Solitonlike base pair opening in a helicoidal DNA: An analogy with a helimagnet and a cholesteric liquid crystal

M. Daniel[*] and V. Vasumathi[†]

Centre for Nonlinear Dynamics, School of Physics, Bharathidasan University, Tiruchirappalli 620 024, India
(Received 8 August 2008; published 20 January 2009)

We propose a model for DNA dynamics by introducing the helical structure through twist deformation in analogy with the structure of a helimagnet and a cholesteric liquid-crystal system. The dynamics in this case is found to be governed by the completely integrable sine Gordon equation, which admits kink-antikink solitons with increased width, representing a wide base-pair opening configuration in DNA. The results show that the helicity introduces a length-scale variation and thus provides a better representation of the base-pair opening in DNA.

The B-form DNA double-helix molecule is usually modeled by two parallel chains of nucleotides known as strands with linkage interms of dipole-dipole interaction along the strands, and the two strands are coupled to each other through hydrogen bonds between the complementary bases [1]. Molecular excitations in DNA based on the above model are generally governed by nonlinear evolution equations [2–4] and in particular by the completely integrable sine Gordon–type equations [5,6]. In the above studies, DNA is treated as two coupled linear chains without involving the helical character of its structure. However, in nature DNA exists in a double-helix form and recently there were attempts by a few authors to study the dynamics by taking into account the helical character of the double helix through different forms of coupling. For instance, Gaeta [7–9], Dauxios [10], and Cadoni *et al.* [11] assumed that the torsional coupling between the nth base on one strand and the $(n+4)$th base on the complementary strand is the responsible force for the helical nature in DNA and found that the localized excitations are governed by solitons and breathers. Barbi *et al.* [12,13] and Campa [14], however, introduced the helicity through a proper choice of the coupling between the radial and angular variables of the helix and obtained breathers and kinks. On the other hand, very recently, Takeno [15] introduced helicity in DNA through a helical transformation and obtained nonbreathing compactonlike modes to represent the base-pair opening through numerical calculations.

In this paper, we propose a model by introducing the helical character in each strand of the DNA molecule through a twist deformation of the chain in analogy with the twist in cholesteric liquid crystal [16] or orientation of spins in a helimagnet [17]. As an illustration in Figs. 1(a)–1(c) we present a schematic representation of the arrangement of bases, spins, and molecules, respectively, in a DNA double-helical chain, in a helimagnet, and in a cholesteric liquid crystal, leading to the formation of helical structure. In Fig. 1(a), R and R' represent the two complementary strands of the DNA double helix and the dots between the arrows represent the hydrogen bonds between the complementary

bases. The arrows and short lines in Figs. 1(b) and 1(c), respectively, represent the spins and molecules at different sites and planes in a helimagnet and in a cholesteric liquid crystal. When we go along the z direction, the orientations of spins and molecules are tilted from one plane to the next through a certain tilt angle. If we join the tips of the arrows representing the spin vectors and also the tips of the molecules, they form a helix as shown in Figs. 1(b) and 1(c), respectively.

In a recent paper, one of the present authors studied the nonlinear spin dynamics of a helimagnet by incorporating the helicity in terms of Frank free energy corresponding to the twist deformation which is responsible for helicity in a cholesteric liquid-crystal system [17,18]. The Frank free-energy density associated with the twist deformation in a cholesteric liquid crystal is given by $[\mathbf{p} \cdot (\boldsymbol{\nabla} \times \mathbf{p}) - q_0]^2$, where the unit vector $\mathbf{p}$ represents the director axis which corresponds to the average direction of orientation of the liquid-crystal molecules, $q_0 = \frac{2\pi}{q}$ is the pitch wave vector, and q is the pitch of the helix. The discretized form of the above twist free energy is written as $\{[\hat{\mathbf{k}} \cdot (\mathbf{p}_n \times \mathbf{p}_{n+1})] - q_0\}^2$, where $\hat{\mathbf{k}}$ is the unit vector along the z direction. In analogy with the above, we write down the free energy associated with the twist deformation in terms of spin vector as $\{[\hat{\mathbf{k}} \cdot (\mathbf{S}_n \times \mathbf{S}_{n+1})] - q_0\}^2$. By taking into account the form of free energy the Heisenberg model of the Hamiltonian for an anisotropic helimagnetic system is written as [17]

$$H_1 = \sum_n \left[-J(\mathbf{S}_n \cdot \mathbf{S}_{n+1}) + A(S_n^z)^2 + h\{[\hat{\mathbf{k}} \cdot (\mathbf{S}_n \times \mathbf{S}_{n+1})] - q_0\}^2 \right].$$

(1)

In Eq. (1), $\mathbf{S}_n = (S_n^x, S_n^y, S_n^z)$ represents the spin vector at the nth site and the terms proportional to J and A, respectively, represent the ferromagnetic spin-spin exchange interaction and uniaxial magnetocrystalline anisotropy with the easy axis along the z direction. h denotes the elastic constant associated with the twist deformation. We identify the above helical spin chain with one of the strands of the DNA double-helical chain. Therefore, in a similar fashion we can write down the spin Hamiltonian H_2 for another helimagnetic system corresponding to the complementary strand with the

─────────
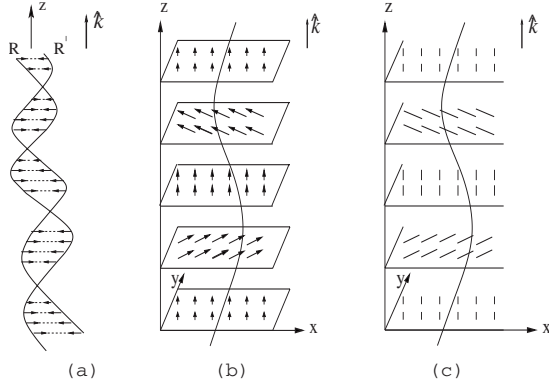*danielcnld@gmail.com
†vasu@cnld.bdu.ac.in

FIG. 1. A schematic representation of (a) a DNA double-helical chain, (b) a helimagnet, and (c) a cholesteric liquid-crystal system.

spin vector $\mathbf{S}_n$ replaced by $\mathbf{S}'_n$. We assume that in the Hamiltonian the exchange, anisotropic, and twist coefficients as well as the pitch in both the helimagnetic systems are equal. Now, for mapping the helimagnetic spin system with the DNA double-helical chain we rewrite the Hamiltonian by writing the spin vectors as $\mathbf{S}_n \equiv (S_n^x, S_n^y, S_n^z) = (\sin\theta_n\cos\phi_n, \sin\theta_n\sin\phi_n, \cos\theta_n)$ and $\mathbf{S}'_n \equiv (S_n^{'x}, S_n^{'y}, S_n^{'z}) = (\sin\theta'_n\cos\phi'_n, \sin\theta'_n\sin\phi'_n, \cos\theta'_n)$, where $\theta_n(\theta'_n)$ and $\phi_n(\phi'_n)$ are the angles of rotation of spins in the x-y and x-z planes, respectively. The new Hamiltonian corresponding to H_1 is written as

$$H_1 = \sum_n [-J\{\sin\theta_n\sin\theta_{n+1}\cos(\phi_{n+1}-\phi_n) + \cos\theta_n\cos\theta_{n+1}\} + A\cos^2\theta_n + h\{\sin\theta_n\sin\theta_{n+1}\sin(\phi_{n+1}-\phi_n) - q_0\}^2]. \tag{2}$$

We now map the two helical spin systems with the two strands of the DNA double helix with the two angles $\theta_n(\theta'_n)$ and $\phi_n(\phi'_n)$ representing the angles of rotation of bases in the x-z and x-y planes of the two strands, respectively. A horizontal projection of the nth base of DNA in the x-y and x-z planes is shown in Figs. 2(a) and 2(b). Here Q_n and Q'_n denote the tips of the nth bases attached to the strands R and R' at P_n and P'_n, respectively. The DNA double-helix chain is stabilized by stacking of bases through an intrastrand dipole-dipole interaction and through hydrogen bonds (interstrand interaction) between complementary bases. The interstrand base-base interaction or hydrogen bonding energy between the complementary bases depends on the distance between them, and using the simple geometry in Figs. 2(a) and 2(b), we can write the distance between the tips of bases as [6]

$$(Q_n Q'_n)^2 \approx 2[\sin\theta_n\sin\theta'_n(\cos\phi_n\cos\phi'_n + \sin\phi_n\sin\phi'_n) - \cos\theta_n\cos\theta'_n]. \tag{3}$$

Now, the above equation represents the hydrogen bonding energy between complementary bases and the Hamiltonian for the interstrand interaction or hydrogen bonds is written as
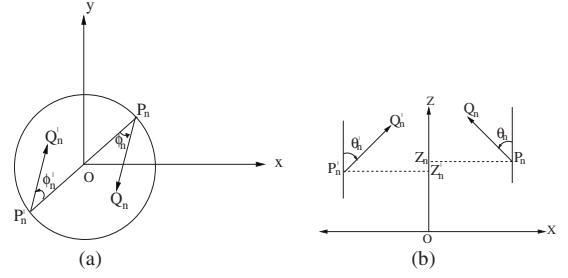

FIG. 2. A horizontal projection of the nth base pair in a DNA double helix (a) in the x-y plane and (b) in the x-z plane.

$$H_{12} = \eta[\sin\theta_n\sin\theta'_n(\cos\phi_n\cos\phi'_n + \sin\phi_n\sin\phi'_n) - \cos\theta_n\cos\theta'_n], \tag{4}$$

where η is a constant. The total Hamiltonian for our helicoidal model of DNA in terms of the angles of rotation of bases using the above Hamiltonians is written as

$$\begin{aligned} H &= H_1 + H_2 + H_{12} \\ &= \sum_n [-J\{\sin\theta_n\sin\theta_{n+1}\cos(\phi_{n+1}-\phi_n) + \cos\theta_n\cos\theta_{n+1} \\ &\quad + \sin\theta'_n\sin\theta'_{n+1}\cos(\phi'_{n+1}-\phi'_n) + \cos\theta'_n\cos\theta'_{n+1}\} \\ &\quad + h\{[\sin\theta_n\sin\theta_{n+1}\sin(\phi_{n+1}-\phi_n) - q_0]^2 \\ &\quad + [\sin\theta'_n\sin\theta'_{n+1}\sin(\phi'_{n+1}-\phi'_n) - q_0]^2\} \\ &\quad + \eta\{\sin\theta_n\sin\theta'_n(\cos\phi_n\cos\phi'_n + \sin\phi_n\sin\phi'_n) \\ &\quad - \cos\theta_n\cos\theta'_n\} + A(\cos^2\theta_n + \cos^2\theta'_n)]. \end{aligned} \tag{5}$$

Using the equation of motion for the corresponding quasispin model [19] in the limit $A \gg J, \eta, h$, we obtain $\dot\phi_n = 2A\cos\theta_n$ and $\dot\phi'_n = 2A'\cos\theta'_n$. Hence, under the absolute minima of the potential the Hamiltonian (5) becomes

$$\begin{aligned} H &= \sum_n \left[\frac{I}{2}(\dot\phi_n^2 + \dot\phi_n'^2) + J[2 - \cos(\phi_{n+1}-\phi_n) \right. \\ &\quad - \cos(\phi'_{n+1}-\phi'_n)] - \eta[1 - \cos(\phi_n - \phi'_n)] + h\{2q_0^2 \\ &\quad \left. - [\sin(\phi_{n+1}-\phi_n) - q_0]^2 - [\sin(\phi'_{n+1}-\phi'_n) - q_0]^2\} \right], \end{aligned} \tag{6}$$

where $I = \frac{1}{2A^2}$ is the moment of inertia of the bases around the axes at $p_n(p'_n)$. While rewriting the Hamiltonian in the above form, we have restricted the bases to be rotating in the plane which is normal to the helical axis. In other words, we have now restricted our problem to a plane base rotator model [6] by assuming $\theta = \theta' = \pi/2$.

Having formed the Hamiltonian, the dynamics of the DNA double-helix molecule can be understood by constructing Hamilton's equations of motion corresponding to the Hamiltonian (6) as
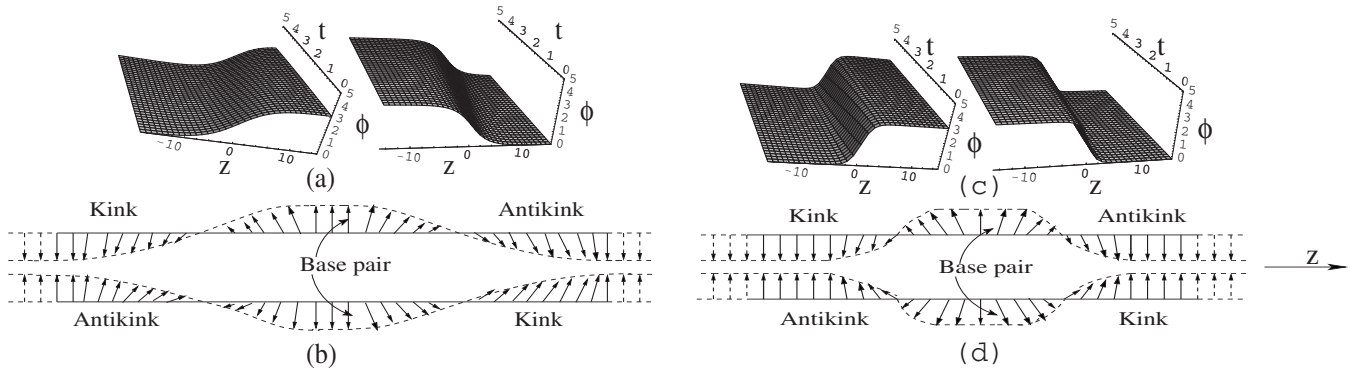
FIG. 3. (a) Kink-antikink one-soliton solutions [Eq. (10)] of the sine Gordon equation when helicity is present ($h \neq 0$). (b) A sketch of the formation of open-state configuration in terms of kink-antikink solitons in a DNA double helix when helicity is present ($h \neq 0$). (c) Kink-antikink one-soliton solutions of the sine Gordon equation when helicity is absent [Eq. (10) when $h=0$]. (d) A sketch of the formation of open-state configuration in terms of kink-antikink solitons in DNA double helix when helicity is absent ($h=0$).

$$I\ddot{\phi}_n = [J + 2h\cos(\phi_{n+1} - \phi_n)]\sin(\phi_{n+1} - \phi_n)$$
$$- [J + 2h\cos(\phi_n - \phi_{n-1})]\sin(\phi_n - \phi_{n-1})$$
$$+ \eta\sin(\phi_n - \phi_n') - 2hq_0[\cos(\phi_{n+1} - \phi_n)$$
$$- \cos(\phi_n - \phi_{n-1})], \tag{7a}$$

$$I\ddot{\phi}_n' = [J + 2h\cos(\phi_{n+1}' - \phi_n')]\sin(\phi_{n+1}' - \phi_n')$$
$$- [J + 2h\cos(\phi_n' - \phi_{n-1}')]\sin(\phi_n' - \phi_{n-1}')$$
$$+ \eta\sin(\phi_n' - \phi_n) - 2hq_0$$
$$\times [\cos(\phi_{n+1}' - \phi_n') - \cos(\phi_n' - \phi_{n-1}')], \tag{7b}$$

where an overdot represents derivative with respective to time. Equations (7a) and (7b) describe the dynamics of the DNA double helix at the discrete level when the helical nature of the molecule is represented in the form of a twistlike deformation.

It is expected that the difference in angular rotation of bases with respect to neighboring bases along the two strands is small [5,20]. Also, very recently Gaeta [8,9] proposed that the helical structure of DNA will introduce qualitative changes only in the small-amplitude regime. Hence, under the small-angle approximation, in the continuum limit, the discrete equations of motion (7a) and (7b) after suitable rescaling of time and redefinition of the parameter η reduce to

$$\phi_{tt} = \frac{(J + 2h)}{I}\phi_{zz} + \eta\sin(\phi - \phi'), \tag{8a}$$

$$\phi_{tt}' = \frac{(J + 2h)}{I}\phi_{zz}' + \eta\sin(\phi' - \phi). \tag{8b}$$

Adding and subtracting Eqs. (8a) and (8b) and after suitable rescaling of the variable z, we obtain

$$\Psi_{tt} - \Psi_{zz} + \sin\Psi = 0, \tag{9}$$

where $\Psi = 2\phi$ and we have further chosen $2\eta = -1$. Also, while deriving Eq. (9), we have chosen $\phi' = -\phi$, because among the possible rotations of bases, rotation of comple-

mentary bases in opposite directions easily facilitate an open-state configuration. Equation (9) is the completely integrable sine Gordon equation which was originally solved for N-soliton solution in terms of kinks and antikinks using the most celebrated inverse scattering transform method [21]. For instance, the kink-antikink one-soliton solution of the sine Gordon equation is written in terms of the original variables as

$$\phi(z,t) = 2\arctan\left[\exp\left(\pm\frac{1}{\sqrt{1-v^2}}\sqrt{\frac{I}{(J+2h)}}(z-vt)\right)\right], \tag{10}$$

where $+$ and $-$ represent the kink and antikink soliton solutions, respectively, and v is the velocity of the soliton. In Fig. 3(a) we plot the angular rotation of bases ϕ in terms of the kink-antikink one-soliton solution as given in Eq. (10) by choosing the stacking, helicity, moment of inertia, and velocity parameters, respectively, as $J=1.5$ eV, $h=3.0$ eV, $I=1.3 \times 10^{-36}$ g cm^2, and $v=0.4$ cm s^{-1} [10,15]. The kink-antikink soliton solution which can propagate infinite distance and time describes an open-state configuration in the DNA double helix, which is schematically represented in Fig. 3(b). In order to understand the effect of helicity on the open-state configuration, in Fig. 3(c), we have also plotted the kink-antikink one-soliton solution of the sine Gordon equation in the absence of helicity—that is, by choosing $h=0$ (keeping all other parameter values the same)—in the solution given in Eq. (10). From Figs. 3(a) and 3(c), we observe that when there is helicity in the model ($h \neq 0$), the kink-antikink soliton becomes broadened. In other words, helicity in DNA makes a larger number of base pairs to participate in the formation of open-state configuration without introducing any qualitative change in the dynamics. This is also schematically represented in Fig. 3(d), which looks evident on comparing Fig. 3(b). In order to highlight the above fact, we have separately plotted the kink one-soliton solution at a given time ($t=1$) for different values of helicity by choosing $h=0,1,2,3,4$ in Fig. 4(a). The increase in width against helicity is explicitly represented in Fig. 4(b). From the figure it may be noted that the increase in helicity slows down the
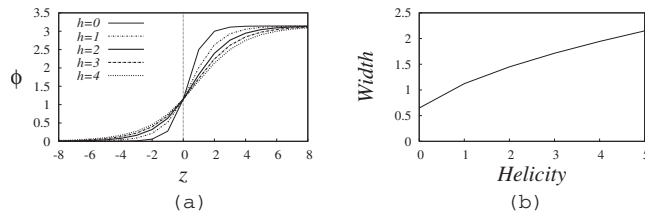
FIG. 4. (a) The kink one-soliton [Eq. (10)] representing base-pair opening at $t=1$ for different values of helicity. (b) Variation of width of the kink soliton against helicity.

rotation of bases and makes a larger and larger number of base pairs to participate in the open-state configuration, thus providing a better representation of base-pair opening in DNA. Thus, helicity introduces a length scale variation in the base-pair opening.

Similar results have also been observed by Dauxios [10] through a perturbation analysis of his helicoidal model of DNA and obtained a soliton with a much broader width. In order to have a more realistic model, dissipative (viscous effect) and noise terms should be added to the equations of motion. Experimentally, the lifetime of a soliton in this case is shown to be a few nanoseconds at room temperature (see, e.g., Ref. [22]). Also, in a recent paper, Yakushevich *et al.* [23] through a numerical analysis showed that when the viscosity is strong the soliton moves a length of only few chain links and it will stop after that. On the other hand, when the viscosity is low the soliton passes more than 3000 chain links like a heavy Brownian particle which is found to be stable with respect to thermal oscillations. When the above two effects are taken into account, Eq. (9) takes the form $\Psi_{tt} - \Psi_{zz} + \sin \Psi = \epsilon [\alpha \Psi_t + \beta \mathsf{F}(z,t)]$, where the terms proportional to α and β are related to viscous surrounding and thermal forces, respectively. The function $\mathsf{F}(z,t)$ is related to the random normally distributed forces describing the interaction of the bases with thermal bath. A soliton perturbation analysis [24] of the above equation shows that when the viscosity is high the soliton moves for a small distance and then stops. But when the viscosity is low, the soliton moves for a long distance along the chain. The detailed analytical calculations of the above study will be separately published elsewhere.

In summary, we proposed a helicoidal model to study DNA dynamics by introducing the helical character in analogy with the twist deformation in a cholesteric liquid-crystal system and the spin arrangement in a helimagnet. The nonlinear dynamics of DNA under the present helicoidal model is found to be governed by the completely integrable sine Gordon equation in the continuum limit which admits kink and antikink soliton solutions. From the nature of solitons, we observe that helicity introduces a length-scale variation without causing any change in the shape of the soliton. Due to this scaling variation, the width of the soliton increases and hence we obtain broader kinks and antikinks. In other words, a large number of bases are involved in the base-pair opening, thus leading to a better representation. This broadened base-pair opening may act as a better energetic activator in the case of RNA-polymerase transport during the transcription process in DNA. As the continuum helicoidal model does not introduce qualitative changes in the DNA dynamics, we propose to study the full nonlinear dynamics of the helicoidal model of DNA (without making a small-angle approximation) by solving Eqs. (7a) and (7b) numerically and the results will be published elsewhere.

[1] L. V. Yakushevich, *Nonlinear Physics of DNA* (Wiley-VCH, Berlin, 2004).

[2] S. W. Englander, N. R. Kallenbanch, A. J. Heeger, J. A. Krumhansl, and S. Litwin, Proc. Natl. Acad. Sci. U.S.A. **77**, 7222 (1980).

[3] M. Peyrard and A. R. Bishop, Phys. Rev. Lett. **62**, 2755 (1989).

[4] V. Muto, P. S. Lomdahl, and P. L. Christiansen, Phys. Rev. A **42**, 7452 (1990).

[5] S. Yomosa, Phys. Rev. A **27**, 2120 (1983); **30**, 474 (1984).

[6] S. Takeno and S. Homma, Prog. Theor. Phys. **70**, 308 (1983); **72**, 679 (1984).

[7] G. Gaeta, Phys. Lett. A **143**, 227 (1990); **168**, 383 (1992).

[8] G. Gaeta, Phys. Rev. E **74**, 021921 (2006).

[9] G. Gaeta, J. Nonlinear Math. Phys. **14**, 57 (2007).

[10] T. Dauxios, Phys. Lett. A **159**, 390 (1991).

[11] M. Cadoni, R. De Leo, and G. Gaeta, Phys. Rev. E **75**, 021919 (2007).

[12] M. Barbi, S. Cocco, and M. Peyrard, Phys. Lett. A **253**, 358 (1999).

[13] M. Barbi, S. Lepri, M. Peyrard, and N. Theodorakopoulos, Phys. Rev. E **68**, 061909 (2003).

[14] A. Campa, Phys. Rev. E **63**, 021901 (2001).

[15] S. Takeno, Phys. Lett. A **339**, 352 (2005).

[16] P. G. de Gennes, *Physics of Liquid Crystals* (Clarendon, Oxford, 1974).

[17] R. M. White, *Quantum Theory of Magnetism* (Springer, New York, 1982).

[18] M. Daniel and J. Beula, Chaos, Solitons Fractals (to be published).

[19] J. Tjon and J. Wright, Phys. Rev. B **15**, 3470 (1977).

[20] G. Fa Zhou, Phys. Scr. **40**, 694 (1989).

[21] M. J. Ablowitz, D. J. Kaup, A. C. Newell, and H. Segur, Stud. Appl. Math. **53**, 249 (1974).

[22] M. Peyrard, Nonlinearity **17**, R1 (2004) and references therein.

[23] L. V. Yakushevich, A. V. Savin, and L. I. Manevitch, Phys. Rev. E **66**, 016614 (2002).

[24] M. Daniel and V. Vasumathi, Physica D **231**, 10 (2007).