The Theoretical Analysis of the Phenomenon of Solitons in DNA

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Abstract—**We have introduced that a DNA supercoil can be considered as a quantum spin system such that spins are located on the axis   formulate an antiferromagnetic chain. These spins can be connected with** $SU(2)$ **gauge field currents when gauge fields recline on the links. We have expressed bending (curvature) and twisting (torsion) with regard to these gauge fields. In fact, the topological property acting as the linking number can be borrowed from the Chern-Simon's topology affiliated with a quantum spin. The current study additionally shows that DNA loops in the supercoil execute topological objects like solitons.**

Keywords—DNA supercoil; antiferromagnetic chain; solitons; Chern-Simons topology

I.   INTRODUCTION

The presence of supercoiled DNA has been confirmed in experiments earlier and it was originated that in vivo chromosomal B-DNA molecules consist of topological domains including supercoiling can occur [1-3]. DNA molecules from prokaryotes (cells without nuclear membranes) frequently adopt the interwound structures which are called "plectonemic" supercoils. In eukaryotes (cells with nuclei and other organelles with their own internal membranes) chromosomal DNA molecules are also known as arranged into topological independent loops [2-5]. Statistical mechanics of supercoiled DNA has been examined by several authors [6]. At length scale of thousands of base pairs DNA is formed into topologically self-sufficient loops. There are position in vivo when topological constraints induce supercoiling. DNA loops in a supercoil may perform as a topological object such as a soliton (skyrmion) which is accomplished when we execute DNA as a spin system. In fact, DNA loops in a supercoil when strained by a change in the linking number due to variation of twisting rate from W_0 compare to the formation of a spin texture when a DNA molecule is treated as a spin system.

II.   THEORETICAL BACKGROUND

A change in the linking number from $L_0 k_o$ as a result of twist of the ends induce a deviation from the planar circle configuration compare to a spin texture and symbolize a alteration of the spin system from the ground state when spin excitations occur. These excitations approach the solitons explained by the nonlinear σ-model.
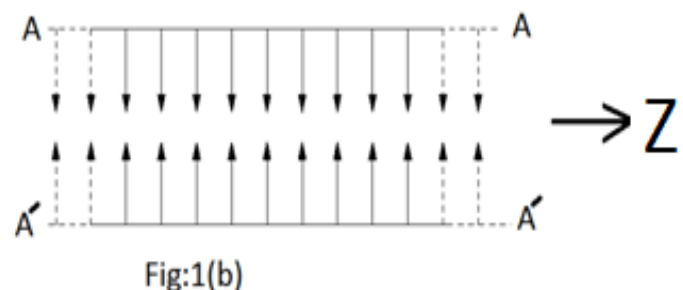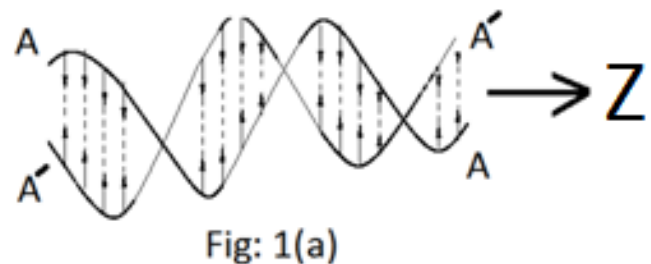

Fig: 1(a)

Fig:1(b)

Fig: 1(a) A diagram configuration B-DNA Chain. (b) A diagram depiction of DNA as an anisotropic fixed spin double helix string model.

We can depict a two-component spinor as $\begin{bmatrix} c_1 \\ c_2 \end{bmatrix}$ with

$$c_1 = \cos\frac{\theta_1}{2} e^{i\varphi_1/2} \qquad (1)$$

$$c_1 = \sin\frac{\theta_1}{2} e^{-i\varphi_1/2} \qquad (2)$$

In terms of the spin system we can consider the ground state wave function depicting the DNA supercoil with linking number $L_0 k_o$

$$|\psi_0\rangle = \prod_{i\langle j}\left(c_{1_i}c_{2_j} - c_{2_j}c_{1_i}\right) \qquad (3)$$

where j and i communicate to the spin sites. When the linking numeral deviates from $L_0 k_o$ owed to divergence of the twisting speed from ω_0, the consequential skyrmion state is described through

$$|\psi\rangle = D\prod_k \begin{pmatrix} c_{2_k} \\ -\Lambda c_{1_k} \end{pmatrix} |\psi_0\rangle \qquad (4)$$

where the spin texture is incorporated within the mechanism c_{1_k} and c_{2_k} and $0 \le \Lambda \le 1$ [7] . If a smooth and monotonical function $f(\theta)$ is defined with $f(0) = 0$ and $f(\pi) = \pi$ then the skyrmion state can be written as

$$\vec{\varphi}(\xi) = \cos(f(\theta) - \theta)\vec{e}_r + \sin(f(\theta) - \theta)\vec{e}_\theta$$
(5)

where $\vec{e}_r$ and $\vec{e}_\theta$ are the foundation vectors. The dimension of a skyrmion is resolute by the function $f(\theta)$ and $f(\theta) = \theta$ describes the hedgehog skyrmion with spin in the radial path $\vec{r}$ [8].

The skyrmion state $\vec{\varphi}(\xi)$ is controlled by the relation $|\vec{\varphi}(\xi)| = 1$. The quantum state for the skyrmion $\vec{\varphi}(\xi)$ can be written as

$$|\psi\rangle = D\prod_k \begin{pmatrix} \sin\frac{f(\theta_k)}{2} e^{-i\varphi_k/2} \\ -\cos\frac{f(\theta_k)}{2} e^{i\varphi_k/2} \end{pmatrix} |\psi_0\rangle \qquad (6)$$

where D is the normalization steady and $f(\theta)$ controls the size of the skyrmion. From equ. (5) and (6) it is seen that $0 \le \Lambda \le 1$ is determined from $f(\theta)$ and Λ pedals the size of the skyrmion [9] . Certainly we can define

$$\theta = 2\arctan\Lambda \qquad (7)$$

which equals $\frac{\pi}{2}$ for the hedgehog skyrmion with $\Lambda = 1$.

Now we may write the nonlinear σ-model Lagrangian in terms of the $SU(2)$ matrices U as [10]

$$G = -\left(m^2/16\right)\left(\partial_u U^\dagger \partial_\mu U\right) - \left(1/32\beta^2\right)\left(\partial_\mu U U^\dagger, \partial_\nu U U^\dagger\right)^2 \qquad (8)$$

where M is a constant having dimension of mass and η is a dimensionless parameter, μ, ν being space -time indices.

Taking the spin variable $\vec{Z} = U\vec{Z}_0$ with $\vec{Z}_0 = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$ and $U \varepsilon SU(2)$

The Λ reliance may be incorporated through m and β where these parameters are taken as functions of Λ.

For a indistinct loop we can believe the radius of the loop R_1 as a function, $R_1(\theta, \varphi)$ corresponding to the core radius of the Soliton. We can define the core size of the Soliton. such that $R_1 = R_0(1-\Lambda)$ where R_0 is the size of the Soliton with minimum energy. The stationary nonlinear σ-model Lagrangian corresponding to eqn. (8) gives increase to the energy integral as

$$H = \int d^3x \left\{ \left(m^2/16\right)Tr\left(\nabla U^\dagger \nabla U\right) + \left(1/32\beta^2\right)Tr\left[\partial_i U U^\dagger, \partial_j U U^\dagger\right]^2 \right\}$$
(9)

where $i, j = 1,2,3$ are special indices.

To calculate the energy we take the Skyrme ansatz

$$U(x) = \exp(iI(r)\vec{\tau}.\hat{x} \qquad (10)$$

where $\vec{\tau}$ are Pauli matrices, $\hat{x} = \frac{\vec{x}}{r}$ and $I(0) = \pi$ and $I(r) \to 0$ as $r \to \infty$. We explicitly write

$$U = \cos I(r) + i\vec{\tau}.\hat{x}\sin I(r) \qquad (11)$$

with

$$\cos I(r) = \left(1 - \frac{r}{R_1}\right)^2 \Big/ \left(1 + \frac{r}{R_1}\right)^2 \qquad \text{and}$$

$$\sin I(r) = 2\left(\frac{r}{R_1}\right)\Big/ 1 + \left(\frac{r}{R_1}\right)^2 \qquad (12)$$

The energy integral becomes

$$H(R_1) = 4\pi^2 m^2 R_1 I_1 + 2\pi^2\left(I_2 / \beta^2 R_1\right) \qquad (13)$$

where

$$I_1 = \frac{1}{\pi}\int_0^\alpha dx\left[\sin^2 I(r) + x^2\left(\partial I/\partial x\right)^2\right] = 3.0 \qquad (14)$$

and

$$I_2 = (1/\pi) \int_0^\alpha dx \left[\left(\sin^4 I(r)/x^2 \right) + \sin^2 I(r) \left(\partial I/\partial x \right)^2 \right] = 1.5$$

(15)

with $x = r/R_1$. This gives the look of energy

$$H(R_1) = 12\pi^2 m^2 R_1 + \left(3\pi^2 / \beta^2 R_1 \right)$$

(16)

The smallest amount of energy $H(R_1)$ is found from the relation

$$\partial H(R_1)/\partial R_1 = 12\pi^2 m^2 - 3\pi^2/\beta^2 R_1^2 = 0$$

(17)

which gives for H_{min} the size as

$$R_0 = 1/2m\beta \qquad (18)$$

and the energy

$$H_{min} = H(R_0) = 12\pi^2 m/\beta \qquad (19)$$

It is well-known that the coupling parameters m and β are functions of Λ such that in the limit $\Lambda \to 0, m(\Lambda) \to 0$ and $\beta(\Lambda) \to 0$ but m/β is fixed. When we take

$$R_1 = R_0 \left(1 - \Lambda \right)$$

we have

$$H(R_1) = \left\{ \left(6\pi^2 m \right)/\beta \right\} \left[(1-\Lambda) + 1/(1-\Lambda) \right] \qquad (20)$$

Now we note that the parameter Λ totally gives a measure of the hilarity associated with twisting strain into the loop given by $\sigma = \left(\Delta L_0 k/Lk_0 \right)$. In fact in the simplest form we can take $\Lambda = k|\sigma|$ where k is a constant. So form the relation $R_1 = R_0(1-\Lambda) = R_0(1-k|\sigma|)$, we can measure the energy of a DNA loop as a function of σ. It is noted that the relation $R_1 = R_0(1-\Lambda)$ gives a nonzero size for $\Lambda = 1(\sigma = 0)$ when R_0 is infinite. Definitely, it has been found that for $|\sigma| < 0.02$ the negligeable free energy state has $R_1 = P = \infty$ demonstrating that no reliable stable supercoiled state exists for small $|\sigma|$. For $|\sigma| > 0.02$ the plectonemic free energy shows a minimum value for finite R_1 and P which indicates that we have a stable supercoiled state. It seems that σ can be varied through unevenly - 0.1 to 0.1 as elsewhere these confines the double helix is unstable [11]. These observations are found to be reliable with this skyrmion model also Skyrmion energy circulate

along Z-axis. In fig: 1(a) A diagram formation B-DNA Chain. (b) A diagram representation of DNA as an anisotropic fixed spin double helix string model.
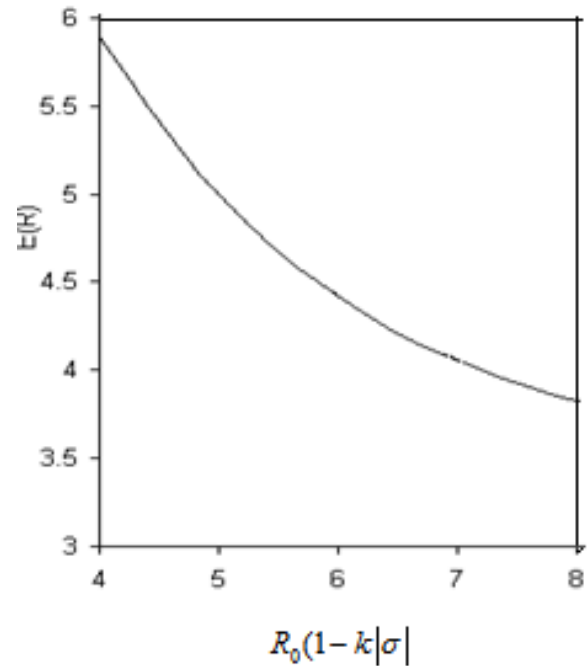
(15)

Fig.2. Skyrmion energy as a function of $R_0(1-k|\sigma|)$

In fig.2.we have designed the Skyrmion energy as a function of $R_0(1-k|\sigma|)$. From our analysis it seems that when the long linear chromosomal DNA molecules are organized into loops, these topological independent loops appear as solitons. Solitons are nonlinear excitations which can travel as coherent solitary waves. The present analysis suggests that soliton excitations may well exist in DNA chains which is reliable with the observations of Englander et.al.[12] The linking number related with a supercoil is given by the topological charge of the loops. As the skyrmion (soliton) showing a loop is designated by the nonlinear σ - model in terms of $SU(2)$ gauge fields, the topological charge of a loop is given by the winding number of the mapping of the 3-space manifold into the group manifold $SU(2) = S^3$ which resembles to homotropy $\pi_3(SU(2)) = \pi_3(S^3) = Z$ where Z signifies the set of numbers [13]. When DNA loops supercoil, the linking number is given by an integer resolute by this homotropy group so that $L_0 k = nZ$ where n is the number of superhelix loops.

III. DISCUSSION

A significant result of our examination is that a DNA loop can be considered as topological object showed as a skyrmion (soliton) which arises due to the excitation of spins caused by the variation of the twisting rate from leading to additional (deficit) of linking number. The spin consistency is determined

by the twist parameterized by the quantity .The energy of the skyromion showing a DNA loop   depends on the radius which is resolute by the parameter The linking number   of a DNA molecule when ordered into loops is associated to the topological charge of a skyrmion showing a loop

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