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Topology and Elastic Theory of DNA Molecule

Subhamoy Singha Roy

Department of Physics, JIS College of Engineering, West Bengal University of Technology, Kalyani, India

Email address:
ssroy.science@gmail.com

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Abstract: We have determined at this point that the DNA molecule may be considered as a long chain of an antiferromagnetic spin adjustment when the spin is accurate to be situated on the axis of the supercoil. Furthermore, we examine that as two polynucleotide chains are coiled regarding the same axis with an exact helical sense in a DNA molecule, this can be considered as if a spin with a specific point of reference is confined on the axis of the coil such that two contiguous coils have reverse direction of the spin. Actually, with each turn two strands move in the opposite side of the axis and so the spin direction accredited for the two adjacent coils should be opposite to each other. As soon as spins are defined in the Lie algebra of SU (2) the linking number can be established from the Chern-Simon's topology linked with the spin system. We shall study the topological property of a DNA supercoil from the angle of such a spin chain. Also, we shall put together the elastic properties of a DNA molecule from on analysis of the spin degrees of freedom. As spins are considered at this time as gauge currents formulated from SU (2) gauge fields we map the elastic properties onto the space of gauge potentials. In quantum field theory the divergence of this current is non-zero which gives increase to chiral anomaly caused by chiral balance contravention.

Keywords: DNA Molecule, Linking Number, Elastic Forces, Gauge Fields

1. Introduction

Statistical mechanics of supercoiled DNA has been studied by several authors [1]. The experiments of Boles et al. [2] propose that thermal alteration regulate the construction of supercoils. Experiments of Bednar et al [3] inscribed that DNA-DNA allure may battle with variation entropy. In this explanation we shall study contrasting analytical mechanical character of DNA supercoils by taking into analysis that a DNA supercoil can be recognize as a chain of spin system. In fact, as two polynucleotide chains are helicoid about the same axle with a definite helical impact in a DNA molecule, we may anticipate it such that a spin with a distinct direction is added on the axle in the coil such that two adjoining coils have opposite locations of the spin. This comes from the fact that with each turn two strands go in the contradictory side of the axle and so the spin set up assigned for two contiguous coils should be opposite to each other. In aspect of this a DNA supercoil may be examined to serve as an antiferromagnetic chain of spins based on the axle of the supercoil. We shall consider the topological features as well as the elastic and thermo dynamical features of a DNA supercoil from a breakdown of this spin structure. Indeed, the topological feature such as the linking number can be derived from the Chern-Simon's topology linked with a quantum spin [4, 5]. The elastic features such as bending (curvature) and twisting (torsion) can be arrange in terms of gauge fields when spins are explained as gauge currents [4, 5]. The added benefit in this system is that it directly implies the interconnection of bending and twisting. The thermo dynamical entropy linked with a DNA supercoil emerges here as the entanglement entropy of the antiferromagnetic spin chain. It may be referred that entanglement entropy of a DNA supercoil actually speaks for the consist of information that can be write out. Thus, we arrive at a significant representation of the genetic information involved in the supercoil and the process of genetic knowledge documentation can be featured in the framework of quantum information theory.

2. Theoretical Background

A. Linking Number: A Topological Feature of DNA.

In length scales of a large number of base pairs DNA in vivo is defined into topologically independent loops. The two strands of a circular DNA molecule acquire as a topological invariant the number of times they curl around each other which is recognized as the linking number. A B-DNA molecule has one right-handed twist per $h = 3.4$ down to its length. When these are folded in a planar circle after twisting of the ends, the culminating linking number is $lk_o = l/h = \omega_0 l/(2\pi)$ where l is the length and ω_0 is the spatial rotation rate of the base pairs nearly the pivotal axle [1]. Adjustment in the coiling rate from ω_0 is calculated relative to lk_o about the parameter deciding the excess associating $\sigma = (\Delta lk/lk_0)$ where $\Delta lk = lk - lk_0$. The linking number lk is declared as $lk = Tw + \phi r$ where Tw portrays the twist interrelated to the cycle of the intrinsic degrees of freedom about the molecule axle and ϕr presents the writhe [6-8]. The twist calibrates the coiling of one curve about the other. It can be scientifically expressed as [1]

$$Tw = \int_0^l (ds/2\pi)\left[\omega_0 + \pi(s)\right] = lk_o + \Delta Tw \tag{1}$$

where π is the twist strain considerate the excess or deficit rotation of the base pairs about the axle and s represents the arc length. The writhe defines the chiral deformation of a curve. One can select a direction to a curve and measure the sum of signed crossings in a planar projection by each way. ϕr is same to the average of such sums over all projections [9].

We can grasp twist and writhe more notably from the subsequent considerations [10]. Let us follow that there are two oriented non- separated closed curves ξ_1 and ξ_2, visualize that ξ_2 bears a unit current in the line of its orientation. Obviously, this brings about a magnetic field. Now applying Ampere's law to reduce the number of times ξ_1 cycles ξ_2 and by taking help of Biot-Savert law which let us do the assessment of the magnetic field cause of the current we can write:

$$lk(\xi_1, \xi_2) = \oint_{r_1} \vec{B}(\vec{r}_1)d\vec{r}_1$$

$$= \frac{1}{4\pi}\oint_{\xi_1}\oint_{\xi_2} \{(\vec{r}_1 - \vec{r}_2)(d\vec{r}_1 \times d\vec{r}_2)\}/|\vec{r}_1 - \vec{r}_2|^3 \tag{2}$$

This is called the Gauss linking number which is proportional to the interchange of $\xi_1 \leftrightarrow \xi_2$. For a closed loop of DNA we describe the curves with the strands. Two such parallel curves (ξ_1, ξ_2) form the edges of a ribbon of width E. We now look at the curve $\vec{r}(t)$ going by the axle of the ribbon midway between ξ_1 and ξ_2 and express it as ξ. The unit tangent to ξ at the point $\vec{r}(t)$ is given by:

$$\vec{t}(t) = \dot{\vec{r}}(t)/|\vec{r}(t)| \tag{3}$$

the dot indicating the differentiation with respect to t. A unit vector $\vec{y}(t)$ perpendicular to $\vec{t}(t)$ lies in the ribbon pointing from $\vec{r}_1(t)$ to $\vec{r}_2(t)$. We can now note:

$$\vec{r}_1(t) = \vec{r}(t) - (1/2)E\vec{y}(t)$$

$$\vec{r}_2(t) = \vec{r}(t) + (1/2)E\vec{y}(t) \tag{4}$$

Expressing

$$\dot{\vec{y}} = \vec{\omega} \times \vec{y} \tag{5}$$

where $\vec{\omega}(t)$ is the angular velocity vector we can define twist as:

$$Tw = 1/2\pi \oint_{\xi} (\vec{\omega}.\vec{t})dt \tag{6}$$

If we let $\vec{r}_1(t)$ and $\vec{r}_2(t)$ match to the single axis curve $\vec{r}(t)$ in the integrand of (2) the self -linking integral defined as the writhe is given by:

$$\phi r = \frac{1}{4\pi}\oint_{\xi}\oint_{\xi} \{(\vec{r}(t_1) - \vec{r}(t_2))((\dot{\vec{r}}(t_1) \times \dot{\vec{r}}(t_2))\}dt_1 dt_2 / |(\vec{r}(t_1) - \vec{r}(t_2)|^3 \tag{7}$$

The writhe is a feature of the comprehensive shape of the curve ξ and is absolute of the ribbon that harbors it. We have the relation:

$$lk = Tw + \phi r \tag{8}$$

which is known as the Calugareanu-White-Fuller relation.

From the perspective that a DNA molecule can be explained as a spin system we can verify the linking number from the spin degrees of freedom. It is notable that the analysis of the current I_μ correlated with the spin given by eqn.

$$I_\mu = (1/16\pi^2)E^{\mu\nu\lambda\sigma}Tr\{Z_\nu \Re_{\lambda\sigma} + (2/3)Z_\nu Z_\lambda Z_\sigma\} \tag{9}$$

approximately correlates to the Chern-Simons secondary attributes class. The topological charge:

$$Q = \int I_0 d^3x \tag{10}$$

correlates to the coiling number corresponded with the homotropy $\pi_3(S^3) = \mathbb{Z}$ and can be considered as:

$$Q = 2\mu = (1/24\pi^2)\int_{S^3} E^{\mu\nu\lambda\sigma}Tr(g^{-1}\partial_\nu g)(g^{-1}\partial_\lambda g)(g^{-1}\partial_\sigma g) \tag{11}$$

This charge Q substantially means the Pontryagin index which is an integer and the relation $Q = 2\mu$ represents that μ correlates to the magnetic monopole strength. This Pontryagin index can be observed as the integral in the 4-dimensional manifold M_4 as:

$$Q = (1/16\pi^2)\int_{M_4} Tr(\Re \wedge \Re) \quad (12)$$

where F is the two-form corresponded to the field strength linked with the $SU(2)$ gauge field A_μ . Now from the association:

$$\int_{M_4} Tr(\Re \wedge \Re) = \int_{M_3} Tr(Z \wedge dZ + (2/3) Z \wedge Z \wedge Z) \quad (13)$$

where M_3 is a three spatial assorted and Z is the one-form related to the $SU(2)$ gauge field Z_μ we see that the R. H. S of eqn.(13) serve as the Chern-Simons invariant and is thus viewed as a form affiliated with the Pontryagin index. Noting that the Pontryagin index equivalent to the charge associated to the gauge current I_μ given by eqn. (9) and eqn. (10) which is corresponded with the spin, we can take spin in the framework of Chern-Simon' stopology.

In fact from eqn.

$$\vec{I}_\mu = E^{\mu\nu\lambda\sigma} \vec{A}_\nu \times \vec{f}_{\lambda\sigma} = E^{\mu\nu\lambda\sigma} \partial_\nu \vec{f}_{\lambda\sigma} \quad (14)$$

we say that any factor of the spin vector can be written as:

$$I^a_\mu (A = 1,2,3) = E^{\mu\nu\lambda\sigma} A_\nu \partial_\lambda A_\sigma \quad (15)$$

where A_ν denotes an Abelian gauge field. When we project it onto a three-dimensional manifold this correlates to the Chern-Simon' sterm $E^{\nu\lambda\sigma} A_\nu \partial_\lambda A_\sigma$. In the Abelian theory we look at the one-form a linked with the gauge field A_ν and adopt the action:

$$S = (k/8\pi) \int_{M_3} E^{ijk} A_i \partial_j A_k \quad (16)$$

where k is an integer. We now acquire some circles C_A and some integers n_A affiliated with illustration of the Abelian gauge group. It is assumed that two curve C_A and C_B do not corresponds for $A \neq b$. As shown by Polyakov [11] the expectation value of the product:

$$W = \Omega_A \exp(i n_A \int_{C_A} A \quad (17)$$

related to the method computed by e^{iS} is given by:

$$\langle \phi \rangle = \exp\left((i/2k) \sum_{A,b} n_A n_b \int_{C_A} dx^i \int_{C_b} dY^j E_{ijk} \left\{ (x-Y)^k / |x-Y|^3 \right\} \right) \quad (18)$$

For $A \neq b$ this integral is originally the linking number:

$$\varphi(C_A, C_b) = \frac{1}{4\pi} \int_{C_A} dx^i \int_{C_b} dY^j E_{ijk} \left\{ (x-Y)^k / |x-Y|^3 \right\} \quad (19)$$

As long as C_A and C_b do not concern $\varphi(C_A, C_b)$ is a known integer. So, ignore the term $A = b$, we have:

$$\langle \phi \rangle = \exp\left((2\pi i/k) \sum_{A,b} n_A n_b \varphi(C_A, C_b) \right) \quad (20)$$

The representation of linking number from the Chern-Simon's term related with the gauge current defining the spin recommend that the linking number can be correlated with a spin system.

From this view it is noted that when a DNA molecule is described as a spin system the linking number can be taken into as a topological invariant related to the Chern-Simon's topology corresponded with the spin system. It is worth noting that though the linking number is a topological invariant when it is divided into twist (Tw) and writhe (ϕr) these entities are not topological invariants. Since the linking number of a closed DNA molecule stays absolute during any defect of the molecule that represents chemical bonding, it can only be interchanged by structures in which chemical bonds are broke into [10].

B. Elastic Mechanicalproperties of the DNA

Here we consider the elastic features of a DNA molecule from ananalysis of the spin degrees of freedom. As spins are taken here as gauge currents composed from $SU(2)$ gauge fields we design the elastic features onto the space of gauge capability. In fact, the tangent vector $\vec{t} = \partial_s \vec{r}(s)$ where $\vec{r}(s)$ represents a space curve specified by arc length s of the helix can be graph onto the spin vector combined by the vector of topological gauge current given by the eqn (14). Now taking account of that these gauge currents act as the cause of $SU(2)$ gauge fields we can describe the tangent vector $\vec{t}$ to the vector of gauge potentials $\vec{A}_\mu$ where the factors combine to the $SU(2)$ gauge fields. Obviously $\partial_s^2 \vec{r}$ represents the vector of $SU(2)$ gauge field strength $\vec{f}_{\mu\nu}$. Accepting the relation $A_\mu = \vec{a}_\mu . \vec{\sigma}$ and $F_{\mu\nu} = \vec{f}_{\mu\nu} . \vec{\sigma}$ the internal energy combining to the curvature (bending) given by $\int ds (\partial_s^2 \vec{r})^2$ can be viewed as $\int d^3x Tr \Re_{\mu\nu} \Re_{\mu\nu}$. The twisting elastic energy can be linked with the spin-spin interaction and can be viewed as the continuum limit as $m^2 \int \vec{I}_\mu \vec{I}_\lambda d^3x$ where $\vec{I}_\mu$ is the gauge current given by eqn. (14) and m is a constant having the dimension of mass. It is noteworthy that this term related to the spin-spin interaction in the continuum limit serve as torsion [12].

The elastic energy of B-DNA of length l is given by [6].

$$\Im_{cL}/k_BT = \frac{1}{2}\int_0^l ds\left[Z(\partial_s^2\vec{r})^2 + C\pi^2\right] \quad (21)$$

where the aberration in the twisting rate from ω_0 is characterized by the scalar field $\pi(s)$, $Z(C)$ being the bending (twisting) elastic constant. When we write this on the configuration space of gauge potentials corresponded with the spin system, we can describe the elastic energy in the continuum limit.

$$\Im_{cL}/k_BT = \frac{1}{2}\int d^3x[ZTr\Re_{\mu\nu}\Re_{\mu\nu} + Cm^2\vec{I}_\mu\vec{I}_\mu] \quad (22)$$

where $\vec{I}_\mu$ is given by eqn. (14). We shall note that the topological current $\vec{I}_\mu$ is linked to the topological Lagrangian.

Knowing this, both bending energy and twisting energy relates to the $SU(2)$ gauge field strength $\Re_{\mu\nu}$. As in a non-Abelian gauge theory the field strength is not gauge invariant but gauge covariant any arbitrary deformation such as bending, twisting and stretching can be joined with gauge transformation. A compelling result of this experiment is that curvature (bending) and torsion (twisting) correlated with the diversion from ω_0 are not different entities. Undoubtedly one is related to the other. This complies from the fact that the gauge field curvature $\Re_{\mu\nu}$ is assimilated in the structure of the current $\vec{I}_\mu$ in eqn. (13a) which gives birth to torsion. This generally depicts that bending causes a dynamical effect on torsional energy. In regard to this it may be consider that Nelson [13] proposed that intrinsic bending can have a huge effect in the carrying of torsional stress along DNA.

It is noteworthy that twisting is calculated by the spatial rotation rate of base pairs about the central axis which for an undistorted DNA is just ω_0 . However, for a distorted DNA twisting elastic energy carries a value when the double-helix twist is changed from ω_0 . In this case we have chiral symmetry collapsing which is demonstrated through torsion. We shall note that in the current situation torsion is created by the topological current $I_\mu^A(A=1,2,3)$ which correlate to the axial vector current $I_\mu^5 = \bar{\psi}\xi_\mu\xi_5\psi$ corresponded with a chiral spinner. In fact, each portion of the vector $\vec{I}_\mu$ in eqn. (14) is correlated to the axial vector current by this relation [14-16]:

$$\partial_\mu I_\mu^2 = -1/2\partial_\mu I_\mu^5, I_\mu^1 = -1/2I_\mu^2,\ I_\mu^3 = 1/2I_\mu^2, \quad (23)$$

In quantum field theory the divergence of this current is non-zero which generates the chiral anomaly result of chiral symmetry breaking.

3. Conclusion

We have gone through the topological features of a DNA molecule and discovered the elastic features such as bending (curvature) and twisting (torsion) in accord of these gauge fields. A noteworthy outcome of this formalism is that bending and twisting are not independent entities. In fact, bending give rise to the propagation of twisting strain along the DNA which has been backed by experiments. Finally, we have realized that the spin chain model gives birth to the salient feature of the RLC model when the partition function is overwritten on the path integral representation of a quantum charged particle in the field of a magnetic monopole with nonquantized charge. In account of this we encounter that twisting elastic energy defined by torsion has a coherence with the chiral anomaly in quantum field theory.

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