E_{n,m,K} = (2n+|m|+1)\hbar\omega + E_K \tag{5}$$

with n=0,1,2,...; m=0, $\pm1, \pm2, \ldots$. (Appendix 1) [14]. $R_{n,m}(\rho)$ is related to a confluent hyper-geometry function that gives coordinate constraints on the wave function of 2D oscillator and

$$\Phi_m(\varphi) = \exp(im\varphi) \tag{6}$$

One may use another set of quantum number n_x and n_y to describe the state. n_x is the quantum number of x-direction oscillator, n_y is the quantum number of y-direction oscillator and one has $n_x + n_y = 2n + |m|$. The ground state of helix has n=0, or n_x=n_y=0; the first excited state has two possibilities, n=0, $m = \pm1$ or n_x =1, n_y = 0 and n_x =0, n_y =1; the second excited state has three possibilities, (n=1, $m = 0$), (n=0, $m = \pm2$); etc. When $m \neq 0$ it describes a helix state, when m=0 the state collapses to a line. The single chain is generally in the ground state of 2D harmonic SCF, while each strand of DNA is in the first excited state of 2D harmonic SCF. That is, as the Watson-Crick coupling is switched on, the nucleotides in SCF generally jump from ground state to the first excited state.

Following Bloch theorem we have

$$\chi_K(z) = \exp(iKz) f_K(z) \tag{7}$$

The subscript K is the Bloch wave number in OZ direction and $f_K(z)$ is a periodic function of z, $f_K(z)$=$f_K(z+h)$. The energy E_k describes the energy level in conducting bands and can be deduced from the periodic potential $V_{sym}(z)$.

Considering

$$R_{nm}(\rho) = R_{n,-m}(\rho)$$

and

$$f_K(z) = f_{-K}(z)$$

we obtain stationary-wave solution

$$\psi_{nmK}(\rho,\varphi,z) = R_{nm}(\rho)\cos(m\varphi + Kz) f_K(z) \tag{8}$$

with the same eigenvalue given by (5).

In Equation (8) $f_K(z)$ is a periodic function and the 2-dimenional wave function cos($m\varphi$+Kz) describes the helix distribution of bases in φ-z subspace with step of helix $h = \frac{n\pi}{K}$ (n=1,2, ...). Moreover, the solution is invariant under the transformation

$$m \to -m \quad K \to -K$$

Suppose the system of N nucleotides is located in a cylinder of height (length) L. The Bloch wave-number is given by $K = \frac{2n\pi}{L}$ (n=0,1,.....). However, for particles moving in a periodicity field the energy levels constitute several sets of conducting bands intermixed with forbidden bands. The boundary between a conducting band and its adjacent forbidden band (wave number denoted as K_b) is determined by the condition [15].

$$\cos K_b h = \pm 1$$

or $K_b h = n\pi$ (n=1,2,.....). Only those K's in conducting band are permitted.

Remarks on Second Quantization and Wannier Representation

For the further applications here we give two remarks. The motion of N nucleotides in a single strand can be regarded as a quantum many-body problem written directly by use of second quantization method. Define annihilation and production operator of the state labeled by quantum number n,m,K as

$$b_{nmK}, \quad b^+_{nmK}$$

and assume they satisfy

$$\{b_{nmK}, b^+_{n'm'K'}\} = \delta_{nn'}\delta_{mm'}\delta_{KK'}$$

$$\{b_{nmK}, b_{n'm'K'}\} = 0 \tag{9}$$

The many-body Hamiltonian of the system is

$$H = \sum_{nmK} E_{nmK} b^+_{nmK} b_{nmK} \tag{10}$$

The annihilation and production operators satisfy Heisenberg's motion equation.

Assume the nucleotides move in a periodic self-consistent field and the helix is composed of many primitive cells characterized by the lattice position z_l. The l's are taken from 1 to N (N cells) or from 1 to L/h (L/h cells). To be definite, we take (l=1,...,N) in the following. Define the Fourier's transformation of Bloch wave function $\chi_{\mathbf{k}}(z)$

$$W_l(z) = \frac{1}{\sqrt{N}} \sum_K \exp(-iKz_l)\chi_{\mathbf{k}}(z) \tag{11}$$

as the Wannier wave function in the periodic potential [16] . Under the tight binding approximation one can deduce a relation between the Bloch wave function in periodic field and the localized bound state wave function φ_i (with energy level ε_i) [17],

$$\chi_K(z) = \frac{1}{\sqrt{N}} \sum_m \exp(iKz_m)\varphi_i(z - z_m) \tag{12}$$

Eq (12) is exactly in the form of the inverse transformation of (11). So, the Wannier wave function $W_l(z)$ is essentially the locally bound state wave function φ_i

$$W_l(z) = \varphi_i(z - z_l) \tag{11a}$$

By use of (7) and (12) one has

$$f_k(z) = \frac{1}{\sqrt{N}} \sum_m \exp(-iK(z - z_m))\varphi_i(z - z_m)$$
$$\cong \frac{1}{\sqrt{N}} \sum_m \varphi_i(z - z_m) \tag{13}$$

due to φ_i not vanishing only as z near $z_{m.}$ It gives an approximate expression for Bloch wave function f_K.

Generally speaking, the *N*-degenerate bound energy levels ε_i of the N-particle system form a band in the periodic field. However, the translational symmetry (periodicity) of $V_{sym}(z)$ is generally broken. It was proved that the small breakdown of the symmetry would cause the strong localization of the solution [18]. This is the so-called Anderson localization. Therefore, the tight binding model is really a good approximation in the present problem. Under local approximation the energy band of N-particle system degenerates to N energy levels with the same value ε_i. Above deduction shows that the Wannier wave function is the eigen-function of H_2 (Eq(3)) under the tight binding approximation. Based on Wannier wave function, the second quantization of the many-body problem in local representation can be deduced immediately. The annihilation and production operators in Wannier representation are denoted by b_{nml}, b^+_{nml} and they satisfy the same relation as Eq (9).

Model: Base Pair Interaction, Double Helix and Quasi-Particle

The formation of double helix must depend on the interaction between bases. Although each strand is localized in a small radius around an axis, the double helix extends to a larger spatial range due to Watson-Crick coupling. To understand the structure and dynamics of DNA one should study base pair interaction first .

By use of the annihilation and production operators in a many-body system the two-body interaction potential of the system can generally be expressed by

$$\begin{aligned} \mathrm{V} &= \frac{1}{2}\sum_{j\neq k} v(\mathrm{r}_j - \mathrm{r}_k) \\ &= \frac{1}{2}\sum_{ll'} (N_l N_{l'} - N_l\delta_{ll'}) v_{ll'} \\ &= \frac{1}{2}\sum_{ll'} b_{l'}{}^{+} b_l^{+} b_l b_{l'} v_{ll'} \end{aligned} \tag{14}$$

where b_l and b_l^+ are the annihilation and production operator of quantum state φ_l respectively and $N_l = b_l^+ b_l$ the particle number operator of the state φ_l . The 4-operator term in the last line of Eq (14) gives the second-quantization formalism for a general two-body interaction $v(\mathbf{r_j}\text{-}\mathbf{r_k})$.

Set the annihilation and production operators on two chains in Wannier representation denoted by

$$b^{(i)}_{nml}, \quad b^{+(i)}_{nml}$$

(the superscript i=1,2 means two chains respectively) and they satisfy the similar relation as Eq (9) in Bloch representation. The total Hamiltonian of the double helix system is given by

$$\mathbb{H} = \sum_{nml} E_{nml}\left(\mathrm{b}^{(1)+}_{nml}\mathrm{b}^{(1)}_{nml} + \mathrm{b}^{(2)+}_{nml}\mathrm{b}^{(2)}_{nml}\right) - \sum_{ll'} V_{ll'}\mathrm{b}^{(1)+}_{nml}\mathrm{b}^{(2)+}_{nml'}\mathrm{b}^{(2)}_{nml'}\mathrm{b}^{(1)}_{nml} \tag{15}$$

The second term in Eq (15) comes from Eq (14) which describes the Watson-Crick interaction between two chains and it can be rewritten as

$$-\sum_{ll'} V_{ll'}(b^{(1)+}_{nml} b^{(2)+}_{nml'} b^{(2)}_{nml'} b^{(1)}_{nml}) = -V\sum_{l} b^{(1)+}_{nml} b^{(2)+}_{nml} b^{(2)}_{nml} b^{(1)}_{nml} \tag{15.1}$$

where only the interaction between corresponding bases (l=l') on two chains is assumed and for simplicity the coupling is assumed independent of position l . Considering nucleotides on two chains are always in the same self-consistent field the same labels (nm) under all operators b and b^+ will be omitted in the following. That is, $b^{(i)}_{nml}(b^{(i)+}_{nml})$ is abbreviated as $b^{(i)}_l(b^{(i)+}_l)$.

As the W-C couplings switch on between corresponding bases of two strands the nucleotides of DNA are no longer in the quantum ground state n=0, m=0 but they jump from the ground state to the first excited state n=0, m=± 1. The corresponding energy level of Wannier state is expressed by

$$E_{0l} = 2\hbar\omega + E_l \tag{16}$$

as seen from Eq (5) where E_l is the energy of the locally bound state φ_l at z_l . The reduced Hamiltonian of the double helix system is

$$\mathbb{H} = \sum_l E_{0l}\left(\mathrm{b}^{(1)+}_l\mathrm{b}^{(1)}_l + \mathrm{b}^{(2)+}_l\mathrm{b}^{(2)}_l\right) - \sum_{ll'} V_{ll'}\mathrm{b}^{(1)+}_l\mathrm{b}^{(2)+}_{l'}\mathrm{b}^{(2)}_{l'}\mathrm{b}^{(1)}_l \tag{17}$$

Due to the interaction term $V_{ll'}$ the Hamiltonian Eq(17) is not diagonal. However, the Hamiltonian can be diagonalized through a quasi-particle transformation as used in BCS theory of superconductivity [19]. Namely, we introduce the annihilation and production operator of quasi-particle

$$\begin{aligned} \alpha^{(1)}_l &= u_l b^{(1)}_l - v_l b^{(2)+}_l \\ \alpha^{(1)+}_l &= u_l b^{(1)+}_l - v_l b^{(2)}_l \\ \alpha^{(2)}_l &= u_l b^{(2)}_l + v_l b^{(1)+}_l \\ \alpha^{(2)+}_l &= u_l b^{(2)+}_l + v_l b^{(1)}_l \end{aligned} \tag{18}$$

u_l and v_l are supposed to be real and satisfy

$$u_l^2 + v_l^2 = 1 \tag{19}$$

Easily prove $a^{(i)}_l, a^{(i)+}_l$ etc satisfy the Fermi type relation as Eq (9). So, $a^{(i)}_l$ is the annihilation operator of quasi-particle and $a^{(i)+}_l$ is the production operator of quasi-particle.

Set

$$\Delta = V\sum_l \left\langle b^{(2)}_l \mathrm{b}^{(1)}_l \right\rangle = V\sum_l \left\langle \mathrm{b}^{(1)+}_l b^{(2)+}_l \right\rangle \tag{20}$$

The reduced Hamiltonian of the helix system Eq (17) can be approximated as

$$\mathbb{H}_0 \approx \sum_l E_{0l}\left(b^{(1)+}_l b^{(1)}_l + b^{(2)+}_l b^{(l)}_l\right) - \Delta\sum_l (b^{(1)+}_l b^{(2)+}_l + b^{(2)}_l b^{(1)}_l) + \frac{\Delta^2}{V} \tag{21}$$

By transformation Eq (18) and under the choice of

$$u_l^2 = \frac{1}{2}\left(1 + \frac{E_{0l}}{\xi_l}\right)$$

$$v_l^2 = \frac{1}{2}\left(1 - \frac{E_{0l}}{\xi_l}\right)$$

$$\xi_l = \sqrt{E_{0i}{}^2 + \ddot{A}^2} \tag{22}$$

we obtain the Hamiltonian diagonalized relative to the quasi-particle operator

$$\mathbb{H}_0 = \sum_l \xi_l \left(\alpha_l^{(1)+}\alpha_l^{(1)} + \alpha_l^{(2)+}\alpha_l^{(2)}\right) + E_0 \tag{23}$$

where

$$= 2\sum_l E_{\ l} v_l - 2\Delta\sum_l u_l v_l + \frac{\ddot{A}}{} \tag{24}$$

Thermal Denaturation of DNA Double Helix

The phase transition of DNA occurs at the temperature T_c where the gap $\Delta = 0$. One should calculate the energy gap at first. At given temperature the thermal average of the gap, Eq (20), is expressed as

$$\Delta = V\sum_l \left\langle b_l^{(2)} \mathrm{b}_l^{(1)} \right\rangle_T \tag{20a}$$

The inverse transformation of Eq (18) is

$$\begin{aligned} b_l^{(1)} &= u_l \alpha_l^{(1)} + v_l \alpha_l^{(2)+} \\ b_l^{(2)} &= u_l \alpha_l^{(2)} - v_l \alpha_l^{(1)+} \end{aligned} \tag{25}$$

Inserting (25) into (20a) and neglecting two or more quasi-particle state we obtain

$$\begin{aligned} \Delta &= V\sum_l u_l v_l \{\left\langle \alpha_l^{(2)} \alpha_l^{(2)+} \right\rangle_T - \left\langle \alpha_l^{(1)+} \alpha_l^{(1)} \right\rangle_T\} \\ &= V\sum_l u_l v_l \{1 - \left\langle \alpha_l^{(2)+} \alpha_l^{(2)} \right\rangle_T - \left\langle \alpha_l^{(1)+} \alpha_l^{(1)} \right\rangle_T\} \\ &= V\sum_l u_l v_l (1 - 2f(\xi_l)) \\ &= V\sum_l \frac{\Delta}{2\xi_l}(1 - 2f(\xi_l)) \end{aligned} \tag{26}$$

Here $f(\xi_l)$ means the distribution of ideal Fermi gas. In high-temperature and low density approximation, namely in case of the thermal wavelength much smaller than the average interparticle separation, the quantum effect can be neglected and the distribution $f(\xi_l)$ can be expressed as [20]

$$\begin{aligned} f(\xi_l) &= Z\exp(\frac{-\xi_l}{k_B T}) \\ Z &= \lambda^3 \rho_N + \frac{1}{2\sqrt{2}}(\lambda^3 \rho_N)^2 + \ldots \end{aligned} \tag{27}$$

where ρ_N denotes the number density of the particles and λ the thermal wavelength

$$\lambda = \sqrt{\frac{2\pi}{M k_B T}}\hbar \tag{28}$$

In experiments DNA undergoes a sharp transition at a definite melting point *T*c around 90°C [21]. The temperature Tc is high enough so that the condition $\lambda^3\rho_N << 1$ is always satisfied in the problem. By using (26)(27) at $T=T_c$ and taking Z<<1 into account we obtain

$$1 = \frac{V}{2}\sum_l \frac{1 - 2f(\xi_l)}{\xi_l} = \frac{V}{2}\sum_l \frac{1 - 2Z\exp(\frac{-\xi_l}{k_B T_c})}{\xi_l} = \frac{V}{2}\sum_l \frac{1}{\xi_l} \tag{29}$$

where $\xi_l = E_{0l}$ should be taken. It leads to

$$\frac{V}{2}\int_{2\hbar\omega}^{E_N} dE\,\rho(E)\frac{1}{E} = 1 \tag{30}$$

where the state density is given by (Appendix 2)

$$\rho(E) \cong \frac{L\sqrt{M}}{\sqrt{2}\pi\hbar\sqrt{E - 2\hbar\omega}} \tag{31}$$

The energy integral in Eq (30) is completed in the harmonic-oscillator n=0, m=±1 band, namely, from the lower edge $2\hbar\omega$ to the upper edge E_N approximately determined by

$$\int_0^N dN = \sqrt{\frac{M}{2}}\frac{L}{\pi\hbar}\int_{2\hbar\omega}^{E_N}\frac{1}{\sqrt{E - 2\hbar\omega}}dE$$

It gives

$$E_N = 2\hbar\omega + a^2 N^2, a = \frac{\pi\hbar}{L\sqrt{2M}} \tag{32}$$

Inserting (31) and (32) into (30) one obtains

$$\frac{VL\sqrt{M}}{2\sqrt{2}\pi\hbar}\frac{aN}{\hbar\omega} = \frac{VN}{4\hbar\omega} = 1 \tag{33}$$

As an typical example, taking $N = 1000$, $V = (0.35\text{-}0.48)\times 10^{-12} erg$ corresponding to AT and GC coupling respectively we obtain

$$\omega = \frac{VN}{4\hbar} = (0.9 - 1.2)\times 10^{17} s^{-1} \tag{34}$$

Above result holds as long as *Tc* is not-too-low so that Z<<1. It means the existence of phase transition at not-too-low temperature provides a clue to determine the frequency parameter of NSCF. The high frequency ω of self-consistent field is consistent with the idea that each strand of DNA is localized in a small radius that is comparable with the dimension of nucleotide ($\sqrt{\frac{\hbar}{M\omega}} \approx 10^{-11} cm$).

The above discussion shows that the molecular mechanism of DNA thermal fluctuation is related to the collective motion of nucleotides in self-consistent field. Therefore, the denaturation temperature is dependent on the frequency of the field. The point can be further clarified by observing the fluctuation of denaturation temperature *Tc*. In fact, instead of Eq (33), more rigorous calculation gives

$$\begin{aligned} &\frac{VN}{4\hbar\omega}F(T_c) = 1 \\ &F(T_c) = 1 - 2Z(T_c)\exp\frac{-E_c^{'}}{k_B T_c} \end{aligned} \tag{35}$$

where $E_c^{'}$ is an intermediate-value of *E* in energy integral from $2\hbar\omega$ to E_N and $(1\text{-}2Z\exp(-E/k_B T_c)$ under the integral has been approximated by $(1\text{-}2Z\exp(-E_c^{'}/k_B T_c)$ and taken out of the integral. Both *N* and *V* have fluctuations. It leads to the fluctuation of *Tc*,

$$\frac{\delta T_c}{T_c} = G\frac{\delta(\frac{VN}{\hbar\omega})}{\frac{VN}{\hbar\omega}}, G = \frac{k_B T_c}{2ZE_c^{'}}\exp\left(\frac{E_c^{'}}{k_B T_c}\right) \quad (36)$$

where G>>1 due to $E_c^{'} > 2\hbar\omega >> k_B T_c$. Therefore, the small fluctuation of N and V possibly causes the large fluctuation in temperature during DNA thermal denaturation This has been observed in experiments [22]. However, most part of fluctuations in N and V may have been canceled by the fluctuation of frequency ω. That is, the self-consistent field frequency ω is automatically adjusted to the fluctuated *N* and *V*. The observed temperature fluctuations are only the remainder of the fluctuation effect of N and V.

Polymorphism of DNA Structure

There are three approaches to the variation of DNA structure. The first approach is due to the change of the quantum number (*n*,*m*) of the single chain in the two-dimensional harmonic self-consistent field. The quantum number *m*=0 describes the non-helix state, while the positive *m* and negative *m* describe right- and left-handed helix respectively. The quantum number *n* describes the nucleotide distribution in radial direction. Since $2n + |m| = n_x + n_y$ where n_x (n_y) the quantum number of x-(y-) directional linear oscillator, the increase of *n* corresponds to the quantum state of particles distributed in larger x and/or in larger y-direction. These structural variation requires the large energy change which is in the order of $\hbar\omega$.

The second approach to the variation of DNA structure is caused by the change of the symmetry existing in the Hamiltonian H_2 (Eq (3)). For a single chain of B-DNA one helix turn (one step) contains 10 nucleotides, for A-DNA 11 nucleotides, for C-DNA 9.33 nucleotides, and for left-handed Z-DNA 12 nucleotides, etc. In solution the number of base pairs contained in one step of DNA further changes, for example, from 10.3 to 10.6 for B-DNA [10]. All above polymorphism of DNA structure can be understood by the periodicity of $V_{sym}(z)$ and the positive/negative directivity in φ-z subspace. In living cell DNA is winding on the histone octamer. The axis of DNA is a curve and in this case the tangent of the curve defines the z-direction. Suppose there are N nucleotides located in a tube-like region of length L and the self-consistent potential $V_{sym}(z)$ has symmetry $V_{sym}(z)=V_{sym}(z+h)$. The step h of helix is determined by the interaction among N nucleotides and the interaction between nucleotides and environment. For a definite h the number of nucleotides in one step is changed as L stretched or contracted. It can be an integer or a fraction. Simultaneously, accompanying z increasing the angle φ may increases or decreases. These lead to polymorphism of DNA.

The third approach to the variation of DNA structure is due to the interaction between base pair in adjacent chains. The commonest structure is double strands paired through Watson-Crick coupling. In triple helix DNA the third strand is coupled with double helix through Hoogsteen or reversed Hoogsteen pairing. The quartet helix DNA is formed of four-stranded complex by guanine-rich motifs in DNA [10]. The theory of DNA thermal denaturation stated in previous section can easily be generalized and applied to the triple and quartet helix DNA.

Discussions and Conclusion

The basic conclusion of the present study is : the double helix structure of nucleic acid originates from its quantum property and it can be deduced from the solution of a quantum many-body problem of nucleotides. Formally, the theory was developed based on two basic assumptions: 1, The nucleotides in a single chain of DNA are independent fermions moving in a 2D harmonic self-consistent potential in the transverse plane and an 1D longitudinal periodical self-consistent field parallel to the helix axis. 2, The Watson-Crick interaction between double chains is described by the two-body interaction potential through the annihilation and production operators of nucleotides in the self-consistent field. Based on above assumptions two main results were obtained. The first is: by introducing the self- consistent harmonic potential and periodic potential, the double helix structure is deduced and the polymorphism of DNA structure is explained or predicted. The second is: by introducing quasi particles in the coupled double helix the problem of DNA thermal denaturation is solved. The denaturation is a kind of collective motion of nucleotides, whose temperature is related to the frequency ω of harmonic potential. A simple relation $\omega = \frac{VN}{4\hbar}$ is obtained. The related discussions are given as follows:

Test of the prediction on harmonic self-consistent field

To test the theoretical prediction on the harmonic SCF of frequency $\omega \approx 10^{17}$/sec we suggest to study the interaction of electromagnetic field with DNA. In experiments DNA photolyases were observed under ultraviolet irradiation and the corresponding repair pathways were investigated [23,24]. It is expected to observe the effect of DNA damage under shorter wave-length of 1-2 hundreds angstroms (corresponding to $\omega \approx 10^{17}$/sec) and checking the proposed model of SCF harmonic field.

Generalization from harmonic potential to self-consistent field of same shape

Set

$$V_{+}(x, a_0) = V_{-}(x, a_1) + R(a_1) \quad (37)$$

where a_0 is a set of parameters, a_1 is a function of a_0, $R(a_1)$ is irrespective of *x*. Following Gendenshtein [25] we call V_+ and V_- are shape invariant. Evidently, the harmonic potential in present theory can be generalized to other potential that is shape-invariant with harmonic.

DNA replication can proceed only when the duplex is unwound. The speed of replication fork movement is 50000 bp/min for bacteria and about 2000 bp/min for eukaryotes [8]. That means the helix unwinding accompanying the replication should proceed in a very high rate. Topoisomerases play important role in helix unwinding. We conjecture that the microscopic mechanism of the topoisomerase may be related to the generation of a special

kind of harmonic self-consistent field or its shape-invariant field.

Generalization to four kinds of bases

In a real DNA there are four kinds of bases,A,T,G and C. The symmetry of self-consistent field V(z) is strongly broken. The problem should be carefully studied. One important result is the annihilation and production operators $b_{nml}^{(i)}$, $b_{nml}^{+(i)}$ will be generalized to four kinds, namely $A_{nml}^{(i)}, A_{nml}^{+(i)}, T_{nml}^{(i)}, T_{nml}^{+(i)}, G_{nml}^{(i)}, G_{nml}^{+(i)}, C_{nml}^{(i)}, C_{nml}^{+(i)}$ and correspondingly the Hamiltonian Eq (15) should also be generalized. Note that there are two hydrogen bonds between A and T and three hydrogen bonds between C and G, the energy gap Δ in Eq (20) will be generalized to two, Δ_1 and Δ_2 , namely

$$\Delta_1 = \mathrm{V}_1 \sum_l \left\langle A_l^{(2)} \mathrm{T}_l^{(1)} \right\rangle = \mathrm{V}_1 \sum_l \left\langle \mathrm{T}_l^{(1)+} A_l^{(2)+} \right\rangle$$

$$\Delta_2 = \mathrm{V}_2 \sum_l \left\langle G_l^{(2)} \mathrm{C}_l^{(1)} \right\rangle = \mathrm{V}_2 \sum_l \left\langle \mathrm{C}_l^{(1)+} G_l^{(2)+} \right\rangle$$

Accordingly, the quasi -particle can be generalized to four kinds.

Vertical interaction of base pairs and the sequence diversity

The W-C interaction between corresponding bases on two chains is called horizontal interaction. The stacking interaction between two neighboring bases on each chain is called vertical interaction. By use of annihilation and production operators the vertical interaction can be expressed as

$$\sum_{j=1,2;l} V^{j}{}_{l,l+1} b_{nml}^{(j)+} b_{n,m,l+1}^{(j)+} b_{n,m,l+1}^{(j)} b_{nml}^{(j)}$$

The vertical and horizontal interactions should be considered simultaneously. When the theory is generalized to four kinds of bases there are ten kinds of independent stacking interactions for DNA double chains. These stacking energies take quite different values, making one sequence differentiated from others. Moreover, the stacking energy is dependent of the local deviation of helix structure. Sometimes, one base mutation in a sequence could make a large variation of DNA structure. Therefore, the vertical interaction produces the sequence diversity and it makes possible that the sequence contains a large amount of biological information.

Acknowledgement

The authors are indebted to Dr Yulai Bao and Ms Aiying Yang for their kind help in literature searching.

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