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An Investigation into DNA Denaturation Temperature

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Abstract

We consider that just below the critical point the two strands of a DNA molecule move apart and the spins begin to be tilted. We consider denaturation of a DNA molecule and show that this corresponds to quantum phase transition induced by a quench when the temperature effect is incorporated in the quench time.

Keywords: DNA Molecule; Denaturation; Quantum Phase Transition (QPT)

Introduction

When the system attains the critical point spins become oriented in such a way that in between a kink and antikink all are in the same direction representing a ferromagnet. When a spin reverses its orientation at the critical point, just below this point the process of reversal occurs through gradual tilting. During this process the DNA loops in a supercoil begin to change their conformational characteristics and the strands begin to move apart which enhances the opening of base pairs. The DNA loops in this stage correspond to spin texture and appear as solitons (skyrmions) and these solitonic excitations drive the system towards the critical point.

Theoretical Background

A spin may be depicted in terms of fermionic oscillators. We can depict a two-component spinor as $\begin{bmatrix} u \\ v \end{bmatrix}$ with

$$u = \cos\theta/2\, e^{i\varphi/2} \qquad (1)$$

$$v = \sin\theta/2\, e^{-i\varphi/2} \qquad (2)$$

In terms of the spin system we can consider the ground state wave function depicting the DNA supercoil

$$|\psi_0\rangle = \prod_{i<j}\left(u_i v_j - v_i u_j\right) \qquad (3)$$

where *i* and *j* correspond to the spin sites. When the spins begin to be tilted just below the critical point, the resulting skyrmion state is described by

$$|\psi\rangle = C\prod_k \begin{pmatrix} v_k \\ -\alpha u_k \end{pmatrix} |\psi_0\rangle \qquad (4)$$

where the spin texture is included within the components ν_k and μ_k with $0 \leq \alpha \leq 1$ [1]. If a smooth and monotonical function g(θ) is defined with g(0) = 0and g(π)= π then the skyrmion state can be written as

$$\vec{\varphi}(\Omega) = \cos(g(\theta)-\theta)\vec{e}_r + \sin(g(\theta)-\theta)\vec{e}_\theta \qquad (5)$$

where $\vec{e}_r$ and $\vec{e}_\theta$ are the basis vectors. The size of a skyrmion is determined by the function g(θ) and g(0) = 0 describes the hedgehog skyrmion with spin in the radial direction $\vec{r}$.

The skyrmion state $\vec{\phi}(\Omega)$ is constrained by the relation $\left|\vec{\phi}(\Omega)\right| = 1$. The quantum state for the skyrmion $\vec{\phi}(\Omega)$ can be written as

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

where *C* is the normalization constant and *g(θ)*controls the size of the skyrmion. From eqns. (4) and (4) it is seen that *α* is determined from *g(θ)* and as such it controls the size of the skyrmion . Indeed we can define

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

which equals π/2 for the hedgehog skyrmion with α=1

Taking the spin variable $\vec{z} = U\vec{z}_0$ with $\vec{z}_o = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$ andU \in SU\left(2 \right)SU\left(2 \right) $matrices$U$ as [2]

$$L = -\left(M^2/16\right)\left(\partial_u U^\dagger \partial_\mu U\right) - \left(1/32\eta^2\right)\left(\partial_\mu UU^\dagger, \partial_\nu UU^\dagger\right)^2 \qquad (8)$$

Where *M* is a constant having dimension of mass and *η* is a dimensionless parameter, *μ,ν* being space -time indices. The α dependence may be incorporated through *M* and *η* where these parameters are taken as functions of α.

We can consider the radius of the DNA loop R (plectoneme radius) as a function, R(θ,φ) corresponding to the core radius of the skyrmion. We can define the core size of the skyrmion such that $R = R_0\,(1-\alpha)$ where R_0 is the size of the skyrmion with minimal energy. The static nonlinear σ -model Lagrangian corresponding to eqn. (8) gives rise to the energy integral as

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

where *i, j =1,2,3* are spacial indices. To compute the energy we take the Skyrme ansatz [2]

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

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

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

with

$$\cos F(r) = \left(1 - r/R\right)^2 \Big/ \left(1 + r/R\right)^2 \qquad (12)$$

$$\sin F(r) = 2\left(r/R\right)\Big/ 1+\left(r/R\right)^2 \qquad (13)$$

The energy integral becomes

$$E(R) = 4\pi^2 M^2 R I_1 + 2\pi^2\left(I_2/\eta^2 R\right) \qquad (14)$$

where

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

and

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

with $x = r/R$. This gives the expression of energy

$$E(R) = 12\pi^2 M^2 R + \left(3\pi^2/\eta^2 R\right) \qquad (17)$$

The minimum of energy $E(R)$ is found from the relation

$$\partial E(R)/\partial R = 12\pi^2 M^2 - 3\pi^2/\eta^2 R^2 = 0 \qquad (18)$$

which gives for E_{min} the size as

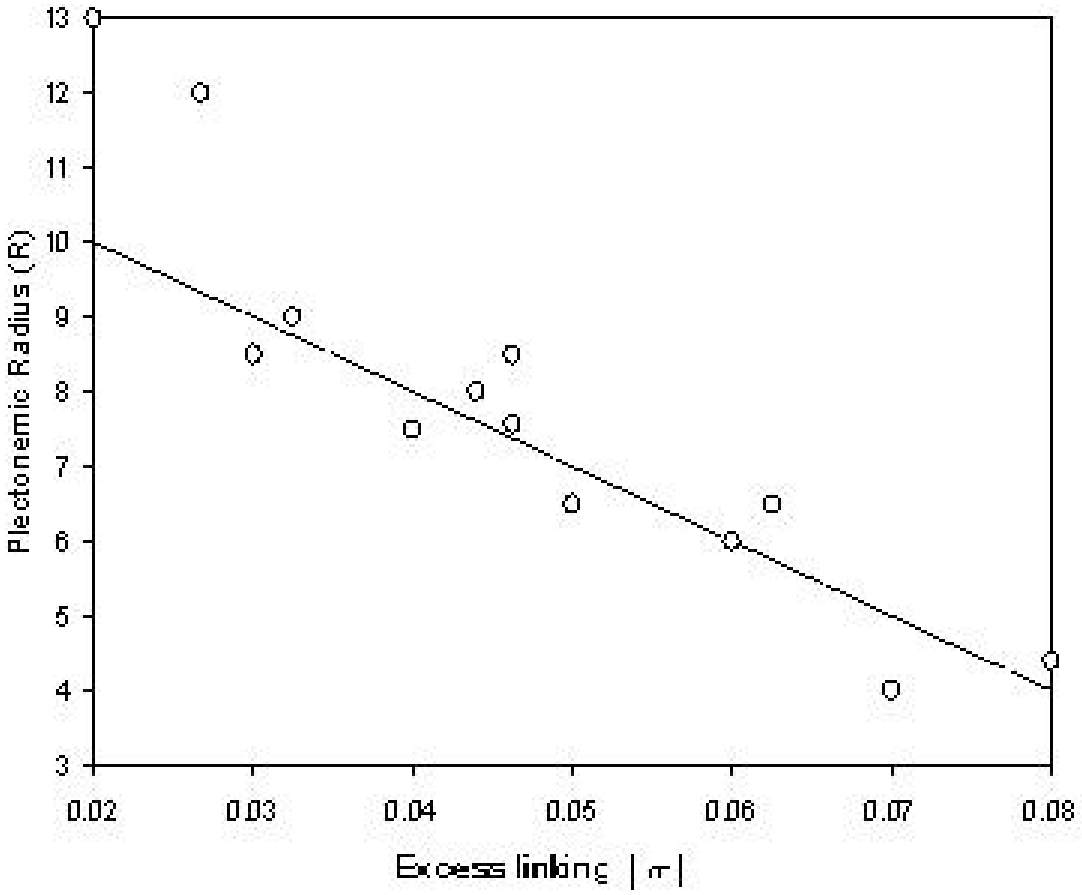
$$R_0 = 1/2M\eta \qquad (19)$$

and the energy

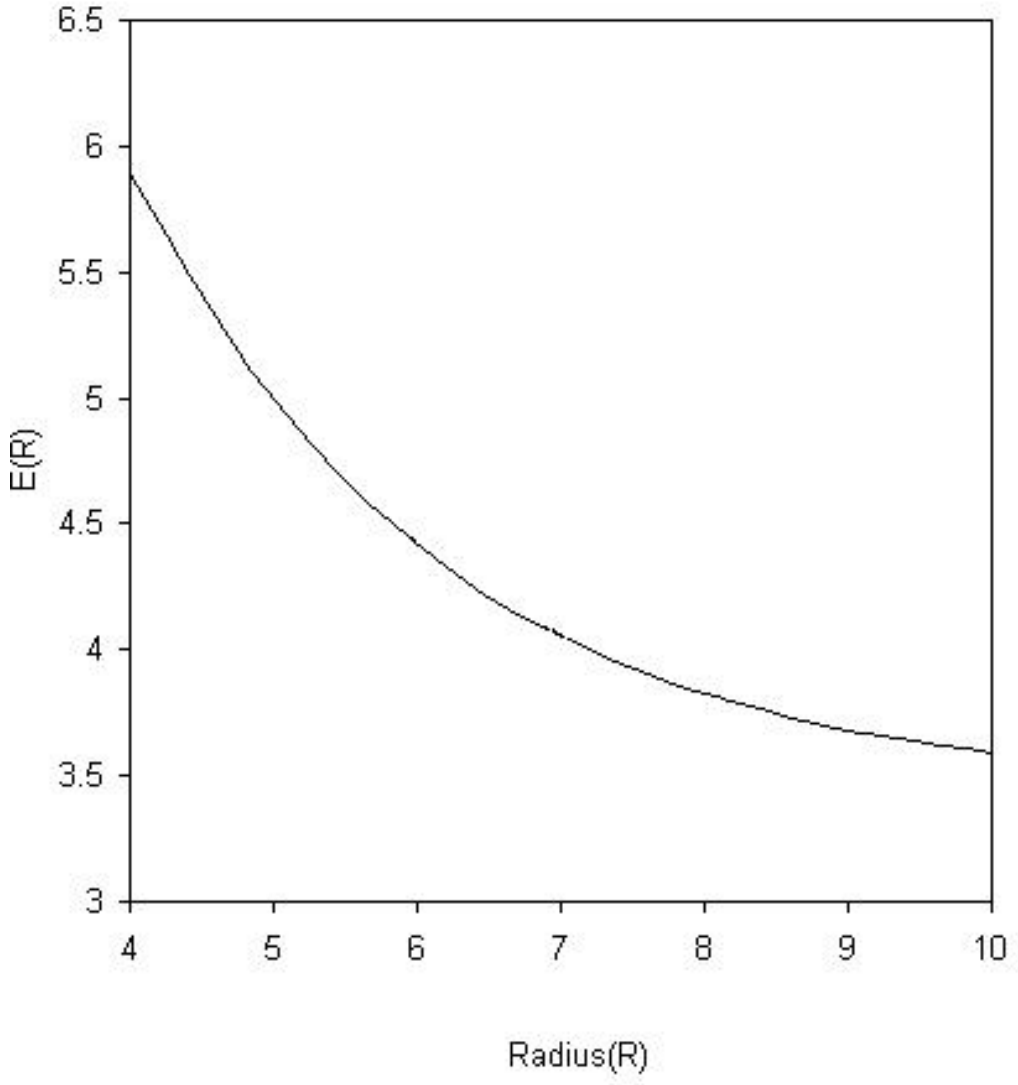
$$E_{\min} = E(R_0) = 12\pi^2 M/\eta \qquad (20)$$

It is noted that the coupling parameters M and η are functions of α such that in the limit $\alpha \to 0$, $M(\alpha)\to 0$ and $\eta(\alpha)\to 0$ but M/η is fixed. When we take $R = R_0(1-\alpha)$ we have

$$E(R) = \left\{\left(6\pi^2 M\right)/\eta\right\}\left[(1-\alpha)+1/(1-\alpha)\right] \qquad (21)$$


Plectonemic Radius (R)
13
12
11
10
9
8
7
6
5
4
3
0.02
0.03
0.04
0.05
0.06
0.07
0.08
Excess linking | σ |

1(a)



1(b)

Figure 1: Here (a) depicts the radius *R* of a plectonemic supercoil as a function of σ where *R* is given by $R = R_0(1- \alpha)$ with $\alpha = k\backslash \sigma \backslash$ .The constant k is determined from the experimental data [3] and the best fit is given by k=8.333 and (b) depicts the skyrmion energy as a function of radius R.

Now we note that we can associate the parameter α with the twisting strain given by $\sigma = (\Delta LK/LK_0)$. In fact in the simplest form we can take $\alpha = k\backslash \sigma \backslash$ where *K* is a constant. It is noted that the relation $R = R_0(1- \alpha)$ gives a nonzero size for $\alpha = 1(\sigma = 0)$ when R_0 is infinite. Indeed it has been found that for $|\sigma| < 0.02$ the minimal free energy state has $R = P = \infty$ indicating that no consistent stable supercoiled state exists for small $|\sigma|$. For $|\sigma| > 0.02$ the plectonemic free energy exhibits a minimum value for finite *R* and *P* which implies that we have a stable supercoiled state [4-5]. Indeed for torque induced denaturation the critical supercoiling parameter is found to be $\sigma_c = -0.015$ which suggests that just near this critical point the stability of the supercoil is disturbed. This leads to the opening of the base pairs when it reaches the critical point.

Discussion

From our above analysis we observe that just below the critical point we have skyrmionic excitation which drives the system towards the critical point [6]. The critical radius of the DNA loop $R_c = R_0(1-|\sigma_c|)$ corresponds to the plectoneme radius involving

opened base pairs and determines the characteristic size of the skyrmion when denaturation occurs.

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