A QUANTITATIVE ANALYSIS OF QUICK DNA DENATURATION

Abstract.

One approach to imagine spins on the axis generating an antiferomagnatic chain is described as simulating a DNA molecule as a Heisenberg spin system. In a DNA molecule, the entanglement entropy of the spin system is shown to be in good agreement with the thermodynamic entropy. At times when the impact of temperature is included during the time of quench, It is shown that denaturation corresponds to a quantum phase change triggered by a quench. The critical point is attained and When the entanglement entropy is eliminated, it equates to a critical torsonal energy. DNA loops now appear as solitonic (skyrmionic) excitations upon base pair opening

Keywords: Heisenberg spin system, Antiferromagnetic chain, DNA molecule, Entanglement entropy, Thermodynamic entropy, Quantum phase transition

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I. INTRODUCTION

The spins are oriented so that, between a kink and an antikink, they are all pointing in the same direction as soon as the system reaches the critical point, which is suggestive of a ferromagnet. At the critical point, a spin's orientation is reversed, and the reversal process occurs by gradually tilting the spin exactly below this critical point. During this stage, the structural properties of the DNA loops start to alter and the DNA strands in a supercoil begin to split, which enhances base pair opening. In this stage, the DNA loops become skyrmions, or solitons, when they align with the spin texture. The system is driven toward the critical point by these solitonic excitations.

II. THEORETICAL BACKGROUND

Fermionic vibration is one method of representing a spin. We represent a spinor with two components by cannistering.

as $\begin{bmatrix} a \\ b \end{bmatrix}$ with

$$a = \cos(\alpha/2)\exp\left((i\beta)/2\right) \tag{1}$$

$$b = \sin(\alpha/2)\exp\left((-i\beta)/2\right) \tag{2}$$

We may think about the spin axis to be the position condition signal purpose that represents the DNA superhelix.

$$\left|\psi_0\right\rangle = \prod_{I\langle J}\{(a_I b_J) - (b_I a_J)\} \tag{3}$$

J and I interact with the revolving positions everywhere they go. When the spins begin to tilt slightly below the critical point, the resulting skyrmion situation is depicted by the following.

$$\left|\psi\right\rangle = (C)\prod_k \begin{pmatrix} b_k \\ -za_k \end{pmatrix} \left|\psi_0\right\rangle \tag{4}$$

wherein the components have the spin texture and with $0 \le z \le 1$ [1].

When a flat and monotonic function $[g(\alpha)]$ is created using $[g(0)] = 0$ and $[g(\pi)] = \pi$, the skyrmion state may be expressed as

$$\begin{aligned} \vec{\beta}(\Omega) &= \{\cos(g(\alpha)-\alpha)\vec{e}_r\} \\ &+\{\sin(g(\alpha)-\alpha)\vec{e}_\alpha\} \end{aligned} \tag{5}$$

Whereas $(\vec{e}_r)$ and $(\vec{e}_\alpha)$ stand for the fundamental vectors. The function $g(\alpha)$ and $g(\alpha)=\alpha$, which define a skyrmion's size, describe the radially orientated $\vec{r}$ hedgehog skyrmion with spin.
where $\vec{\beta}(\Omega)$ and $\left|\vec{\beta}(\Omega)\right|=1$ stand for the basic vectors. The function DD and EE, which define a skyrmion's size, describe the radially orientated $\vec{\beta}(\Omega)$ hedgehog skyrmion with spin.

$$|\psi\rangle = C\prod_k \begin{pmatrix} \sin g(\alpha_k)/2 \; e^{-(i\beta_k)/2} \\ -\cos g(\alpha_k)/2 \; e^{(i\beta_k)/2} \end{pmatrix} |\psi_0\rangle \tag{6}$$

where the skyrmion's dimension is represented by $g(\alpha)$ gearstick and the normalization invariable by C. Equations (4) and (6) demonstrate that $g(\alpha)$ is invariant with respect to , and as such, it rotates the skyrmion's dimension.

Definitely we can describe

$$\alpha = 2(\arctan z) \tag{7}$$

which equals $(\pi/2)$ for the hedgehog skyrmion with $z=1$. Enchanting the spin changeable $\vec{Z} = (U\vec{z}_0)$ with $\vec{z}_o = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$ and $U \in \{SU(2)\}$
In circumstances of the $SU(2)$matrices U, we might inscribe the nonlinear σ -model Lagrangian as [2].

$$L = -((m^2/16)(\partial_u U^\dagger \partial_\mu U)) - [(1/(32\eta^2))((\partial_\mu UU^\dagger),(\partial_\nu UU^\dagger))^2] \tag{8}$$

where η is a parameter without dimensions, m is a constant with a mass dimension, and μ,ν are space-time indices. If θ is viewed as a function of m and η, then one method to include the dependency is through these elements.

The DNA loop's radius may be considered as an apparatus $w(\alpha,\beta)$, based on the skyrmion's core radius, denoted as plectoneme radius w. By calculating the skyrmion's core size, we can get $w = w_0(1-z)$ where w_0, is the skyrmion's minimum energy size. The energy integral is obtained as the Lagrangian of the equation (8)'s related static nonlinear (σ) -model.

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

where $(I, J) = 1, 2, 3$ are indexes of space. We use the Skyrme ansatz to compute the energy [2].

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

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

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

with $$\cos F(r) = \left\{\left(1-(r/w)\right)^2 \Big/ \left(1+(r/w)\right)^2\right\} \tag{12}$$

$$\sin F(r) = \left(2\left(r/w\right) \Big/ 1+\left(r/w\right)^2\right) \tag{13}$$

The power essential becomes

$$E(w) = \left(4\pi^2 M^2 w I_1\right) + 2\pi^2 \left(I_2/\eta^2 w\right) \tag{14}$$

where $$I_1 = \frac{1}{\pi}\int_0^\infty dx\left[\{\sin^2 F(r)\} + \{x^2\left(\partial F/\partial x\right)^2\}\right] = 3.0 \tag{15}$$

and $$I_2 = (1/\pi)\int_0^\infty dx\left[\left(\left\{\sin^4 F(r)\right\}/x^2\right) + \left\{\sin^2 F(r)\left(\partial F/\partial x\right)^2\right\}\right] = 1.5 \tag{16}$$

with $x = \left(r/w\right)$. where radius of the DNA loop w (plectoneme radius). This give the face of power $$E(w) = \left(12\pi^2 m^2 w\right) + \left(3\pi^2/\eta^2 w\right) \tag{17}$$

where η is a parameter with no dimensions and m is a constant with a mass dimension.

The connection yields the minimum of energy $E(w)$.

$$\{\partial E(w)/\partial w\} = \left(12\pi^2 m^2 - 3\pi^2/\eta^2 w^2\right) = 0 \tag{18}$$

This provides the size for $E_{\min}$ as

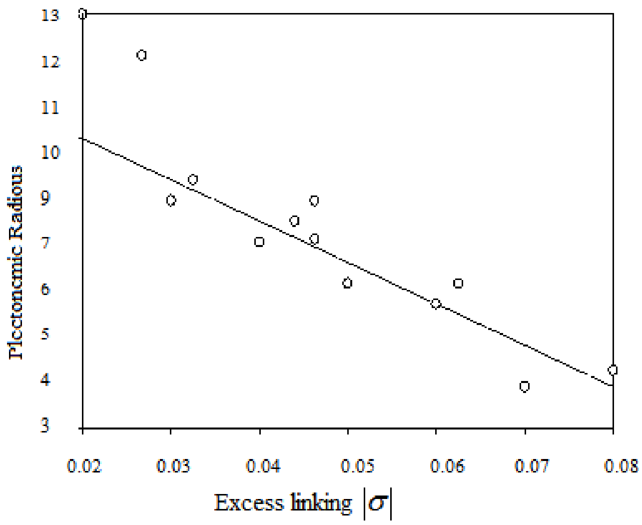
$$w_0 = \left(1/2m\eta\right) \tag{19}$$

and the energy

$$E_{\min} = E(w_0) = \left(12\pi^2 m\right)/\eta \tag{20}$$

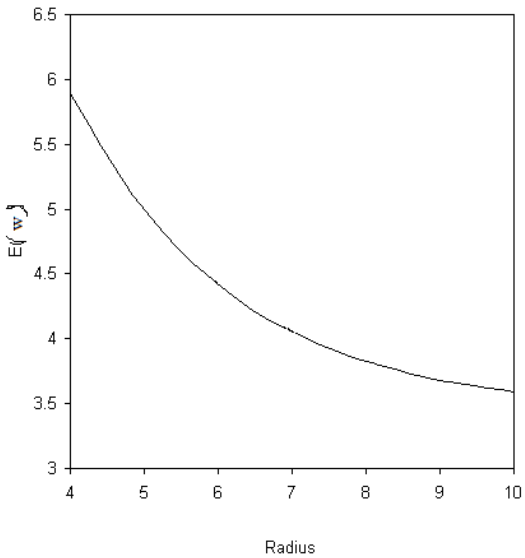
It should be observed that the combination parameters η and are functions of z, meaning that m/η is fixed while $z \to 0, m(z) \to 0$ and $\eta(z) \to 0$ are not in the limit. As we use $w = w_0(1-z)$, we have

$$E(w) = \left\{\left(6\pi^2 m\right)/\eta\right\}\left[\left\{(1-z)+1/(1-z)\right\}\right] \tag{21}$$



1(a)

Figure 1: Here (a) illustrates the radius of a a plectonemic supercoil depending on where



1(b)

$w = w_0(1-z)$ gives forth together with $z = k|\sigma|$. The constant k=8.333 is determined using the experimental data [3], and k offers the best fit. Additionally, (b) illustrates the link between the skyrmion energy and radius w .

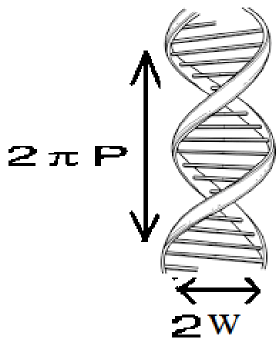


Figure 2: The solid, plectonemic superhelix line illustrates the double helix structure of B-DNA. Pitch and radius are represented by the numbers and , respectively.

The entanglement entropy serves as a useful illustration of the thermodynamic entropy. The collapse of a supercoil is prevented by this repulsive entropic potential, even at zero temperature when elastic forces would normally allow it to happen. When accounting for the temperature influence during the time of the quench, It is shown that a DNA molecule's denaturation correlates to a quantum phase transition produced by a quench at zero temperature. At the moment when the entanglement entropy disappears, the pivotal moment is equivalent to the torsonal energy's essential value.

Now we note that we can associate the parameter z with the twisting strain given by (excess linking) $\sigma = (\Delta Lk/Lk_0)$. Within information in the most submissive manner possible $z = (k|\sigma|)$ where k is a stable. It is observed that when w_0 is infinite, the relation $w = w_0(1-z)$ yields a nonzero size for $z = 1(\sigma = 0)$. It has been discovered that the least free energy state for $|\sigma| < 0.02$ possesses $w = P = \infty$, indicating that the small $|\sigma|$ does not exist in a stable, continuous supercoiled condition. The plectonemic free energy for finite w and P for $|\sigma| > 0.02$ has a low value, indicating that our situation is a stable and supercoiled state [4-5]. In fact, the essential supercoiling parameter for torque-induced denaturation is discovered to be $\sigma_c = -0.015$, indicating that the supercoil's stability is disrupted very close to this critical point. When it approaches the critical point, this causes the base pairs to open [6-8].

III. DISCUSSION

The entropic potential connected through the without charge power per unit span, this is equivalent to the entropy charge of containing a stiff polymer within a small tube, is encouraged by the description of the DNA molecule as an anti-ferromagnetic spin chain. This entanglement entropy is obtained using this method. The entanglement entropy serves as a useful illustration of the entropy of thermodynamics [9-11] . The collapse in a supercoil is prevented by this repulsive entropic potential, even at zero temperature when elastic forces would normally allow it to happen.

Denaturing a DNA molecule is shown to correlate to zero temperature quantum phase transition produced by a quench, taking into consideration the impact of temperature during the quench period.The critical point is the value of the torsonal energy at which the entanglement entropy vanishes[12] . As a consequence, spin patterns are produced just below the threshold value where solitonic (skyrmionic) excitations of DNA loops within a supercoil are seen. It is observed that the system is pushed toward the critical point by skyrmionic excitation, which happens just below the critical point [13]. The skyrmion's dimensions upon denaturation is established by the critical radius of the DNA loop (plectoneme radius) $w_c = w_0(1-k|\sigma_c|)$, which is equivalent to the plectoneme radius involving opened base pairs.

REFERENCES

[1] Basu.B.,Dhar.S., and Bandyopadhyay.p., Skyrmions In Arbitrary Polarized Quantum Hall States, Phys. B., 18, 171 (2004).

[2] Skyrme.T. H. R., A Nonlinear Field Theory, Proc. Roy. Soc. A 260 127 (1962).

[3] Bednar.J., Furrer.P., Stasrak.A., Dubochet.J., Engelman.C.H. and Bates.A.D., J.Mol.Biol., 235, 825 (1994).

[4] Marko.J. F., and Siggia.F. D., Statistical mechanics of supercoiled DNA, Phys.Rev.E.,52, 2912 (1990).

[5] Roy.S.Singha. and Bandyopadhyay.P., Quantum perspective on the localized strand separation and cyclization of DNA double helix, Phys. Lett. A., 382,1973 (2018) .

[6] Roy.S.Singha., Reverse –Transcription Spin chain reaction of RNA molecule into DNA molecule.Journal of Physics: Conference Series 1797 , 012038 (2021).

[7] Roy. S.Singha. and Bandyopadhyay.P, Entropy-driven denaturation and bubble nucleation in DNA melting, Europhys.Lett.109, 48002 (2015).

[8] Roy.S.Singha.and Bandyopadhyay.P., Torsion and entropy driven denaturation of DNA, Phys. Lett. A., 337,2884 (2013).

[9] Roy.S.Singha, Surface Free Energy of Photon echo on DEOXYRIBONUCLEIC ACID Molecules, Theoretical Study, European Journal of Biophysics 8(2), 16-19, (2020).

[10] Roy.S.Singha, Quantum effects in DNA, ISBN : 978-620-3-30866-2, Lambert Academic Publishing, (2021).

[11] Roy.S.Singha, S. Karfa, S. Sharma , S.Ghosh, Nonlinear Molecular Quantum Dynamics in an Entirely Nonhomogeneous DNA Chain Voltage, PP-1-4, IEEE explore , (2025).

[12] Roy.S.Singha, Topology and Elastic Theory of DNA Molecule, Science Journal of Applied Mathematics and Statistics, 10(1), 10-14 , (2022).

[13] Roy.S.Singha, Reverse –Transcription Spin chain reaction of RNA molecule into DNA molecule.Journal of Physics: Conference Series 1797 012038, (2021).