DNA Spin Dynamics and Thermodynamic Entropy

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We show that when the conformational properties of a DNA supercoil mapped onto an antiferomagnetic spin system the entanglement entropy effectively corresponds to the thermodynamic entropy . The free energy per unit length is found to be in good agreement with that derived by other authors.

The existence of supercoiled DNA was established in experimental studies almost 50 years ago . It has been observed that DNA molecules, however small, contain topological domains along which supercoiling can occur through the attachments of the DNA to itself , cell membranes and other structures. Thermal fluctuations compete with elastic forces to determine supercoil structure [1].Fluctuation effects on supercoils were studied by Vologodskii et . al . [2,5] who have carried out numerical Monte Carlo simulations. A solenoidal single helix supercoil is closed by slow distortion of the coil into a toroidal structure. An interwound plectonemic supercoil consists of two helices of the same handedness and at the end of the cylindrical structure the two helices are connected. A supercoiled DNA is characterized by a right helix of radius R and pitch P , the helix repeat length being $2\pi P$ .The length of molecule in 1 rad of superhelix is $l=\sqrt{R^2+P^2}$ and the helix angle is defined by $\sin\gamma = P/l$ .where γ takes values between 0(a circle) and $\pi/2$ (a straight line). The writhes of plectonemic and solenoidal coils are

$$Wr=\begin{cases} \mp 2n\sin\gamma & (\text{plectonemic}) \\ \pm n(1-\sin\gamma) & (\text{solenoidal}) \end{cases}$$

where n is the number of superhelix repeats.

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The two strands of a circular DNA molecule possess as a topological invariant the number of times they wind around each other which is known as the linking number. A B-DNA molecule has one right-handed twist per $h=3.4$ nm along its length. When these are closed in a planar circle without twisting of the ends the resulting linking number is $Lk_o = L/h = \omega_0 L/(2\pi)$ where L is the length and ω_0 is the spatial rotation rate of the base pairs about the central axis. Deviations in the twisting rate from ω_0 is measured relative to Lk_o through the parameter defining the excess linking $\sigma = (\Delta Lk/Lk_0)$ where $\Delta Lk = Lk - Lk_0$ .The linking number Lk is expressed as $Lk = Tw + Wr$ where Tw represents the twist corresponding to the rotation of the internal degrees of freedom about the molecule axis and Wr represents the writhe . The twist measures the winding of one curve about the other. At zero temperature a long elastic wire or tube will collapse into a plectonemic supercoil when we have $\Delta Lk/L \neq 0$ [6]. Indeed taking all the ΔLk into Wr , we can make the twist energy vanishing . Then making $\sin\gamma = 1$,the plectoneme become a line which makes the bending energy zero also. It is now noted that for a tube of nonzero radous the elastic energy cannot be reduced to zero. However for a plectoneme a lowest energy configuration can be obtained for tube radius small compared to superhelix pitch. It is to be mentioned that for a solenoid as Wr is maximum for $\gamma = 0$ when the curvature becomes nonzero both the twist and bend energies cannot be reduced to zero simultaneously. Thermal fluctuation swells up the supercoil radius to larger than the supercoil hard core radius. In fact it has been shown that a repulsive effective entropic potential arises opposing the elastically driven collapse at zero temperature [1]. It implies that thermodynamic entropy plays a significant role in a DNA supercoil.

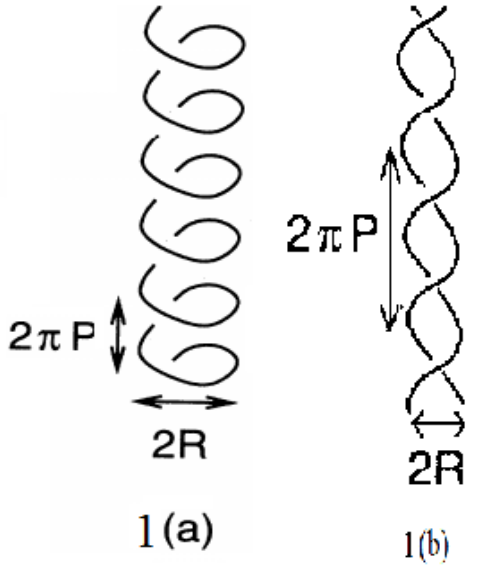

Fig.1(a) Solenoidal superhelix; (b) Plectonemic superhelix , Solid line represents double helix structure of B-DNA . R and πP correspond to the radius and the pitch respectively.

Recently a theory of the denaturation transition of a DNA molecule has been proposed in the framework of the mapping of the conformational properties of DNA onto a Heisenberg spin system[7]. As two polynucleotide chains are twisted about the molecule axis with a specific helical sense in a DNA molecule, this can be viewed as if a spin with a specific orientation is inserted on the axis such that two adjacent coils have opposite orientations of the spin. In fact with each turn two strands move in the opposite side of the axis and so the spin orientation assigned for the two adjacent coils should be opposite to each other. Indeed twisting of the two strands in mutually opposite directions can be taken to imply that two strands can be designated by two spins having orientations $+1/2$ and $-1/2$.When these two spins having opposite orientations are inserted on the axis such that these are located in the two adjacent sites with lattice spacing of one period of helix this represents an antiferromagnetic spin system. In this scenario denaturation transition can be formulated in terms of quantum phase transition induced by a quench when the temperature effect is incorporated in the quench time and torsion takes the role of the external field. In a recent letter [8] we have computed the melting profiles for the different sequence-specific DNA molecules and the results are found to be in excellent agreement with experiment. Here we consider the entropy of a supercoiled DNA in the framework of the mapping of a DNA molecule onto a Heisenberg spin system. In a supercoil we can consider that the spins associated with each DNA loop are arranged along the axis of the supercoil. As we have pointed out that in a DNA molecule spins are considered to be arranged in an antiferromagnetic chain, the supercoil axis may be treated as a lattice of antiferromagnetic spin system. To have the minimal energy two adjacent spins of opposite orientations will form a singlet. Due to chirality caused by twisting strain into the loop related to torsion the spin system will be in a frustrated state as frustration leads to chirality. This frustration suggests that spin singlets are formed by resonating valence bond (RVB) [9].

In summary we observe that when a supercoiled DNA is mapped onto an antiferomagnetic spin chain, the entanglement entropy effectively represents the thermodynamic entropy. The free energy per unit length is found to be in good agreement with that derived by other authors.

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