Quantum Logic in DNA

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Abstract

We are here to consider the DNA molecules' spin system to consider when the antiferromagnetic spin chain is formed by the top remains' axis. It ap-pears that the turning and twist are not two separate entities, not the one the other on the set. This formality assistances us in depicting the thermodynamic entropy as entanglement entropy, and hence the concurrence of two-set entanglement is appraised for transverse Ising model, and antiferromagnetic chain for the assess-ment is that the other methods are to obtain agreements with the excellent deal appeared to be.

Keywords: DNA molecules; entanglement entropy; antiferromagnetic chain

Introduction

Please note that the first paragraph of a section or subsection is not indented. The first paragraphs that follows a table, figure, equation etc. does not have an indent, either. This note shall study the specific properties of DNA by considering that a DNA mole-cule can be mapped onto a Heisenberg spin system [1]. A spin is represented as a 'SU (2)' gauge bundle. This essentially implies that two strands twisting about the axis in opposite direction can be designated by two spins having orientations +1/2 and -1/2.

We shall also learn about the topological properties and the elastic and ther-modynamical properties of a DNA molecule from an analysis of this spin system. The thermodynamical entropy associated with a DNA supercoil appears here as the entan-glement entropy of the antiferromagnetic spin chain and also a probable relationship between the Berry phase and the measure of entanglement viz. concurrence of the two-set entanglement is appraised for transverse Ising model has been pointed out in ref[2]. Here we will also try to quantify concurrence in terms of the geometric phase in several spin systems. This helps us consider mapping the Heisenberg spin chain's fea-tures onto the quantum mechanical features related to the RLC model. In fact, the spin can be depicted in terms of a magnetic monopole [1].

Theoretical Background

When DNA molecules are treated as spin systems, these attain the entanglement en-tropy due to the entanglement of spins. As we have pointed out, in a DNA molecule, spins are considered to be arranged in an antiferromagnetic chain.

The supercoil axis may be treated as a lattice of an antiferromagnetic spin system. To have minimal en-ergy, two adjacent spins of opposite orientations will form a singlet (fig.).

Due to chi-rality caused by twisting strain into the loop related to torsion, the spin system will be frustrated as frustration leads to chirality. This frustration suggests that spin singlets are formed by resonating valence bond (RVB) [3].

It has been shown that a repulsive sig-nificant entropic potential arises opposing the elastically driven collapse at zero tem-perature [4].

It implies that thermodynamic entropy plays a significant role in DNA molecules.

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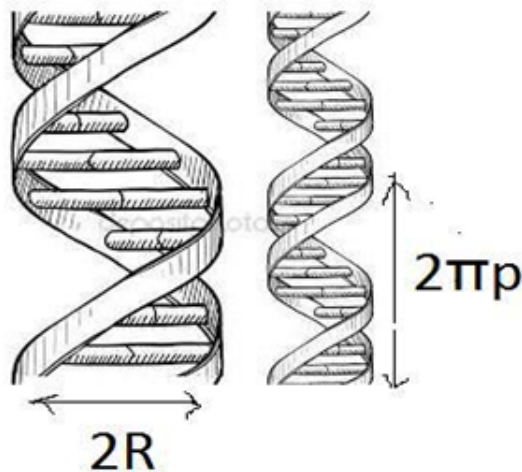
Figure: A plectonemic superhelix, the solid line represents the double-helical structure of B-DNA.

And πP correspond to the radius and the pitch, respectively.

It has been shown in some earlier papers [5, 6] that the measure of the entanglement of formation given by concurrence 'G' for the entanglement of a pair of

nearest neighbor spins is related to the Berry phase [7] provided by $e^{i\phi_B} = e^{i2\pi\tilde{\phi}_B}$

which is ac-quired by a spin state when the spins in the system are rotated about the quantization axis (z-axis) in a closed circuit. We have the relation

$$G = \left|\tilde{\phi}_B\right| = \left|\phi_B\right|/2\pi$$

It has been observed that the concurrence associated with the entanglement of formation for a pair of nearest neighbor spins in a frustrated system is given by G = 0.5 [5]. Thus the total concurrence accumulated in the spin chain is given by

$$G = \sum_{i=1}^{N/2} \left|\tilde{\phi}_B\right| = \left|\tilde{\phi}_B\right|(N/2) = (1/2)(N/2) = N/4$$

where N is the total number of spins in the chain and N/2 is the number of singlets. It is noted that the von Neumann entropy for an entangled spin system in a pure state is reduced to the entanglement of formation given by concurrence in a mixed state [8]. Thus the above expression (2) represents the entanglement entropy of the spin system. Now we consider that the supercoiled stiff polymer (DNA) is confined inside a narrow tube of radius 'r' The area of a DNA loop in a supercoil is

determined by the number of coils in the spiral and hence by the number of spins in the circle. When the super-coiled stiff polymer is confined in a narrow tube of radius 'r', we can associate the area of the tube's surface with the number of spins in the DNA loop at that surface. Now from the holographic principle, which states that for closed surface entropy is given by the surface area, the entanglement entropy is found to be provided by the area of the tube's surface. Thus using Eqn. (2) the entanglement entropy can be written in the form

$$U \approx \pi r^2 / 4r_0^2$$

'r' being the radius of the tube and r_0 a fundamental area unit. We now identify $r \approx J$ J being the bending elastic constant, and r_0 is taken to represent the radial displace-ment of a given point on the coil, which satisfies the condition $|r_0| \leq R$ [9]. Taking the mean value $|r_0| = R/2$, the entanglement entropy is given by

$$U \approx \pi J^2 / R^2$$

Similarly for the displacement of a given point on the coil along the supercoil axis which

is of the order of πP, P being the pitch

$$U \approx \pi J^2 / (\pi P)^2$$

So the total entropy is given by

$$U = \pi J^2 / R^2 + \pi J^2 / (\pi P)^2$$

Now we observe that this entanglement entropy effectively corresponds to the thermodynamic entropy. Indeed, a tube of narrow radius entanglement entropy cannot vanish. In contrast, in the limiting case of radius, we can think of zero radii (straight line) when the total elastic energy evaporates at zero temperature. In this case, the en-tanglement entropy also vanishes. In fact, at zero temperature, a flexible tube will collapse into a plectonemic supercoil when subject to the constraint

$$\Delta Nk / N \neq 0 \text{ [10] When } \Delta Lk \text{ is put into writhe,}$$

the twist energy becomes zero. Then we can make the plectoneme collapsed into a line, which makes the bending energy zero also. Now at zero temperature, the area of the loop vanishes. In this case, the entanglement entropy even vanishes. Given this, we can identify the entanglement entropy as the thermody-namic entropy of the supercoil.

This helps us to compute the free energy associated with the supercoil. We note that from the relation dF = UdT, F(T) being

the free energy (temperature), the free energy per unit volume is related to the entropy given by Eqn. (6) can be written as

$$\Delta F / (K_B TV) \approx \pi J^2 / (R^2 r^3) + \pi J^2 / \{(\pi P)^2 r^3\}$$

This gives the free energy per unit length

$$\Delta F / (K_B TN) \approx \pi^{1/3} J^{2/3} / (R^{2/3} r) + \pi^{1/3} J^{2/3} / \{(\pi P)^{2/3} r\}$$

Now, as argued above, is taken to be of the order of and hence we find

$$\Delta F / (K_B TN) \approx \pi^{1/3} J^{2/3} / (R^{2/3} J) + \pi^{1/3} U^{2/3} / \{(\pi P)^{2/3} J\}$$

$$\pi^{1/3} / (J^{1/3} R^{2/3}) + \pi^{1/3} / (J^{1/3} (\pi P)^{2/3})$$

In terms of the diameter D (D = 2R), the confinement free energy per unit length is found to be given by

$$\Delta F / (K_B TN) \approx \pi^{1/3} 2^{2/3} / (J^{1/3} D^{2/3} + J^{1/3} (2\pi P)^{2/3})$$

$$\approx 2.32 / (J^{1/3} D^{2/3} + J^{1/3} (2\pi P)^{2/3})$$

In this context, it may be mentioned that for a semiflexible polymer in a cylindrical tube of diameter D, the confinement free energy per unit length is given by [11].

$$(\Delta F / k_B TN) = c(1 / J^{1/3} D^{2/3})$$

We now pick up some circles G_a and some integers n_a corresponding to the Abelian gauge group's representations. As long as G_a and G_b do not intersect, $\varphi(G_a, G_b)$ is a well-defined integer, where k is an integer. Thus ignoring the term $a = b$, we have

$$\langle W \rangle = \exp\left((2\pi i / k) \sum_{a,b} n_a n_b \varphi(G_a, G_b) \right)$$

The appearance of linking numbers from the Chern-Simons term associated with the gauge current representing the spin suggests that the linking number can be associated with a spin system.

The dimensionless constant G was estimated as 2.46 ± 0.07 on computer simulation [12]. Burkhardt [9] considered a continuum model of a fluctuating semiflexible polymer chain confined along an axis and concluded that G>3/2 is consistent with a com-puter simulation prediction. From our above analysis, we note that the first term in Eqn. 10 represents the free energy per unit length when the displacement of a point on the coil is in the radial direction and corresponds to a strongly

confined polymer in a tube. We have derived the coefficient, which is in excellent agreement with that derived from computer simulations and also satisfies the constraint G>3/2. It may be mentioned that when we take the upper limit for the displacement

$$|r_0| = R$$, we have from eq (10, 12)

the constraint G ≥ 1.46 , which is very close to the relation G>3/2 derived by Burkhardt [9].

The Hamiltonian for the anisotropic XY- model on a 1D lattice with N sites in a trans-verse field is given by

$$I = -\sum_{i=-E}^{E} \Omega \left[\left(\frac{1+\xi}{2} \right) \chi_i^x \chi_{i+1}^x + \left(\frac{1-\xi}{2} \right) \chi_i^y \chi_{i+1}^y + \chi_i^x \right]$$

Where χ_i the Pauli matrix at the site i, ξ is the degree of anisotropy, and Ω is the inverse strength of the external field.

Here E = (B-1)/2 for B odd. For, the sys-tem corresponds to the transverse Ising model. This model's geometric phase has been calculated on the extra furnish to appreciate this phase's criticality [13, 14]. Following these works, we can calculate the geometric phase at the decisive point and explain its relative with the significance of concurrence at that peak.

A relation of Hamiltonians is introduced by applying a turning round of φ around the z-direction to every spin that is

$$I_\varphi = g_\varphi I g_\varphi^+$$

Where $$g_\varphi = \exp\left[\frac{i\varphi \chi_i^+}{2} \right]$$

From the procedure, we can obtain the ground state |g> given by

$$|g\rangle = -\prod_{k\rangle 0} (\cos \frac{\theta_k}{2} |0\rangle k |0\rangle - k - i e^{2i\varphi} \sin \frac{\theta_k}{2} |1\rangle k |1\rangle - k)$$

Where |0>k and |1>k are the vacua and single fermionic excitation of the kth mode, respectively.

The angle θ_k is defined by $$\cos\theta_k = \frac{1 + \Omega \cos\varphi_k}{\sqrt{1 + \Omega^2 + 2\Omega \cos\varphi_k}}$$

with $$\cos\theta_k = \frac{2\pi k}{B}$$, $k = -E, -E+1, \ldots\ldots\ldots\ldots + E$

The geometric phase of the ground state accumulated by varying the angle φ from 0 to

π is described by $\Im = -i\int\limits_0^\pi \left\langle g \left| \dfrac{\partial}{\partial\varphi} \right| g \right\rangle d\varphi = \sum\limits_{k>0} \pi(1-\cos\theta_k)$

In the thermodynamic limit, we have

$$\Im = \int\limits_0^\pi \left(1 - \dfrac{1+\Omega\cos\varphi_k}{\sqrt{1+\Omega^2+2\Omega\cos\varphi_k}} \right) d\varphi$$

which at the critical point $\Omega = \Omega_C = 1$ gives, $\Im_C = \pi - 2$

Referring to Eqn. (1) we have the value of the concurrence for the nearest neighbor entanglement at the critical point

$$G = |\Im_C| / 2\pi = 0.18$$

This is in perfect agreement with the closest neighbor concurrence value at the critical point obtained by the standard procedure G = .1946 [15]. We should point out here that at other points of 'ohm', the concurrence will depend on a function related to the external field. Indeed, as Carollo and Paschos [13] have shown, the geometric phase witnesses the singular point.

Discussion

The formulation of DNA molecule in terms of an antiferromagnetic spin chain gives rise to the entanglement entropy, which induces the entropic potential associated with the free energy per unit length entropy cost of confining a stiff polymer inside a narrow tube. The entanglement entropy effectively represents the thermodynamic entropy. This repulsive entropic potential opposes the elastically driven collapse of a supercoil, which can occur at zero temperature.

Finally, we have observed that the spin chain model reproduces the salient feature of the relation between concurrence and the geometrical phase becomes much more pro-nounced by the fact that near the critical point, both concurrence and the Berry phase follow the scaling behavior as has been shown in refs.[14, 16], respectively. This anal-ysis implies that spin entanglement is associated with the spatial entanglement between electrons at different spatial points. As Vedral [17] has pointed out, entanglement is a consequence of Fermi statistics.

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