Knot soliton in DNA and geometric structure of its free-energy density

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Abstract In general, the geometric structure of DNA is characterized using an elastic rod model. The Landau model provides us a new theory to study the geometric structure of DNA. By using the decomposition of the arc unit in the helical axis of DNA, we find that the free-energy density of DNA is similar to the free-energy density of a two-condensate superconductor. By using the φ –mapping topological current theory, the torus knot soliton hidden in DNA is demonstrated. We show the relation between the geometric structure and free-energy density of DNA and the Frenet equations in differential geometry theory are considered. Therefore, the free-energy density of DNA can be expressed by the curvature and torsion of the helical axis.

Keywords Landau model · DNA · Free energy · Elastic rod model · Euler angles

1 Introduction

Recently, the chiral transform from right-handed B-DNA to left-handed Z-DNA under the torsion torque was observed [1]. In order to explain this transformation theoretically, some theories can be considered e.g., the modified ZZO model [2], Poland-Scheraga model [3], and Peyrard–Bishop–Dauxois model [4, 5]. Especially, the authors [6] consider the Landau model in the study of DNA transformation. In this model, the free-energy density of B- and Z-DNA is obtained by introducing the two-component spin wave function. The free energy can be used to explain the interaction between the structure and function of biological macromolecules, such as protein folding [7–10] and ion channel conduction [11]. The free energy is the bridge between theoretical calculation and experiment. For explanation of the experiment, the chiral transformation in DNA is considered as a local transformation. In order to keep the free-energy density gauge invariance under the chiral

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change in DNA molecules, the chiral gauge potential ρ is introduced; which is defined for the internal structure of base pairs. When $\rho > 0$, it represents the right-hand rotation; when $\rho < 0$, it represents the left-hand rotation. This dynamic model extends the traditional elastic rod model by considering the chiral gauge transformations. However, when B-Z structural transitions in DNA occur under the torsion torque, the geometrical structures of DNA are also changed. This means there must be some relationships between the free-energy density and geometric structure of DNA. This interesting question has not yet been clarified [6].

The purpose of this article is to show the relationships between the geometric structure and the free-energy density of DNA molecules. First, by using the decomposition of the arc unit in the helical axis, a new expression of the free-energy density is deduced. It is similar to the free-energy density of a two-condensate superconductor. For this reason, the torus knot soliton hidden in DNA is observed. The torus knot soliton can be described by the winding number in the frame of the φ -mapping topological current theory. Second, the helical axis is studied as a space curve and a curve on a surface in detail. Some equations associated with the Frenet equations are considered. Then the relationships between the geodesic curvature, normal curvature, and geodesic torsion of the helical axis are presented. Finally, we find the free-energy density of DNA is given by the curvature and geodesic torsion of the helix axis.

2 Landau model in DNA and its knot structure

DNA is composed of a phosphate backbone bridged by base pairs, forming a double helix. The double strands in space are a banded geometric surface, which twist around the DNA helical axis. In addition, the DNA helical axis can also be twisted in space to form supercoiling. The two-component spin wave function is introduced for describing DNA in Ref. [6]. The spin wave function is usually written as:

$$\tilde{\psi} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}. \quad (1)$$

Here the quantum effects are not considered. In order to obtain the wave function in an arbitrary direction, we only need to execute the Euler rotation on the spin wave function:

$$\psi = R\tilde{\psi}, \quad (2)$$

where $R(\phi, \theta, \chi) = R(\phi)R(\theta)R(\chi)$ [12] is the Euler rotation and ϕ, θ, χ are three Euler angles. The Euler rotation is the general rotation in three dimensions, characterized by the Euler angles. First, rotate the rigid body counterclockwise about the z -axis by angle ϕ . Second, perform the rotation about the y' -axis by angle θ . The final rotation is about the t -axis by angle χ . The Euler rotation is shown in Fig. 1 and is expressed as

$$\begin{aligned} R(\phi, \theta, \chi) &= R(\phi)R(\theta)R(\chi) \\ &= \exp\left(\frac{-i\sigma_3\phi}{2}\right)\exp\left(\frac{-i\sigma_2\theta}{2}\right)\exp\left(\frac{-i\sigma_3\chi}{2}\right) \\ &= \begin{pmatrix} \exp\left(\frac{-i\phi}{2}\right) & 0 \\ 0 & \exp\left(\frac{i\phi}{2}\right) \end{pmatrix} \begin{pmatrix} \cos\left(\frac{\theta}{2}\right) & -\sin\left(\frac{\theta}{2}\right) \\ \sin\left(\frac{\theta}{2}\right) & \cos\left(\frac{\theta}{2}\right) \end{pmatrix} \begin{pmatrix} \exp\left(\frac{-i\chi}{2}\right) & 0 \\ 0 & \exp\left(\frac{i\chi}{2}\right) \end{pmatrix} \\ &= \begin{pmatrix} \exp\left(\frac{-i(\phi+\chi)}{2}\right)\cos\left(\frac{\theta}{2}\right) & -\exp\left(\frac{-i(\phi-\chi)}{2}\right)\sin\left(\frac{\theta}{2}\right) \\ \exp\left(\frac{i(\phi-\chi)}{2}\right)\sin\left(\frac{\theta}{2}\right) & \exp\left(\frac{i(\phi+\chi)}{2}\right)\cos\left(\frac{\theta}{2}\right) \end{pmatrix}, \end{aligned} \quad (3)$$

Fig. 1 Euler angles

where $(\sigma_1, \sigma_2, \sigma_3)$ is the Pauli matrix:

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \quad (4)$$

By introducing (3) into (2), the spin wave function is:

$$\psi = \begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix} = \left(\exp\left(-\frac{i(\phi+\chi)}{2}\right) \cos\left(\frac{\theta}{2}\right) \exp\left(\frac{i(\phi-\chi)}{2}\right) \sin\left(\frac{\theta}{2}\right) \right)^t. \quad (5)$$

This wave function consists of two superpositions ψ_1 and ψ_2 . They also can be rewritten as:

$$\begin{aligned} \psi_1 &= \psi_1^1(\phi, \theta, \chi) + i\psi_1^2(\phi, \theta, \chi), \\ \psi_2 &= \psi_2^1(\phi, \theta, \chi) + i\psi_2^2(\phi, \theta, \chi). \end{aligned} \quad (6)$$

Then the superpositions can be considered as the map: $R^3 \rightarrow E^2$. The first superposition ψ_1 describes the DNA conformation, and the second superposition ψ_2 describes the internal structure of the base pair connected by hydrogen bonds. According to the Landau model [6], the free-energy density of DNA can be given from the spin wave function:

$$\mathcal{F}' = \frac{k_1}{2} \frac{d\psi^\dagger}{ds} \frac{d\psi}{ds} + \frac{k_2}{2} \left| \psi^\dagger \frac{d\psi}{ds} \right|^2, \quad (7)$$

where s is the arc unit on the helical axis. By introducing (5) into (7), the free-energy density can be represented by the Euler angles:

$$\mathcal{F}' = \frac{B}{2} \left[\left(\frac{d\theta}{ds} \right)^2 + \left(\frac{d\phi}{ds} \right)^2 \sin^2(\theta) \right] + \frac{C}{2} \left(\frac{d\phi}{ds} \cos \theta + \frac{d\chi}{ds} \right)^2, \quad (8)$$

where $\frac{B}{2}$ represents the isotropic elastic bending and $C = \frac{k_1+k_2}{4}$ equates to torsional elasticity (when the DNA molecule satisfies the linear model, $\theta = 0, \phi = 0$). If one assumes

that the twist persistence length is 75 nm, then $C = 91 \times 10^{-20} \text{ J}$ [6]. In (8), $\frac{d\theta}{ds}$, $\frac{d\phi}{ds}$ and $\frac{d\chi}{ds}$ are the spatial variation of the Euler angle with the rotation of the DNA helical axis. $\frac{d\theta}{ds}$ represents the bending degree of the helical axis. $\frac{d\phi}{ds}$ provides the degree of rotation of the helical axis. $\frac{d\chi}{ds}$ indicates the degree of deviation from the plane perpendicular to the helical axis. Formula (8) is same as the free-energy density in the elastic rod model [6]. When the negative torsion is applied to the B-DNA, the curvature and torsion of the DNA change but we cannot find these changes directly from the free-energy density. In the next section, the relations between the curvature, torsion and free-energy density are studied in detail.

We only consider the variation of χ with the change of the arc s element of the helical axis. When χ changes, the wave function describing DNA changes accordingly. Here, in order to find the change of the free-energy density, we employ the rotation transformation $\exp(i\alpha(s))$ on the spin wave function:

$$\psi' = \psi \exp(i\alpha(s)), \quad (9)$$

where $\alpha(s)$ is the parameter describing the rotation. In this transformation, the free-energy density in the Landau model is:

$$\mathcal{F}' = \frac{B}{2} \left[\left(\frac{d\theta}{ds} \right)^2 + \left(\frac{d\phi}{ds} \right)^2 \sin^2(\theta) \right] + \frac{C}{2} \left(\frac{d\phi}{ds} \cos \theta + \frac{d\chi}{ds} - 2i \frac{d\alpha(s)}{ds} \right)^2. \quad (10)$$

By comparing (8) and (10), we find that this free-energy density is not gauge invariant [13]. To ensure the free-energy density is the gauge invariance, we need to introduce the chiral gauge potential ρ . In fact, the chiral gauge field is the rotation angle between successive base pairs in the helix. It represents the internal interactions of DNA base pairs; $\rho > 0$ for the right-handed rotation and $\rho < 0$ for the left-handed rotation. ρ transforms as:

$$\rho' = \rho - 2i \frac{d\alpha(s)}{ds}. \quad (11)$$

Under this transformation, $\frac{d\psi}{ds}$ should be the covariant derivative $\frac{D\psi}{Ds}$ [13]:

$$\frac{D\psi}{Ds} = \frac{d\psi}{ds} - \rho\psi. \quad (12)$$

The free-energy density associated with this chiral gauge potential is:

$$\mathcal{F}_\rho = -iC\rho \left(\psi^\dagger \frac{d\psi}{ds} - \frac{d\psi^\dagger}{ds} \psi \right) + C \frac{\rho^2}{2}. \quad (13)$$

The representation of the above formula based on the Euler angles is:

$$\mathcal{F}_\rho = -C\rho \left(\frac{d\chi}{ds} + \frac{d\theta}{ds} \cos(\theta) \right) + C \frac{\rho^2}{2}. \quad (14)$$

The total free-energy density is:

$$\mathcal{F} = \mathcal{F}' + \mathcal{F}_\rho. \quad (15)$$

Finally, by introducing the spin wave function into (13) and recalling (8), the free-energy density is given as:

$$\mathcal{F} = \frac{B}{2} \left[\left(\frac{d\theta}{ds} \right)^2 + \left(\frac{d\phi}{ds} \right)^2 \sin^2(\theta) \right] + \frac{C}{2} \left(\frac{d\phi}{ds} \cos \theta + \frac{d\chi}{ds} - \rho \right)^2. \quad (16)$$

This formula is similar to the expression in the elastic rod model [14–17], but the difference exists in the gauge potential ρ , which guarantees the free-energy density gauge invariance.

In order to find the torus knot soliton hidden in this free-energy density, the unit vectors are introduced. The unit vectors are derived by projecting the arc unit ds onto the coordinate axes x_i , where $i = 1, 2, 3$. The meaning of the projection is displayed in Fig. 2. The unit vectors are defined as:

$$e^i = \frac{dx_i}{ds}. \quad (17)$$

Hence, $ds^2 = dx_1^2 + dx_2^2 + dx_3^2$ and the unit vector e^i satisfies the relation:

$$e^i e^j = \begin{cases} 0 & i \neq j \\ 1 & i = j \end{cases} \quad (18)$$

The gradient of the wave function ψ is:

$$\nabla\psi = \left(\frac{d\psi}{dx_1}, \frac{d\psi}{dx_2}, \frac{d\psi}{dx_3} \right). \quad (19)$$

Then the derivative of ψ with s can be expressed as:

$$\frac{d\psi}{ds} = \partial_i \psi e^i. \quad (20)$$

where $\partial_i \psi = \frac{\partial \psi}{\partial x_i}$. The free-energy density (7) without gauge potential changes to:

$$\begin{aligned} \mathcal{F}' &= \frac{k_1}{2} \frac{\partial \psi^\dagger}{\partial x_i} \frac{\partial \psi}{\partial x_i} + \frac{k_2}{2} \left| \psi^\dagger \frac{\partial \psi}{\partial x_i} \right|^2 \\ &= \frac{k_1}{2} \nabla \psi^\dagger \nabla \psi + \frac{k_2}{2} \left| \psi^\dagger \nabla \psi \right|^2. \end{aligned} \quad (21)$$

By using the unit vectors e^i , the gauge potential ρ is defined as:

$$\rho = A_i e^i. \quad (22)$$

Here, we use the Einstein summation convention in (18), (20) and (22). Then the total free-energy density changes to:

$$\mathcal{F} = \frac{k_1}{2} \mathbf{D}\psi^\dagger \mathbf{D}\psi + \frac{k_2}{2} \left| \psi^\dagger \mathbf{D}\psi \right|^2, \quad (23)$$

Fig. 2 Unit vectors

where the covariant derivative $\mathbf{D}$ is:

$$\mathbf{D} = \left(\frac{\partial}{\partial x_1} - A_1, \frac{\partial \psi}{\partial x_2} - A_2, \frac{\partial \psi}{\partial x_3} - A_3 \right). \quad (24)$$

It should be noted that the free-energy costs due to the base-pair structures and the changing base-pair structure along s are not considered here. By introducing the two-component spin wave function (5) into this free-energy density, one has:

$$\mathcal{F} = \frac{k_1}{2} \mathbf{D}\psi_1^* \mathbf{D}\psi_1 + \frac{k_1}{2} \mathbf{D}\psi_2^* \mathbf{D}\psi_2 + \frac{k_2}{2} |\psi_1^* \mathbf{D}\psi_1 + \psi_2^* \mathbf{D}\psi_2|^2. \quad (25)$$

This free-energy density can be well compared with the two-condensate Ginzberg–Landau free-energy density. In Ref. [18, 19], the authors show there is a torus knot soliton in the Ginzberg–Landau free-energy density. As an example, the knot soliton (3,1) with different directions is shown in Fig. 3. By using $\frac{\delta \mathcal{F}}{\delta A_i}$, one can obtain:

By using $\frac{\delta \mathcal{F}}{\delta A_i}$, one has

$$\begin{aligned} \mathbf{J} &= \frac{\delta \mathcal{F}}{\delta A_i} \\ &= \frac{k_1}{2} (\psi_1^* \nabla \psi_1 - \psi_1 \nabla \psi_1^*) + \frac{k_1}{2} (\psi_2^* \nabla \psi_2 - \psi_2 \nabla \psi_2^*) \\ &\quad + \frac{k_1}{2} (\psi_1^* \psi_1 + \psi_2 \psi_2^*) \mathbf{A} + \frac{k_2}{2} |(\psi_1^* \mathbf{D}\psi_1 + \psi_2^* \mathbf{D}\psi_2)| |(\psi_1^* \psi_1 + \psi_2 \psi_2^*)|. \end{aligned} \quad (26)$$

The first and second terms are expressions for the two strands on the torus surface. They can be denoted as:

$$\begin{aligned} \mathbf{J}_1 &= \frac{k_1}{2} (\psi_1^* \nabla \psi_1 - \psi_1 \nabla \psi_1^*), \\ \mathbf{J}_2 &= \frac{k_1}{2} (\psi_2^* \nabla \psi_2 - \psi_2 \nabla \psi_2^*). \end{aligned} \quad (27)$$

Because the component ψ_1 is perpendicular to the component ψ_2 , the direction of the strand $\mathbf{J}_1$ is perpendicular to the strand $\mathbf{J}_2$. Let us assume the direction of $\mathbf{J}_1$ is in a poloidal direction, then the strand $\mathbf{J}_2$ is in a toroidal direction. The two strands have $S^1 \times S^1$ symmetry and construct the torus knot. In order to study the knot in detail, the strand $\mathbf{J}$ is rewritten as:

$$\begin{aligned} \mathbf{J} &= \frac{k_1}{2} \psi_1^* \psi_1 \frac{(\psi_1^* \nabla \psi_1 - \psi_1 \nabla \psi_1^*)}{\psi_1^* \psi_1} + \frac{k_1}{2} \psi_2^* \psi_2 \frac{(\psi_2^* \nabla \psi_2 - \psi_2 \nabla \psi_2^*)}{\psi_2^* \psi_2} \\ &\quad + \frac{k_1}{2} (\psi_1^* \psi_1 + \psi_2 \psi_2^*) \mathbf{A} + \frac{k_2}{2} |(\psi_1^* \mathbf{D}\psi_1 + \psi_2^* \mathbf{D}\psi_2)| |(\psi_1^* \psi_1 + \psi_2 \psi_2^*)|. \end{aligned} \quad (28)$$

Fig. 3 Torus knot with different directions

Let us define new strands as:

$$\begin{aligned} \mathbf{j}_1 &= \frac{k_1}{2} \frac{(\psi_1^* \nabla \psi_1 - \psi_1 \nabla \psi_1^*)}{\psi_1^* \psi_1}, \\ \mathbf{j}_2 &= \frac{k_1}{2} \frac{(\psi_2^* \nabla \psi_2 - \psi_2 \nabla \psi_2^*)}{\psi_2^* \psi_2}, \end{aligned} \quad (29)$$

where $\mathbf{j}_1$ and $\mathbf{j}_2$ are shown in Fig. 3. The strands can be expressed by new unit vectors as:

$$\begin{aligned} j_{1i} &= \frac{k_1}{2} \varepsilon_{ab} n_1^a \partial_i n_1^b, \\ j_{2i} &= \frac{k_1}{2} \varepsilon_{ab} n_2^a \partial_i n_2^b, \end{aligned} \quad (30)$$

where $a, b = 1, 2$ and $i = 1, 2, 3$. The unit vectors n_1^a and n_2^a are:

$$\begin{aligned} n_1^a &= \frac{\psi_1^a}{\|\psi_1^* \psi_1\|}, \\ n_2^a &= \frac{\psi_2^a}{\|\psi_2^* \psi_2\|}, \end{aligned} \quad (31)$$

which satisfy the relations:

$$\begin{aligned} n_1^a n_1^a &= 1 \\ n_2^a n_2^a &= 1 \end{aligned} \quad (32)$$

The unit vectors are the map: $R^3 \rightarrow C^1$. By considering the φ -mapping topological current theory [20–22], the vorticities of the strands j_1 and j_2 are:

$$\begin{aligned} \Gamma_1 &= \int_{S_1} (\nabla \times \mathbf{j}_1) \cdot d\mathbf{S}_1 = W_1, \\ \Gamma_2 &= \int_{S_2} (\nabla \times \mathbf{j}_2) \cdot d\mathbf{S}_2 = W_2, \end{aligned} \quad (33)$$

where W_1, W_2 are the winding numbers, which are topological. In general, the meaning of the winding number is as follows. Let us consider that the superposition ψ_i is the map: $R^3 \rightarrow E^2$; when the coordinates x travel around the zero point of the superposition once, the superposition covers the zero point W_i times. When the superposition covers the zero point counterclockwise, the winding number is positive. Otherwise, the winding number is negative. By considering (5), the winding number of the single zero point of the superposition is +1 or -1 (Fig. 4).

Fig. 4 The winding number in *a* is +1 and in *b* is -1

Let us consider two cross sections of the torus, which are plotted in Fig. 5. One cross section is given as a , but the cross section cannot touch the inner part S of the torus. When the knot passes through the cross section one time, there is a zero point in the cross section. The total winding number W_1 shows that the knot rotates in a poloidal direction by angle $2W_1\pi$. For the same reason, we consider another cross section shown as b where the winding number W_2 shows that the knot rotates in a toroidal direction by angle $2W_2\pi$. Finally, the torus knot soliton hidden in DNA can be expressed by (W_1, W_2) .

3 Geometric structure of DNA

In general, the helical axis is treated only as a curve in three-dimensional space and the Frenet frame [23] on the curve is used to describe the spatial configuration of DNA. To do this, the helical axis can be considered as a curve in three-dimensional space expressed as:

$$\mathbf{r} = \mathbf{r}(s). \quad (34)$$

The unit tangent vector $\mathbf{t}$ at point p in the helical axis is defined as:

$$\mathbf{t} = \frac{d\mathbf{r}(s)}{ds}. \quad (35)$$

Based on the Pauli matrix and two-component spin wave function, the expression of the tangent vector $\mathbf{t}$ is given as:

$$\mathbf{t} = \boldsymbol{\alpha} = \psi^\dagger \boldsymbol{\sigma} \psi = (\sin \theta \cos \phi, \sin \theta \sin \phi, \cos \theta). \quad (36)$$

To derive the Frenet formula of the helical axis, it is necessary to establish a three-dimensional orthogonal frame on the helical axis and introduce two other unit vectors $\boldsymbol{\beta}(s)$ and $\boldsymbol{\gamma}(s)$. They are called the principal normal vector and sub-normal vector, respectively, and are defined as:

$$\boldsymbol{\beta}(s) = \frac{\dot{\boldsymbol{\alpha}}}{k}, \quad (37)$$

$$\boldsymbol{\gamma}(s) = \boldsymbol{\alpha}(s) \times \boldsymbol{\beta}(s), \quad (38)$$

where k is:

$$k = \left| \frac{d\mathbf{t}}{ds} \right| = |\dot{\boldsymbol{\alpha}}|. \quad (39)$$

Fig. 5 Cross sections of the torus knot

Substituting (36) into this equation, one has:

$$k = \sqrt{\left(\frac{d\theta}{ds}\right)^2 + \left(\frac{d\phi}{ds}\right)^2 \sin^2(\theta)}. \quad (40)$$

According to differential geometry, k is the curvature at point p in the helical axis curve $\mathbf{r}(s)$. $\dot{\boldsymbol{\alpha}}$ is called the curvature vector, which is normal to the tangent vector. Introducing formulas (36) and (40) into (37), the principal normal vector $\boldsymbol{\beta}(s)$ is:

$$\begin{aligned} \boldsymbol{\beta}(s) &= \frac{\dot{\boldsymbol{\alpha}}}{k} \\ &= \frac{\left(\cos \theta \cos \phi \frac{d\theta}{ds} - \sin \theta \sin \phi \frac{d\phi}{ds}, \cos \theta \sin \phi \frac{d\theta}{ds} + \sin \theta \cos \phi \frac{d\phi}{ds}, -\sin \theta \frac{d\theta}{ds}\right)}{\sqrt{\left(\frac{d\theta}{ds}\right)^2 + \left(\frac{d\phi}{ds}\right)^2 \sin^2(\theta)}}. \end{aligned} \quad (41)$$

Substituting formulas (36) and (41) into (38), the sub normal vector is:

$$\boldsymbol{\gamma}(s) = \frac{\left(-\sin \phi \frac{d\theta}{ds} - \sin \theta \cos \theta \cos \phi \frac{d\phi}{ds}, \cos \phi \frac{d\theta}{ds} - \sin \theta \cos \theta \sin \phi \frac{d\phi}{ds}, \sin^2 \theta \frac{d\phi}{ds}\right)}{\sqrt{\left(\frac{d\theta}{ds}\right)^2 + \left(\frac{d\phi}{ds}\right)^2 \sin^2(\theta)}}. \quad (42)$$

$\{r(s); \boldsymbol{\alpha}, \boldsymbol{\beta}, \boldsymbol{\gamma}\}$ is the Frenet frame at point p along the helical axis.

In fact, the double helix can form a twist surface in space. Therefore, the helical axis is located in the surface. In the study of the geometry structure of the helical axis, it should not be separated from the helical axis from the surface. Therefore, a new three-dimensional orthogonal frame is redefined as $\{r(s); \mathbf{t}, \mathbf{b}, \mathbf{n}\}$. The unit tangent vector $\mathbf{t}$ on the curve is the same as the previous definition. The unit tangent vector is rotated counterclockwise by $\frac{\pi}{2}$ and another unit vector $\mathbf{n}(s)$ is obtained:

$$\mathbf{n} = (\cos \theta \cos \phi, \cos \theta \sin \phi, -\sin \theta). \quad (43)$$

The third unit vector is calculated by $\mathbf{b} = \mathbf{n} \times \mathbf{t}$:

$$\mathbf{b} = \mathbf{n} \times \mathbf{t} = (\sin \phi, -\cos \phi, 0). \quad (44)$$

The three unit vectors $\mathbf{t}, \mathbf{b}, \mathbf{n}$ constitute another three-dimensional orthogonal frame on the helical axis and satisfy the equations:

$$\frac{d\mathbf{t}}{ds} = k_g \mathbf{b} + k_n \mathbf{n}, \quad (45)$$

$$\frac{d\mathbf{b}}{ds} = -k_g \mathbf{t} + \tau_g \mathbf{n}, \quad (46)$$

$$\frac{d\mathbf{n}}{ds} = -k_n \mathbf{t} - \tau_g \mathbf{b}. \quad (47)$$

By substituting $\mathbf{t}, \mathbf{b}, \mathbf{n}$ into these equations, one has:

$$\begin{aligned} \frac{d}{ds}(\sin \theta \cos \phi, \sin \theta \sin \phi, \cos \theta) &= k_g(\sin \phi, -\cos \phi, 0) + k_n(\cos \theta \cos \phi, \cos \theta \sin \phi, -\sin \theta), \\ \frac{d}{ds}(\sin \phi, -\cos \phi, 0) &= -k_g(\sin \theta \cos \phi, \sin \theta \sin \phi, \cos \theta) + \tau_g(\cos \theta \cos \phi, \cos \theta \sin \phi, -\sin \theta), \\ \frac{d}{ds}(\cos \theta \cos \phi, \cos \theta \sin \phi, -\sin \theta) &= -k_n(\sin \theta \cos \phi, \sin \theta \sin \phi, \cos \theta) - \tau_g(\sin \phi, -\cos \phi, 0). \end{aligned} \quad (48)$$

The coefficients of the right-hand side of the equations are:

$$\begin{aligned}k_g &= -\sin \theta \frac{d\phi}{ds}, \\k_n &= \frac{d\theta}{ds}, \\\tau_g &= \cos \theta \frac{d\phi}{ds},\end{aligned}\tag{49}$$

where k_n is the normal curvature of the helical axis, k_g is the geodesic curvature of the helical axis and τ_g is the geodesic torsion of the helical axis. By introducing (40) into (49), an important relation can be obtained:

$$k^2 = k_g^2 + k_n^2.\tag{50}$$

The expression of free-energy density with curvature and torsion is:

$$F = \frac{B}{2} (k_g^2 + k_n^2) + \frac{C}{2} \left(\tau_g + \frac{d\chi}{ds} - \rho \right)^2,\tag{51}$$

where the Euler angular χ and gauge potential ρ are functions of arc element s . Namely, the variation rate of χ with s and the gauge potential ρ contribute to the torsion. The new torsion can be defined as $\tau'_g = \left(\tau_g + \frac{d\chi}{ds} - \rho \right)$ and (51) can be simplified as:

$$F = \frac{B}{2} k^2 + \frac{C}{2} \tau_g'^2.\tag{52}$$

With this formula, we can intuitively understand that the free-energy density of DNA is determined by the curvature and torsion of the helical axis.

4 Conclusions

In this paper, the free-energy density of the DNA in theory of the Landau model is reviewed. In order to guarantee the gauge invariance of free-energy density, the chiral gauge field is introduced. By using the φ -mapping topological current theory, the knot soliton hidden in DNA is observed and represented by winding number (W_1, W_2). Moreover, we regard the helical axis as the curve in the twist surface of DNA and the equations analogous to the Frenet equations are presented. Therefore, the normal curvature, geodesic curvature and geodesic torsion and their relationship are presented. This provides us with a new way to make study the geometric properties of the twist surface of DNA. By using the relationships between the free-energy density and curvature and torsion, it is possible to reconstruct the geometrical structure of DNA. Furthermore, the geometric structure of the twist surface of the DNA can be studied in detail. Also, it is interesting to discuss how to relate the supercoiling of the DNA to its free-energy density. It is also important to study the relations between the free-energy density and the twisting number and writhing number.

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Compliance with Ethical Standards

Conflict of interest This article does not contain any studies, by any of the authors with human participants or animals.

References

1. Lee, M., Kim, S.H., Hong, S.-C.: Minute negative superhelicity is sufficient to induce the B-Z transition in the presence of low tension. *Proc. Natl. Acad. Sci. U.S.A.* **107**, 4985–4990 (2010)
2. Dong, R., Yan, X., Yu, G., et al.: B- to S-form transition of double-stranded DNA in solutions of various salt concentrations. *Phys. Lett. A* **318**, 600–606 (2003)
3. Poland, D., Scheraga, H.A.: Phase transitions in one dimension and the Helix—Coil transition in polyamino acids. *J. Chem. Phys.* **45**, 1456–1463 (1966)
4. Peyrard, M., Bishop, A.R.: Statistical mechanics of a nonlinear model for DNA denaturation. *Phys. Rev. Lett.* **62**, 2755–2758 (1989)
5. Dauxois, T., Peyrard, M., Bishop, A.R.: Dynamics and thermodynamics of a nonlinear model for DNA denaturation. *Phys. Rev. E* **47**, 684–695 (1993)
6. Okushima, T., Kuratsuji, H.: DNA As a one-dimensional chiral material: Application to structural B-Z transition. *Phys. Rev. E* **84**, 021926 (2011)
7. Andrec, M., Felts, A.K., Gallicchio, E., Levy, R.M.: Protein folding pathways from replica exchange simulations and a kinetic network model. *Proc. Natl. Acad. Sci. U.S.A.* **102**, 6801–6806 (2005)
8. Finkelstein, A., Galzitskaya, O.: Physics of protein folding. *Phys. Life. Rev.* **1**, 23–56 (2004)
9. Ghosh, K., Ozkan, S.B., Dill, K.A.: The ultimate speed limit to protein folding is conformational searching. *J. Am. Chem. Soc.* **129**, 11920–11927 (2007)
10. Dill, K.A., Ozkan, S.B., Weikl, T.R., Chodera, J.D., Voelz, V.A.: The protein folding problem: when will it be solved? *Curr. Opin. Struct. Biol.* **17**, 342–346 (2007)
11. Piccinini, E., Affinito, F., Brunetti, R., Jacoboni, C., Ceccarelli, M.: Exploring free-energy profiles through ion channels: Comparison on a test case. *J. Comput. Electr.* **6**, 373–376 (2007)
12. Sakurai, J.J., Napolitano, J.J.: *Modern Quantum Mechanics*, 2nd edn., pp. 171–174. Addison Wesley, Reading (2010)
13. Ryder, L.H.: *Quantum Field Theory*, 2nd edn., pp. 105–125. Cambridge University Press, Cambridge (1996)
14. Marko, J.F., Siggia, E.D.: Fluctuations and supercoiling of DNA. *Science* **265**, 506–508 (1994)
15. Marko, J.F., Siggia, E.D.: Statistical mechanics of supercoiled DNA. *Phys. Rev. E* **52**, 2912–2938 (1995)
16. Bouchiat, C., Mézard, M.: Elasticity model of a supercoiled DNA molecule. *Phys. Rev. Lett.* **80**, 1556–1559 (1998)
17. Fain, B., Rudnick, J.: Conformations of closed DNA. *Phys. Rev. E* **60**, 7239–7252 (1999)
18. Babaev, E., Faddeev, L.D., Niemi, A.: Hidden symmetry and knot solitons in a charged two-condensate Bose system. *Phys. Rev. B* **65**, 100512 (2002)
19. Babaev, E.: Vortices with fractional flux in two-gap superconductors and in extended Faddeev model. *Phys. Rev. Lett.* **89**, 067001 (2002)
20. Duan, Y.S., Ge, M.L.: SU(2) Gauge theory and electrodynamics of N moving magnetic monopoles. *Sci. Sin.* **11**, 1072–1086 (1979)
21. Shi, X., Duan, Y.S.: Reduced quantum topological trajectory in coherence and decoherence. *Mod. Phys. Lett. A* **26**, 1363–1373 (2011)
22. Shi, X., Yu, M., Duan, Y.S.: Topological solution of Bohmian quantum mechanics. *Mod. Phys. Lett. A* **24**, 453–461 (2009)
23. Chern, W.H.: *Differential Geometry (Chinese Edition)*, pp. 24–30. Peking University Publication, Beijing (1990)