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# Quantum Quench Dynamics in DNA Molecules at Finite Temperatures

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## Abstract

In order to analyze denaturation, we take into account a mapping from the finite temperature phase transition onto a zero temperature quantum phase transition caused by a quench, where the control parameter is the torsion-associated magnetic field and the quench duration handles the temperature effect. It is, in fact, the main forecast made by the current model. It is observed that the topological current linked to the topological Lagrangian provides the torsion term. The introduction of the topological Lagrangian in a non-Abelion gauge field theory essentially corresponds to the presence of a magnetic flux line. Given this, we may conclude that the torsional energy and the magnetic field's energy basically match. Therefore, the term connected to this field may be taken to be related to the torsional energy when a DNA molecule is represented in an external magnetic field by an antiferromagentic spin chain.

**Keywords:** Quantum; Bioinformatics; Biomedical; Dynamics; DNA

## Introduction

Transcription depends critically on the denaturation of DNA molecules. Experimentally, it has been found that when abrupt opening of base pairs happens at a crucial temperature, there exists a thermally induced melting transition [1]. A semiquantitative understanding of DNA melting based on the Ising model has been available for a long time [2]. However a quantitative study of the transition remains elusive. The Ising model has been formulated by considering that a base pair is a two state system where it is either closed or open .Evidently this could not describe the precursor effects and the large amplitude fluctuational openings observed well below the denaturation temperature [3]. Although it is known that phase transitation does not occur in 1D Ising system, several authors [4] tried to waive this argument by considering certain types of many body or long range interactions. Azbel [5] has pointed out that the winding entropy which is released when the two strands are separated contributes to the denaturation . These concepts appear in the Ising model through phenomenological parameters. Peyrard and Bishop [6] proposed a variant of the 1D Ising model introducing a nonlinear dynamics of the DNA denaturation . Instead of a two state variable the status of each base pair is described by a scalar variable representing the transverse stretching of the hydrogen bonds connecting the two base pairs. The onsite morse potential was introduced to depict the hydrogen bonds connecting the two bases belonging to two opposite strands as well as the repulsion of the phosphates and the surrounding solvent effects. Later an Dauxois, Peyrard and Bishop [7] extended this model to incorporate the cooperativity effect which implies that a closed base pair at the boundary of an open domain has a higher probability to open. Apart from the thermally driven melting transition there exists a torque induced denaturation of DNA [8]. Indeed it has been observed that at a critical value of the parameter where $\sigma = (Tw - Tw_0)/Tw_0$ measures the twist *Tw* with respect to the counterpart $Tw_0$ for an unconstrained molecule $\sigma_c = -0.015$ and an associated critical torque $\Gamma_c = -0.05ev/rad$ the twisted molecule separates into a pure B-DNA phase and denaturated region. Cocco and Monasson [8] have shown that denaturation can be described in the framework of first order phase transition with control parameters being the temperature and external torque.

### Theoretical Background

The Hamiltonian for the 1D Heisenberg antiferromagentic spin system (XXX model) is given by

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

Here λ is a parameter representing the external magnetic field. So far as the quantum phase transition (QPT) is concerned, the XXX model has two limit behavior. At λ =2 the system represents the ferromagnetic state which is a product state so that the entanglement entropy vanishes. At λ =0 the system corresponds to the antiferromagentic state with maximum entanglement entropy. The interval $2\rangle\lambda\rangle 0$ is gapless and hence critical. The criticality of the finite temperature phase transition can be studied by mapping it onto the zero temperature QPT, when we incorporate nonequilibrium effects. Indeed the nonequilibrium effect in zero temperature QPT exposes a remarkable analogy between phase transitions at finite and zero temperature [9]. There is an interesting interplay between classical and quantum fluctuations near quantum criticality. Quantum criticality can be approached in two different ways. At T = 0 the nonthermal control parameter such as the magnetic field λ approaches the critical value λ → λ c. Also we may view that as T⟶0 the magnetic field approaches the critical value λ = λ c. Thus in quantum critical region both quantum and thermal fluctuations have definite role [10]. As the critical point is approached the spatial correlation of the order parameter fluctuations becomes long ranged. In addition to this there is an analogous temporal long range correlation of the order parameter fluctuations. The typical time scale for the decay of the fluctuations is the correlation time which diverges near criticality. The crossover from the quantum to classical behavior will occur when the correlation time exceeds $\beta = \dfrac{1}{K_B T}$ in a quench induced quantum phase transition. Indeed this happens when we incorporate the Kibble-Zurek [11-12] mechanism taking into account the time dependent control parameter in quantum phase transition which gives rise to nonequilibrium effects near criticality. This suggests that zero temperature phase transition induced by a quench can be mapped onto a classical finite temperature phase transition when the temperature effect is incorporated in the quench time $\tau$ with T $1/\tau$

Recently the Kibble-Zurek mechanism has been investigated in the context of zero temperature quantum phase transition induced by a quench when the driving parameter is considered to be time dependent [13-18]. A crucial feature of the phase transition induced by a quench is the formation of defects .It has been observed that the nonadiabatic evolution of the driving parameter at the critical region produces defects such that the system becomes a mosaic of ordered domains separated by the formation of kinks (antikinks) where the size of the domains corresponding to the Kibble-Zurek (KZ) correlation length depends on the quench time. Recently the Hamiltonian (1) for the XXX model has been studied in this framework taking into account the time evolution of the driving parameter λ (t) given by the relation

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

So that at $t = \tau$ we have the critical point λ =2 [18]. It has been found that the number density of defects (kinks and antikinks) is given by

$$n = (1/8\pi)(1/\sqrt{\tau}) \quad (3)$$

Implying that the KZ correlation length scales as $\tau^{1/2}$.

Now for the DNA molecule represented by antiferromagnetic chain we note that when due to the fluctuation of the twist the system attains the critical point λ =2 the entanglement entropy vanishes and we have denaturation. This implies that at a certain critical value of the torsional energy Vc we will have opening of base pairs. This is analogous to the results of Cocco and Monasson [8] who considered the torque induced denaturation. It is noted that the torsional energy is related to torque $\Gamma$ through the relation V = $\Gamma$θ, θ, being the twist angle. However in their analysis, Cocco and Monasson considered the process of denaturation to be analogous to the first order phase transition where the driving parameters are both temperature and troque.

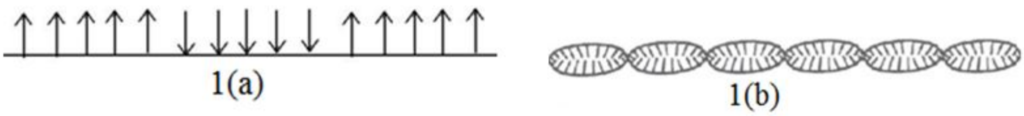


**Figure 1:** QPT induced by a quench and denaturation. Here (a) shows ordered domains separated by kinks (antikinks) during QPT induced by quench and(b) shows chain of opened base pairs

In this instance, we have examined the system when the quench time takes into account the temperature impact and the driving parameter is the torsion-related, time-dependent magnetic field. It is observed that in this framework opening of base pairs is accompanied by the formation of kinks and antikinks as discussed above it may be mentioned that in the expression for torsional energy *V* in terms of torque $\Gamma$ given by V = - $\Gamma\theta$, the twist angle θ is directly related to temperature.

## Discussion

It has been observed that at room temperature the critical value of the torque is $\Gamma_c = -0.05ev/rad$ and the parameter $\sigma_c = -0.015$. For thermal fluctuation, it has been experimentally observed that the ratio of the fluctuation of the twist angle to that of temperature is given by $(\dfrac{\Delta\theta}{\Delta T})$ = - 1.7 \times $10^{-4}$ rad/K at $\Gamma$ = 0 [19]. In view of this we note that the critical value of the torsional energy incorporates the temperature effect also apart from that of the torque [20]. When the temperature effect is included in the quench period, it is demonstrated that denaturation of a DNA molecule corresponds to zero temperature quantum phase transition triggered by a quench. The torsonal energy's critical value, at which the entanglement entropy disappears, is the critical point.

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