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# Bending Dynamics of DNA

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*Abstract-* It is here pointed out that the local opening of base pairs induces the formation of kinks which facilitates the bending of double helix. The conformational properties of DNA can be mapped onto the Heisenberg spin system and denaturation occurs through quantum phase transition (QPT) induced by a quench when the temperature effect is incorporated through the quench time . The nonequilibrium effect in QPT introduced through the quench generate defects like kinks end antikinks, the density of which depends on the quench time and hence on temperature. It is here argued that when we transcribe this result in the rod –like-chain (RLC) model of DNA, these defects lead to bends. This suggests that we have dynamical generation of kinks leading to the formation of bends during local denaturation.

*Keywords:* *DNA, bends, kinks.*

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BENDINGDYNAMICSOFDNA

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# Bending Dynamics of DNA

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*Abstract-* It is here pointed out that the local opening of base pairs induces the formation of kinks which facilitates the bending of double helix. The conformational properties of DNA can be mapped onto the Heisenberg spin system and denaturation occurs through quantum phase transition (QPT) induced by a quench when the temperature effect is incorporated through the quench time . The nonequilibrium effect in QPT introduced through the quench generate defects like kinks end antikinks, the density of which depends on the quench time and hence on temperature. It is here argued that when we transcribe this result in the rod –like-chain (RLC) model of DNA, these defects lead to bends. This suggests that we have dynamical generation of kinks leading to the formation of bends during local denaturation.

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## I. Introduction

It is wellknown that DNA experiences bending due to thermal fluctuation . Also the bending occurs owing to the influence of special proteins or through an external force which deforms it to a circle. It is noted that the elastic properties of DNA can be best formulated when it is considered as an elastic object. The Worm-like-chain (WLC) model was introduced [1] which describes a chain by elastic continuous curve at thermal equilibrium with a single elastic constant, the persistent length P, characterizing the bending energy. The WLC can be solved analytically by mapping it onto a quantum mechanical problem. Indeed the partition function is a Euclidean path integral for a quantum dumbbell. Bouchiat and Mezard [2] generalized this model introducing twist rigidity and it appears that a DNA molecule can be depicted as a thin elastic rod . The rod-like-chain( RLC) model is characterized by the fact that the partition function can be mapped onto the path integral representing the charged particle in the field of a nonquantized magnetic monopole. Cloutier and Widom [3] have shown that the prediction of the WLC model is not consistent with the cyclization of short DNA fragments of around 100 base pairs. Crick and Klug [4] predicted earlier that strong bending of DNA is facilitated by kinks of the double helix. Vologodskii and Frank-Kamenetskii [5] have reviewed the situation of strong bending and pointed out that kinks in strongly bent DNA segments is not a property of short DNA fragments as it is equally possible in large DNA molecules. Indeed these authors have noted that kinks may represent opening of isolated base pairs which had been experimentally detected in linear DNA molecules. In this note we argue that kinks are produced dynamically when we have local denaturation of DNA which play a crucial role in bending of the double helix. Indeed the dynamical generation of kinks leading to the bending of the double helix is a specific property of local denaturation caused by thermal effect.

Recently we have pointed out that the conformational properties of a DNA molecule can be mapped onto a Heisenberg spin system [6]. In this framework denaturation transition can be formulated in terms of quantum phase transition induced by a quench where the temperature effect is incorporated in the quench time [6, 7]. In a DNA molecule two polynucleotide chains are twisted about the molecule axis with a specific helical sense. We can view this such that a spin with a specific helicity is inserted on this axis and two nearest neighbour spins having opposite helicities are located in the axis covering two adjacent coils. The system then represents a spin chain when two nearest neighbour spins have opposite orientations $+1/2$ and $-1/2$ with lattice spacing of the period of helix. Evidently this represents an antiferromagnetic spin chain. When the entanglement entropy of the system vanishes we have denaturation transition [6, 7].

## II. Data And Method

The Hamiltonian of the one dimensional Heisenberg spin chain (XXX model), with nearest neighbor interaction is given by

$$H = \sum_i (\sigma_i^X \sigma_{i+1}^X + \sigma_i^Y \sigma_{i+1}^Y + \sigma_i^Z \sigma_{i+1}^Z) + \lambda \sum_i \sigma_i^2 \qquad (1)$$

$\sigma_i^{X(Y,Z)}$ is the Pauli matrix at the site $i$, which represents the spin vector through the relation $\vec{S} = (1/2)\vec{\sigma}$ and $\lambda$ is the parameter representing the external magnetic field. In the context of DNA, $\lambda$ represents torsion energy [6]. When the spin system undergoes quantum phase transition (QPT) the criticality corresponds to a two-limit behavior. At $\lambda = 0\,(2)$ we have the antiferomagnetic (ferromagnetic ) state. The region between $\lambda = 0$ and $\lambda = 2$ represents the critical region. The entanglement entropy is maximum at $\lambda = 0$ and it decreases as $\lambda$ increases when at $\lambda = 2$ it vanishes.

It is now observed that the criticality of a finite temperature transition can be mapped onto a zero temperature QPT induced by a quench. Indeed as

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pointed out by Schutzhold [8] the nonequilibrium effect in zero temperature QPT shows a remarkable analogy between phase transition at finite and zero temperature. Vojta [9] has argued that quantum criticality can be approached in two different ways. It may be considered that at as $T \to 0$ the control parameter $\lambda$ attains the critical value $\lambda = \lambda_c$. Also it may be argued that at $T = 0$, $\lambda \to \lambda_c$ [9]. In the vicinity of the critical point the spatial correlation as well as the temporal correlation of the order parameter fluctuations become long ranged. The crossover form the quantum to classical behaviour occurs when the correlation time exceeds $\beta = 1/k_B T$ in a quench induced QPT. This arises when we take into account the Kibble –Zurek (KZ) mechanism [10, 11] in QPT having time dependent control parameter which gives rise to nonequilibrium effect near criticality. This implies that zero temperature QPT induced by a quench can be mapped onto a classical finite temperature phase transition when temperature effect is incorporated in the quench time $\tau_q$ having the relation $T \sim 1/\tau_q$. In QPT induced by a quench in Heisenberg spin chain we can take

$$\lambda(t\langle 0) = 2 - 2t/\tau_q \qquad (2)$$

so that at $t = \tau_q$ we have $\lambda = 0$ and as $t$ approaches zero starting from $\tau_q$, $\lambda$ increases so that at $t = 0$, $\lambda = 2$ when the entanglement entropy vanishes. In a recent paper [12] it has been shown that in the Heisenberg spin chain the $\lambda$ dependence of the entanglement entropy $S$ is given by

$$S(\lambda) = S(\lambda = 0) + \Delta S \qquad (3)$$

with

$$\Delta S = (1/6)\log_2(1 - \lambda/2) \qquad (4)$$

It may be mentioned here that in studying denaturation of DNA in terms of QPT induced bya quench the temperature dependence of $\lambda$ is taken to be [6]

$$\lambda = \overline{A}T + \overline{B} \qquad (5)$$

where $\overline{A}$ and $\overline{B}$ are constants given by $\overline{A} = 0.0385$ and $\overline{B} = -11.47$

From eqns (4, 5, 6) we can now determine the entropy at a given temperature which gives a measures of the opening of base pairs at a given temperature [7]. A general property of QPT induced by a quench is that it generates defects in the form of kinks and antikinks and introduces a new lenhth scale known as the Kibble – Zurek (KZ) correlation length defined by the average distance between a kink and the nearest antikink [13, 14]. The density of defects $\rho$ depends on the quench time $\tau_q$ through the relation $\rho \sim 1/\sqrt{\tau_q}$ so that the KZ correlation length $\xi$ satisfies the relation $\xi \sim \sqrt{\tau_q}$ [13, 14]. Utilising the relationship between the quench time $\tau_q$ with temperature $T$ through the relation $T \sim 1/\tau_q$ as mentioned above, we note that the KZ correlation length $\xi$ depends on the temperature through the relation $1/\sqrt{k_B T}$.

## III. Analysis And Discussion

Now we transcribe our above results derived from the situation where a double helix is mapped onto the Heisenberg spin chain into the elastic rod model. It is noted that local denaturation caused by QPT induced by a quench leads to the generation of defects like kinks and antikinks which correspond to the bends of the axis of the DNA molecule and represent dynamical bending of the elastic rod. The KZ correlation length corresponds to the bend length. These bends are dynamically produced and the associated bend length $A$ is different from the structural persistent length P which is the geometrical property of the rod . As the formation of the defects is such that a kink is followed by an antikink, this would mean that every joint periodically bends oppositely to each other .From the relation that the KZ correlation length $\xi \sim \sqrt{\tau_q}$ and $\tau_q \sim 1/T$ we note that when we consider $\xi$ as the bend length $A$, we can write the relation $A \sim 1/\sqrt{T}$. From this we write

$$(A^2/P) = k/K_B T \qquad (6)$$

Where $k$ is the bend stiffness having dimension of $energy.length$. Here we have introduced the structural persistent length P in the L.H.S for dimensional reason as this corresponds to a fixed length scale for the system. Now observing that experimentally we have bend stiffness $k = 45nm(K_B T)$ and $P = 130nm$ [15] we have $A = 76.5nm$. This is to be compared with the experimental value $80nm$ [15].

From this we have the total persistence length given by

$$A_{tot} = (A^{-1} + P^{-1})^{-1} \qquad (7)$$

From eqn. (8) we have $A_{tot} = 48.3nm$ which is to be compared with the standard value $50nm$.

Thus we find that our results are consistent with experiments.

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It may be recalled here that Nelson [16] proposed that natural bends in DNA hinder the axial rotation of the transcribed DNA causing the propagation of torsional stress. The bends are taken to be random but their effects do not average to zero. In contrast the present analysis suggests that bends are produced dynamically during local denaturation associated with transcription. These bends follow a specific pattern having a more or less same distance between them determined by the KZ correlation length so that the bend length $A$ satisfies the eqn (7) . According to Nelson's prescription the total effect of random natural bends makes DNA a random coil with total persistence length $A_{tot}$ . However according to the present formulation the bends are produced dynamically which make DNA a systematic coil having a well defined bend length and total persistence length[17-18].

## IV. Conclusion and Summary

In summary, we argue that local denaturation leads to the generation of defects like kinks and antikinks which correspond to bends in the elastic rod formulation of DNA. This dynamical formation of bends during transcription shut down spinning motion completely and generates significant torsional stress near the point of transcription.

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