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**PERTURBED SOLITON EXCITATIONS
IN INHOMOGENEOUS DNA**

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Abstract

We study nonlinear dynamics of inhomogeneous DNA double helical chain under dynamic plane-base rotator model by considering angular rotation of bases in a plane normal to the helical axis. The DNA dynamics in this case is found to be governed by a perturbed sine-Gordon equation when taking into account the interstrand hydrogen bonding energy and intrastrand inhomogeneous stacking energy and making an analogy with the Heisenberg model of the Hamiltonian for an inhomogeneous anisotropic spin ladder with ferromagnetic legs and antiferromagnetic rung coupling. In the homogeneous limit the dynamics is governed by the kink-antikink soliton of the sine-Gordon equation which represents the formation of open state configuration in DNA double helix. The effect of inhomogeneity in stacking energy in the form of localized and periodic variations on the formation of open states in DNA is studied under perturbation. The perturbed soliton is obtained using a multiple scale soliton perturbation theory by solving the associated linear eigen value problem and constructing the complete set of eigen functions. The inhomogeneity in stacking energy is found to modulate the width and speed of the soliton depending on the nature of inhomogeneity. Also it introduces fluctuations in the form of train of pulses or periodic oscillation in the open state configuration.

I. INTRODUCTION

Deoxyribonucleic acid (DNA) plays an important role in the conservation and transformation of genetic information in biological systems [1]. Genes which specify the kinds of proteins that are to be made by a cell are coded in the form of sequence of bases in DNAs. Thus understanding the mechanism of DNA functions and in particular understanding the replication and transcription which are backbone of our life remains a major challenge in molecular biology. While replication is the process of production of duplicate DNA, transcription is the process of synthesis of proteins. For protein synthesis the template is the RNA molecule which has to be obtained from DNA through the process of transcription in which DNA synthesises mRNA according to the instructions (genetic code) given by a DNA template. RNA polymerase binds to the specific promotor site depending on the protein to be synthesised and the transcription begins at this site. The transcription process ends with the terminator site and mRNA is generated. For the above two functions namely for replication and transcription, opening (denaturation) of base pairs in DNA is a precursor [2]. The opening of bases in DNA corresponds to breaking of hydrogen bonds between the bases. The opening of bases or base flipping in DNA induced by protein-DNA interaction has been indentified by several authors [3–6]. Also, recently it is found that the nonlinearity associated with hydrogen bonding energy plays an important role in bringing out localized open states through molecular excitations [7, 8]. In particular, solitons have been found to govern the fluctuations of double helix between an open state and its equilibrium states [9, 10]. These local excitations in DNA double helix are induced by different types of motions of the base pairs including these nonlinear studies explain open state dynamics [11, 12], hydrogen-deuterium exchange [13], microwave absorption [14, 15], conformation transition [16–18], long range effect [19], regulation of transcription [19, 20], denaturation [21] and others [22]. Thus the study of nonlinear molecular excitations in DNA molecular chain has become an important study since it is related to its major functions.

A number of theoretical models have been proposed to describe the nonlinear properties of DNA. They are based on longitudinal and transverse motions, bending, stretching and rotational motions [23]. Among the different motions, the rotational motion of bases in DNA was found to contribute more towards the opening of base pairs. The first contribution towards nonlinear dynamics of DNA was made by Englander and his co-workers [24] who studied the dynamics of DNA open states by taking into account only the rotational motion of nitrogenous bases, which made the main contribution towards the formation of open states. They suggested that open states in DNA are thermally excited solitons [25]. Yamosa [26, 27] developing this idea further proposed a dynamic plane base rotator model which is a generalized version of the Frenkel-Kontrova [28] model that was later improved by Takeno and Homma [29, 30] in which attention was paid to the degree of freedom, characterizing base

rotations in the plane perpendicular to the helical axis around the backbone structure. To model this motion it was assumed that each base of the strand was coupled with the next nearest neighbouring base of the same strand by the elastic backbone restoring force and the complementary base in the opposite strand by the anharmonic potential used to model the hydrogen bond. Then Peyard and Bishop [21] studied the process of denaturation in which only the transverse motion of bases along the hydrogen bond was taken into account. There was one more model studied by Christiansen and his colleagues (see for e.g.[31]) in which two types of internal motions namely, transverse motion along the hydrogen bond direction and longitudinal motion along the backbone direction, were found to contribute to DNA denaturation process. Their model was constructed out of two polynucleotide strands linked together through hydrogen bonds described by Lennard-Jones potential and phosphate diester bridge described by an anharmonic Toda potential. Further developments, in this approach for several years was limited to small improvements of the models and involving only numerical methods of simulation of the internal dynamics of DNA [32, 33]. Also, discrete breathers and non-breathing compacton-like modes were represented by solving the DNA-lattice model [34–38].

In all the above studies DNA double helix with homogeneous stiff strands have been considered for the analysis. However in nature the presence of different sites along the strands such as promotor, coding, terminator etc. each of which having a very specific sequence of bases and particular functions makes the strands site-dependent or inhomogeneous(soft). Also, inhomogeneity occurs when an electron or a hole is injected into DNA it will induce local distortion in the structure [39]. Further at very low temperatures DNA shows large-amplitude motions known as "fluctuational openings" in which the base pairs open for a very short time and then close again. During the base pair reclosing process they can trap some external molecules causing a defect in the sequence [40] leading to inhomogeneity. One more characteristic dynamical feature of DNA is the occasional local disruption of hydrogen bonds and hence the bases are more solvent-exposed. This phenomenon is known as breathing which was detected in the molecular dynamics simulation of DNA duplex containing a difluorotoluene base which is a nonpolar mimic of thymine [41]. Therefore in this paper we study the nonlinear dynamics of DNA double helix with inhomogeneous strands by considering a plane base rotator model along the lines of Yamosa. The paper is organized as follows. In Sec II we introduce a dynamic plane base rotator model for the site-dependent DNA double helix chain and derive the nonlinear dynamical equation. In sec III, we study the effect of inhomogeneity in stacking energy on the open state of DNA in terms of kink-antikink solitons by solving a perturbed sine-Gordon equation using a multiple scale soliton perturbation theory. The results are concluded in section IV. Detailed evaluation of few integrals using residue theorem given in Appendices.

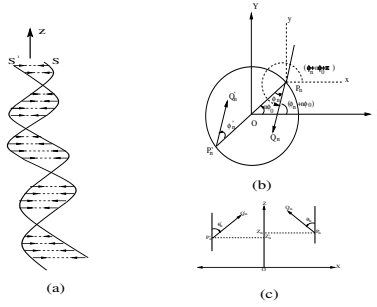


FIG. 1: (a) A Schematic structure of B-form of DNA double helix (b) A horizontal projection of the n th base pair in the XY-plane (c) A Projection of the n th base pair in the XZ-plane.

II. PLANE-BASE ROTATOR MODEL AND DYNAMICAL EQUATION

In Fig.1a we have presented a schematic structure of the B-form DNA double helix. Here S and S' represent the two complementary strands in the DNA double helix. Each arrow in the figure represents the direction of the base attached to the strand and the dots between arrows represent the net hydrogen bonding effect between the complement bases. The major and minor grooves of the DNA helix are seen in the sketch. While a horizontal projection of the n^{th} base pair in the XY-plane is represented in Fig.1b, in Fig. 1c, we have given the projection of the same in the XZ-plane. The Z-axis is chosen along the helical axis of the DNA. In Fig.1b, Q_n denotes the tip of the n^{th} base belonging to the S-strand and Q'_n denotes the tip of the complementary base belonging to the S' -strand which in combination form a hydrogen bonded base pair in an ordered state. P_n and P'_n represent the points where bases in the n^{th} base pair are attached to the strands S and S' respectively. Let (θ_n, ϕ_n) and (θ'_n, ϕ'_n) represent the angles of rotation of the bases in the n^{th} base pair around the points P_n and P'_n in the XZ and XY-planes respectively. The quantities (θ_n, ϕ_n, z_n) and $(\theta'_n, \phi'_n, z'_n)$ measure the deviation of the positions of the n^{th} pair of bases from the exact B-form of the double helix. Thus the directions of $\mathbf{P}_n\mathbf{Q}_n$ and $\mathbf{P}'_n\mathbf{Q}'_n$ in the XY-plane are specified by the rotational angles ϕ_n and ϕ'_n . The coordinates of P_n and P'_n with respect to the point O are $(r \cos n\phi_0, r \sin n\phi_0, z_n)$ and $(r \cos(n\phi_0 + \pi), r \sin(n\phi_0 + \pi), z_n)$ respectively with $\phi_0 = \frac{2\pi}{p}$, where r is the radius of the circle depicted in Fig.(1b), p is the number of bases per turn in S and S' and n is a number. The co-ordinates of Q_n and Q'_n with respect to P_n and P'_n can be given by $(-\sin \theta_n \cos(\phi_n + n\phi_0), -\sin \theta_n \sin(\phi_n + n\phi_0), \cos \theta_n)$ and $(\sin \theta'_n \cos(\phi'_n + n\phi_0), \sin \theta'_n \sin(\phi'_n + n\phi_0), \cos \theta'_n)$ respectively.

The conformation and stability of DNA double helix is mainly determined by the stacking energy between the intrastrand adjacent bases, the hydrogen bonding energy between the interstrand complementary bases and other energies. From a heuristic argument it was assumed that the interstrand base-base interaction or hydrogen bonding energy of the given base pair depends on the distance between them. Thus, from Fig.1b we can write down the square of the

distance between the edges of the arrows $(Q_n Q'_n)^2$ as

$$\begin{aligned}
(Q_n Q'_n)^2 &= 2 + 4r^2 + (z_n - z'_n)^2 + 2(z_n - z'_n) \\
&\times (\cos \theta_n - \cos \theta'_n) - 4r [\sin \theta_n \cos \phi_n \\
&+ \sin \theta'_n \cos \phi'_n] + 2 [\sin \theta_n \sin \theta'_n \\
&\times (\cos \phi_n \cos \phi'_n + \sin \phi_n \sin \phi'_n) \\
&- \cos \theta_n \cos \theta'_n].
\end{aligned} \tag{1}$$

The base-base interaction energy can be understood in a more clear and transparent way by introducing quasi-spin operators $\mathbf{S}_n = (S_n^x, S_n^y, S_n^z)$ and $\mathbf{S}'_n = (S_n'^x, S_n'^y, S_n'^z)$ in the form

$$\begin{aligned}
S_n^x &= \sin \theta_n \cos \phi_n, & S_n^y &= \sin \theta_n \sin \phi_n, \\
S_n^z &= \cos \theta_n,
\end{aligned} \tag{2a}$$

$$\begin{aligned}
S_n'^x &= \sin \theta'_n \cos \phi'_n, & S_n'^y &= \sin \theta'_n \sin \phi'_n, \\
S_n'^z &= \cos \theta'_n,
\end{aligned} \tag{2b}$$

for the n^{th} bases in the S^{th} and S'^{th} strands respectively. In view of this, Eq. (1) can be written in terms of the given spin operators as follows.

$$\begin{aligned}
(Q_n Q'_n)^2 &= 2 + 4r^2 + 2 [S_n^x S_n'^x + S_n^y S_n'^y \\
&- S_n^z S_n'^z] - 4r [S_n^x + S_n'^x].
\end{aligned} \tag{3}$$

While writing Eq.(3) we have neglected the longitudinal compression along the direction of the helical axis thereby choosing $z_n = z'_n$. It may be noted that the form of $(Q_n Q'_n)^2$ given in Eq.(3) is the same as the Hamiltonian for a generalized form of the Heisenberg spin model. Therefore, the intrastrand base-base interaction in DNA can be written using the same consideration. It is also reasonable to think that if such a quasi-spin model Hamiltonian can be used in this problem, the double strand DNA and the rung-like base pairs can be conceived as an anisotropic coupled spin chain model or spin ladder. This is schematically presented in Fig.2. In the figure, S and S' which previously represented two strands of the DNA here correspond to two ferromagnetic lattices of a spin ladder with antiferromagnetic coupling among the rungs. In the case of spin chains each arrow represents the magnetic moment corresponding to a group of atoms at that lattice point. Due to antiferromagnetic type of rung coupling the arrows in the lattice S and S' are marked anti-parallel to each other. Here Z-direction (i.e) the direction of the helical axis is chosen as the easy axis of magnetization in the spin chain. Further the spin-spin exchange interaction is restricted to the nearest neighbours, (i.e) the n^{th} spin is coupled to the spins at the $(n+1)^{\text{th}}$ and $(n-1)^{\text{th}}$ sites.

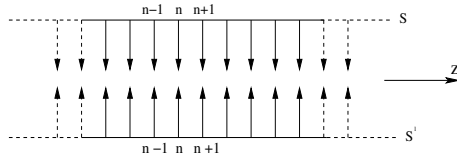


FIG. 2: A Schematic representation of DNA as an anisotropic coupled spin chain model or spin ladder.

With this consideration we use the following Heisenberg model of the Hamiltonian for an anisotropic coupled spin chain model or spin ladder with site-dependent or inhomogeneous ferromagnetic-type exchange interaction between nearest neighbouring spins in the same lattice (equivalent to coupling among bases in the same strand i.e. intrastrand interaction) and antiferromagnetic rung-coupling (between bases belonging to the complementary strands i.e. interstrand interaction).

$$\begin{aligned}
H = \sum_n & \left[-J f_n (S_n^x S_{n+1}^x + S_n^y S_{n+1}^y) - K f_n \right. \\
& \times S_n^z S_{n+1}^z - J' f'_n (S_n^x S_{n+1}^x + S_n^y S_{n+1}^y) \\
& - K' f'_n S_n^z S_{n+1}^z + \eta (S_n^x S_n^x + S_n^y S_n^y) \\
& \left. + \mu S_n^z S_n^z + A (S_n^z)^2 + A' (S_n^z)^2 \right]. \quad (4)
\end{aligned}$$

In the above Hamiltonian J and J' correspond to the intrastrand interaction constant or the stacking energy between the n^{th} base and its nearest neighbours in the plane normal to the helical axis in the strands S and S' respectively. When K and K' are not equal to J and J' respectively, they introduce anisotropy in the intrastrand interaction. μ and η represent a measure of interstrand interaction or hydrogen bonding energy between the bases of similar sites in both the strands along the direction of the helical axis and in a plane normal to it respectively. Here we have assumed that there exists on an average an almost uniform interaction A and A' which assume positive values are the uniaxial anisotropy coefficients leading to rotation of the bases in a plane normal to the helical axis. The quantities f_n and f'_n in Hamiltonian (4) indicate that the intrastrand stacking energy between bases in the S^{th} and S'^{th} strand varies in a specified site dependent fashion which lead to inhomogeneity in the DNA double helical chain. In general f_n and f'_n may take different values for different base sequences. The inhomogeneity in DNA double helix may arise due to any one of the reasons mentioned in the previous section. The effect of inhomogeneity in DNA nonlinear dynamics has been studied in the past by several authors in various contexts such as variational mass density of bases [41], defect [42], hydrophobic interaction among bases [43] and charge transport [38].

To proceed further we rewrite Hamiltonian (4) in terms of the variables (θ_n, ϕ_n) and (θ'_n, ϕ'_n)

using Eqs.(2) and obtain

$$\begin{aligned}
H = \sum_n & \left[-J f_n \sin \theta_n \sin \theta_{n+1} \cos(\phi_{n+1} - \phi_n) \right. \\
& - K f_n \cos \theta_n \cos \theta_{n+1} - J' f'_n \sin \theta'_n \sin \theta'_{n+1} \\
& \cos(\phi'_{n+1} - \phi'_n) - K' f'_n \cos \theta'_n \cos \theta'_{n+1} \\
& + \eta \sin \theta_n \sin \theta'_n \cos(\phi_n - \phi'_n) + \mu \cos \theta_n \\
& \left. \times \cos \theta'_n + A \cos \theta_n^2 + A' \cos \theta_n'^2 \right]. \tag{5}
\end{aligned}$$

The quasi-spin model thus introduced implies that the dynamics of bases in DNA is described by the following equations of motion.

$$\dot{\theta}_n = \frac{1}{\sin \phi_n} \frac{\partial H}{\partial \phi_n}, \quad \dot{\phi}_n = \frac{-1}{\sin \theta_n} \frac{\partial H}{\partial \theta_n}, \tag{6a}$$

$$\dot{\theta}'_n = \frac{1}{\sin \phi'_n} \frac{\partial H}{\partial \phi'_n}, \quad \dot{\phi}'_n = \frac{-1}{\sin \theta'_n} \frac{\partial H}{\partial \theta'_n}. \tag{6b}$$

In Eqs.(6) the overdot represents time derivative. When the anisotropy energies A and A' are much larger than the other interactions, (i.e) when $A, A' \gg J, J', K, K', \eta, \mu$, then the equations of motion (6) on substituting the Hamiltonian (5) become

$$\dot{\phi}_n = 2A \cos \theta_n, \quad \dot{\phi}'_n = 2A' \cos \theta'_n. \tag{7}$$

The other two equations in (6) satisfy indentically. Using Eqs. (7) in the Hamiltonian (5) we obtain

$$\begin{aligned}
H = \sum_n & \left[\frac{I}{2} \dot{\phi}_n^2 + \frac{I'}{2} \dot{\phi}'_n{}^2 - J f_n \sin \theta_n \sin \theta_{n+1} \right. \\
& \times \cos(\phi_{n+1} - \phi_n) - K f_n \cos \theta_n \cos \theta_{n+1} \\
& - J' f'_n \sin \theta'_n \sin \theta'_{n+1} \cos(\phi'_{n+1} - \phi'_n) \\
& - K' f'_n \cos \theta'_n \cos \theta'_{n+1} + \eta \sin \theta_n \sin \theta'_n \\
& \left. \times \cos(\phi_n - \phi'_n) + \mu \cos \theta_n \cos \theta'_n \right]. \tag{8}
\end{aligned}$$

where $I = \frac{1}{2A}$ and $I' = \frac{1}{2A'}$. The above Hamiltonian can be rewritten in the limits of plane-base rotator ($\theta_n = \theta'_n = \pi/2$) and absolute minima of potential as

$$\begin{aligned}
H = \sum_n & \left[\frac{I}{2} \dot{\phi}_n^2 + \frac{I'}{2} \dot{\phi}'_n{}^2 + J f_n [1 - \cos(\phi_{n+1} - \phi_n)] \right. \\
& \left. + J' f'_n [1 - \cos(\phi'_{n+1} - \phi'_n)] - \eta [1 - \cos(\phi_n - \phi'_n)] \right]. \tag{9}
\end{aligned}$$

It may be noted that the above limit corresponds to the XY-spin model of two coupled inhomogeneous ferromagnetic spin system. In Hamiltonian (9) the first two terms represent the kinetic energies of the rotational motion of the n^{th} nucleotide bases accompanied by the potential energy associated with the n^{th} nucleotide sugar and phosphate and its complementary unit around the

axes at P_n and P'_n (see Figure 1b). I and I' are the moments of inertia of the nucleotides around the axes at P_n and P'_n respectively. It may be noted that in the new Hamiltonian the term proportional to μ vanishes. Now, using Hamiltonian (9), the Hamilton's equations of motion can be immediately written as

$$I\ddot{\phi}_n = J [f_n \sin(\phi_{n+1} - \phi_n) - f_{n-1} \sin(\phi_n - \phi_{n-1})] + \eta \sin(\phi_n - \phi'_n), \quad (10a)$$

$$I'\ddot{\phi}'_n = J' [f'_n \sin(\phi'_{n+1} - \phi'_n) - f'_{n-1} \sin(\phi'_n - \phi'_{n-1})] + \eta \sin(\phi'_n - \phi_n). \quad (10b)$$

Eqs.(10) describe the dynamics of DNA in a plane-base rotator model at the discrete level while considering the dominant angular rotation of the bases in a plane normal to the helical axis and ignoring all other small motions of the bases.

It is expected that in the B-form of DNA double helix the difference in the angular rotation of bases with respect to neighbouring bases along the two strands is small [29, 30]. Hence we assume that $\sin(\phi_{n\pm 1} - \phi_n) \approx (\phi_{n\pm 1} - \phi_n)$ and $\sin(\phi'_{n\pm 1} - \phi'_n) \approx (\phi'_{n\pm 1} - \phi'_n)$ in Eqs.(10). Also, as the length of the DNA chain is very large compared to the distance between the neighbouring bases along the strands we make a continuum approximation which is valid in the long wavelength, low temperature limit by introducing two fields of rotational angles, $\phi_n(t) \rightarrow \phi(z, t)$, $\phi'_n(t) \rightarrow \phi'(z, t)$ and two inhomogeneous stacking fields, $f_n \rightarrow f(z)$ and $f'_n \rightarrow f'(z)$ along with the following expansions.

$$\phi_{n\pm 1} = \phi(z, t) \pm a \frac{\partial \phi}{\partial z} + \frac{a^2}{2!} \frac{\partial^2 \phi}{\partial z^2} \pm \frac{a^3}{3!} \frac{\partial^3 \phi}{\partial z^3} + \dots, \quad (11a)$$

$$f_{n\pm 1} = f(z) \pm a \frac{\partial f}{\partial z} + \frac{a^2}{2!} \frac{\partial^2 f}{\partial z^2} \pm \frac{a^3}{3!} \frac{\partial^3 f}{\partial z^3} + \dots, \quad (11b)$$

where 'a' is the lattice parameter along the strands S and S' . In a similar way we write down expansions for $\phi'_{n\pm 1}$ and $f'_{n\pm 1}$. As the inhomogeneity here is site-dependent and associated with the bases themselves, we have chosen same lattice parameter 'a' for both $\phi_{n\pm 1}$ and $f_{n\pm 1}$. Under this continuum approximation the equations of motion (10) upto $O(a^2)$ is written as

$$I\phi_{tt} = Ja^2 [f(z)\phi_{zz} + f_z\phi_z] + \eta \sin(\phi - \phi'), \quad (12a)$$

$$I'\phi'_{tt} = J'a^2 [f'(z)\phi'_{zz} + f'_z\phi'_z] + \eta \sin(\phi' - \phi). \quad (12b)$$

In Eqs.(12) the suffices t and z respectively represent partial derivatives with respect to time t and the spatial variable z .

In a DNA chain, the two strands are expected to exhibit similar type of macroscopic physical behaviour and hence we assume that $I = I'$, $J = J'$ and $f = f'$. In view of this, Eqs. (12)

after rescaling the time variable $\hat{t} = \sqrt{\frac{Ja^2}{I}}t$ and choosing $\eta = -\frac{Ja^2}{2}$ for future convenience can be written as

$$\phi_{\hat{t}\hat{t}} = [f(z)\phi_{zz} + f_z\phi_z] - \frac{1}{2}\sin(\phi - \phi'), \quad (13a)$$

$$\phi'_{\hat{t}\hat{t}} = [f(z)\phi'_{zz} + f_z\phi'_z] - \frac{1}{2}\sin(\phi' - \phi). \quad (13b)$$

It is more convenient to describe the transverse motion of the bases in DNA strands in terms of the centre of mass co-ordinates. For this, we rewrite Eqs. (13a) and (13b) by subtracting and adding them respectively.

$$\begin{aligned} (\phi - \phi')_{\hat{t}\hat{t}} &= f(z)(\phi - \phi')_{zz} + f_z(\phi - \phi')_z \\ &\quad - \sin(\phi - \phi'), \end{aligned} \quad (14a)$$

$$(\phi + \phi')_{\hat{t}\hat{t}} = f(z)(\phi + \phi')_{zz} + f_z(\phi + \phi')_z. \quad (14b)$$

In a different context while studying the magnetoelastic effect induced by interaction between two ferromagnetically coupled XY-spin chains Dandolo and Saxena [44] obtained similar equations however the static case. To commence the open state configuration in DNA, the two complementary bases are expected to rotate in opposite directions so that $\phi = -\phi'$, and in this case Eq. (14b) satisfies identically and Eq. (14a) becomes

$$\Psi_{\hat{t}\hat{t}} = f\Psi_{zz} + f_z\Psi_z - \sin\Psi, \quad (15)$$

where $\Psi = 2\phi$. Assuming small inhomogeneity along the strands by choosing $f(z) = 1 + \epsilon g(z)$ where ϵ is a small parameter and $g(z)$ a measure of the inhomogeneity, Eq. (15) can be written as

$$\Psi_{\hat{t}\hat{t}} - \Psi_{zz} + \sin\Psi = \epsilon [g(z)\Psi_z]_z. \quad (16)$$

Eq. (16) describes the dynamics of bases under rotation in a plane-base rotator model of an inhomogeneous DNA double helical chain. When $\epsilon = 0$, Eq. (16) reduces to the completely integrable sine-Gordon equation which admits kink and antikink-type of soliton solutions and hence we call Eq.(16) as a perturbed sine-Gordon equation. The integrable sine-Gordon equation ($\epsilon = 0$) case was originally solved for N-soliton solutions using the most celebrated Inverse Scattering Transform (IST) method by Ablowitz and his co-workers [47]. The kink and antikink soliton solutions of the integrable sine-Gordon equation (Eq.(16) when $\epsilon = 0$) are depicted in Figs. 3a and 3b. The kink-antikink solitons of the sine-Gordon equation describe an open state configuration in the DNA double helix. The formation of open state configuration in terms of kink-antikink pair in DNA double helical chain is schematically represented in Fig. 3c. In this figure the base pairs are found to open locally in the form of kink-antikink structure in each strand and propagate along the direction of the helical axis.

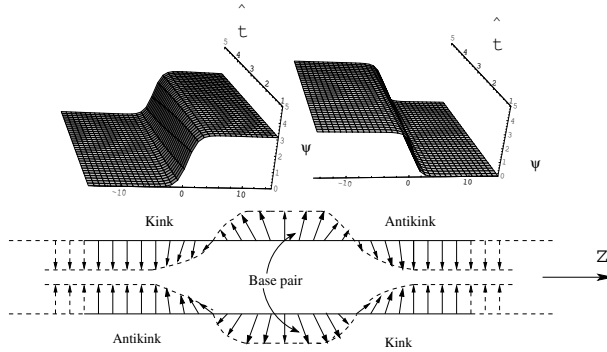


FIG. 3: (a) Kink and (b) antikink soliton solutions of the sine-Gordon equation (Eq.(16) when $\epsilon = 0$). (c) A sketch of the formation of open state configuration in terms of kink-antikink solitons in DNA double helix.

III. EFFECT OF STACKING ENERGY INHOMOGENEITY ON THE OPEN STATE

A. A Perturbation approach

When inhomogeneity in stacking is present (i.e) when terms proportional to ϵ are present in Eq.(16), the inhomogeneity is expected to perturb the kink and antikink solitons corresponding to the open state of DNA. One of the most powerful techniques in dealing with perturbed soliton equations is the soliton perturbation theory which is based on the IST method [45–47]. However, as the method is very sophisticated it is very difficult to use the same in several cases. In view of this, a direct method to study the soliton perturbation was first introduced by Gromshkov and Ostrovskii [48] and later on many authors used different types of direct methods to study soliton perturbation for e.g. see Refs. [49–54]. The characteristic feature of this method is that the perturbed nonlinear equation is linearized by expanding its solution about the unperturbed solution and the eigen functions for the operator associated with linearized equation are found out. The complete solution is then written in terms of these eigen functions [55, 56]. In these methods the basic fact that the presence of perturbation not only modifies the shape of the soliton by a correction of linear dispersion but also undergoes a slow time change of the soliton parameters have been acknowledged. In this paper, we use one such direct perturbation method which is also dealt in reference [57] to solve the perturbed sine-Gordon equation (16) and to understand the effect of inhomogeneity in stacking energy on the open state configuration of DNA. The procedure we adapt here is based on the derivative expansion method to linearize the perturbed sine-Gordon equation in the co-ordinate frame attached to the moving frame. The parameters of the kink-antikink soliton are assumed to depend on a slow time scale in order to eliminate

the secular terms. The linearized equations will be solved using the method of separation of variables which ultimately will be related to an eigen value problem, the eigen functions of which form the bases of the perturbed solution. The eigen functions contain information about the time dependence of the soliton parameters and help to calculate the perturbed soliton. In the following we use the above approach to find the perturbed soliton solution of Eq.(16).

B. Linearization of the perturbed sine-Gordon equation

When the perturbation is absent (i.e) when $\epsilon = 0$ in Eq. (16) the unperturbed integrable sine-Gordon equation provides N-soliton solutions and the one kink-soliton solution (see also Fig. (3a,b)) is written as

$$\Psi(z, \hat{t}) = 4 \arctan \exp[\pm m(z - v\hat{t})], \quad m = \frac{1}{\sqrt{1 - v^2}}. \quad (17)$$

In Eq.(17) while the upper sign corresponds to kink soliton, the lower sign represents the antikink soliton. Here v and m^{-1} are real parameters that determine the velocity and width of the soliton respectively. In order to study the effect of perturbation the time variable \hat{t} is transformed into several variables as $t_n = \epsilon^n \hat{t}$ where $n=0,1,2,\dots$ and ϵ is a very small parameter. In view of this, the time derivative in Eq. (16) is replaced by the expansion

$$\frac{\partial}{\partial \hat{t}} = \frac{\partial}{\partial t_0} + \epsilon \frac{\partial}{\partial t_1} + \epsilon^2 \frac{\partial}{\partial t_2} + \dots \quad (18)$$

Simultaneously Ψ is expanded in an asymptotic series as

$$\Psi = \Psi^{(0)} + \epsilon \Psi^{(1)} + \epsilon^2 \Psi^{(2)} + \dots \quad (19)$$

Using the above expansions for \hat{t} and Ψ in Eq. (16) and equating the coefficients of different powers of ϵ , we obtain the following equations.

$$\epsilon^{(0)} : \quad \Psi_{t_0 t_0}^{(0)} - \Psi_{zz}^{(0)} + \sin \Psi^{(0)} = 0, \quad (20a)$$

$$\begin{aligned} \epsilon^{(1)} : \quad & \Psi_{t_0 t_0}^{(1)} - \Psi_{zz}^{(1)} + \cos \Psi^{(0)} \Psi^{(1)} = g \Psi_{zz}^{(0)} \\ & + g_z \Psi_z^{(0)} - 2 \Psi_{t_0 t_1}^{(0)}, \end{aligned} \quad (20b)$$

etc.

The initial conditions for perturbation in the case of the single soliton given in Eq. (17) is written as

$$\Psi^{(0)}(z, 0) = 4 \arctan \exp mz, \quad (21a)$$

$$\Psi^{(n)}(z, 0) = 0, \quad \Psi_{t_0}^{(n)}(z, 0) = 0, \quad n = 0, 1, 2, \dots \quad (21b)$$

The equation obtained at order of $\epsilon^{(0)}$, (i.e) Eq.(20a) is just the integrable sine-Gordon equation for $\psi^{(0)}$. The single soliton solution of which can be written from Eq. (17) immediatley as

$$\Psi^{(0)}(z, t_0) = 4 \arctan \exp \zeta, \quad \zeta = m_0(z - \xi), \quad \xi_{t_0} = v_0, \quad (22)$$

where v_0 is the velocity of soliton in the t_0 -time scale. Due to perturbation, the soliton parameters namely m and ξ are now treated as functions of the slow time variables t_0, t_1, t_2, \dots . However m is treated independent of t_0 . In view of the above, Eq. (20b) becomes

$$\Psi_{t_0 t_0}^{(1)} - \Psi_{zz}^{(1)} + (1 - 2 \operatorname{sech}^2 \zeta) \Psi^{(1)} = F^{(1)}(z), \quad (23a)$$

where

$$F^{(1)}(z) = 2 [g(z) \operatorname{sech} z]_z + 4v_0 \operatorname{sech} z \times [m_{t_1} + (m^2 \xi_{t_1} - z m_{t_1}) \tanh z]. \quad (23b)$$

While writing the above equation we have used the result $\cos \Psi^{(0)} = 1 - 2 \operatorname{sech}^2 \zeta$ obtained from the solution of the unperturbed equation (20a). In order to represent everything in a co-ordinate system moving with the soliton, we transform $z = \frac{\zeta}{m} + vt_0$ and $t_0 = t_0 + \zeta$, so that Eqs. (23) and the initial conditions given in Eq. (21b) can be written as

$$\Psi_{t_0 t_0}^{(1)} - 2mv_0 \Psi_{t_0 \zeta}^{(1)} - \Psi_{\zeta \zeta}^{(1)} + (1 - 2 \operatorname{sech}^2 \zeta) \Psi^{(1)} = F^{(1)}(\zeta, t_0), \quad (24a)$$

where

$$F^{(1)}(\zeta, t_0) = 2 [g(\zeta) \operatorname{sech} \zeta]_{\zeta} + 4v_0 \operatorname{sech} \zeta \times [m_{t_1} + (m^2 \xi_{t_1} - \zeta m_{t_1}) \tanh \zeta], \quad (24b)$$

and

$$\Psi^{(1)}(\zeta, 0) = 0, \quad \Psi_{t_0}^{(1)}(\zeta, 0) = 0. \quad (24c)$$

We now introduce one more transformation $\tau = \frac{t_0}{2m} - \frac{(1+v_0)\zeta}{2}$ on the independent variable to eliminate the first term in the left-hand side of Eq. (24a). Thus on using the above transformation Eq. (24a) becomes

$$\Psi_{\tau \zeta}^{(1)} - \Psi_{\zeta \zeta}^{(1)} + (1 - \operatorname{sech}^2 \zeta) \Psi^{(1)} = F^{(1)}(\zeta, \tau), \quad (25)$$

where $F^{(1)}(\zeta, \tau)$ equals exactly the right-hand side of Eq. (24b). The solution of Eq. (25) is searched by assuming

$$\Psi^{(1)}(\zeta, \tau) = X(\zeta)T(\tau), \quad (26a)$$

$$F^{(1)}(\zeta, \tau) = X_{\zeta}(\zeta)H(\tau). \quad (26b)$$

Substituting Eqs. (26a) and (26b) in Eq. (25) we obtain

$$\frac{1}{X_{\zeta}} [X_{\zeta \zeta} + (2 \operatorname{sech}^2 \zeta - 1)X] = \frac{1}{T} [T_{\tau} - H(\tau)]. \quad (27)$$

In Eq. (27) the left-hand side is independent of τ and the right-hand side is independent of the variable ζ . Hence we can equate the left and right-hand sides of Eq. (27) to a constant say λ_0 and write

$$X_{\zeta\zeta} + (2\text{sech}^2\zeta - 1)X = \lambda_0 X_{\zeta}, \quad (28a)$$

$$T_{\tau} - \lambda_0 T = H(\tau). \quad (28b)$$

Thus, the problem of constructing the perturbed soliton at this moment turns out to be solving Eqs. (28a) and (28b) by constructing the eigen functions and finding the eigen values. It may be noted that Eq. (28a) is a generalized eigen value problem which is not a self-adjoint eigen value problem and differing from the normal eigen value problem with X_{ζ} in the right-hand side instead of X . And Eq. (28b) is a first order linear inhomogeneous differential equation which can be solved using known procedure.

C. Solving the eigen value problem

Before actually solving the eigen value equation (28a) we first consider it in a more general form given by

$$L_1 X = \lambda \tilde{X}, \quad L_1 = \partial_{\zeta\zeta} + 2\text{sech}^2\zeta - 1, \quad (29)$$

where λ is the eigen value. In order to find the adjoint eigen function to X , we consider another eigen value problem

$$L_2 \tilde{X} = \lambda X, \quad (30)$$

where the operator L_2 is still to be determined. The eigen value equations (29) and (30) can be combined to give

$$L_2 L_1 X = \lambda^2 X, \quad (31a)$$

$$L_1 L_2 \tilde{X} = \lambda^2 \tilde{X}. \quad (31b)$$

Since we already know the form of L_1 as given in Eq.(29), if we choose the operator L_2 as $L_2 = \partial_{\zeta\zeta} + 6\text{sech}^2\zeta - 1$, it can be verified that $L_1 L_2$ is the adjoint of $L_2 L_1$. Thus X and \tilde{X} are expected to be adjoint eigen functions.

Now for solving the eigen value equations (29) and (30), we choose the eigen functions X and \tilde{X} to be in the form

$$X(\zeta, k) = \gamma(\zeta, k)e^{ik\zeta}, \quad (32a)$$

$$\tilde{X}(\zeta, k) = \delta(\zeta, k)e^{ik\zeta}. \quad (32b)$$

where $\gamma(\zeta, k)$ and $\delta(\zeta, k)$ are assumed to have the asymptotic behaviour $\gamma(\zeta, k) \rightarrow$ a constant and $\delta(\zeta, k) \rightarrow$ a constant as $\zeta \rightarrow \pm\infty$ and k is the propagation constant. On using these asymptotic forms for $\gamma(\zeta, k)$ and $\delta(\zeta, k)$ in Eqs. (32a) and (32b) and then substituting the resultant $X(\zeta, k)$ and $\tilde{X}(\zeta, k)$ in Eqs. (29) and (30) we obtain the eigen value as

$$\lambda = -(k^2 + 1). \quad (33)$$

On substituting the exact forms of X and \tilde{X} from Eqs. (32a) and (32b) in Eqs. (29) and (30) we get the following set of ordinary differential equations for $\gamma(\zeta, k)$ and $\delta(\zeta, k)$.

$$L_1\gamma + 2ik\gamma_\zeta - k^2\gamma + (1 + k^2)\delta = 0, \quad (34a)$$

$$L_2\delta + 2ik\delta_\zeta - k^2\delta + (1 + k^2)\gamma = 0. \quad (34b)$$

For solving the above equations we expand $\gamma(\zeta, k)$ and $\delta(\zeta, k)$ in the following series [24].

$$\begin{aligned} \gamma(\zeta, k) = & \gamma_0 + \gamma_1 \frac{\sinh \zeta}{\cosh \zeta} + \gamma_2 \frac{1}{\cosh^2 \zeta} + \gamma_3 \frac{\sinh \zeta}{\cosh^3 \zeta} \\ & + \gamma_4 \frac{1}{\cosh^4 \zeta} + \gamma_5 \frac{\sinh \zeta}{\cosh^5 \zeta} + \dots, \end{aligned} \quad (35a)$$

$$\begin{aligned} \delta(\zeta, k) = & \delta_0 + \delta_1 \frac{\sinh \zeta}{\cosh \zeta} + \delta_2 \frac{1}{\cosh^2 \zeta} + \delta_3 \frac{\sinh \zeta}{\cosh^3 \zeta} \\ & + \delta_4 \frac{1}{\cosh^4 \zeta} + \delta_5 \frac{\sinh \zeta}{\cosh^5 \zeta} + \dots, \end{aligned} \quad (35b)$$

where the coefficients γ_j and δ_j , $j=0,1,2,\dots$ are functions of k which are to be determined. We substitute the series expansions given in Eqs. (35a) and (35b) in Eqs. (34a) and (34b) and collect the coefficients of $1, \frac{\sinh \zeta}{\cosh \zeta}, \frac{1}{\cosh^2 \zeta}, \dots$ and obtain the following algebraic equations.

$$\gamma_0 = \delta_0, \quad \gamma_1 = \delta_1, \quad (36a)$$

$$2\gamma_0 + 2ik\gamma_1 + (3 - k^2)\gamma_2 - 4ik\gamma_3 + (1 + k^2)\delta_2 = 0, \quad (36b)$$

$$6\delta_0 + 2ik\delta_1 + (3 - k^2)\delta_2 - 4ik\delta_3 + (1 + k^2)\gamma_2 = 0, \quad (36c)$$

$$-4ik\gamma_2 + (3 - k^2)\gamma_3 + (1 + k^2)\delta_3 = 0, \quad (36d)$$

$$4\delta_1 - 4ik\delta_2 + (3 - k^2)\delta_3 + (1 + k^2)\gamma_3 = 0. \quad (36e)$$

etc.

By assuming $\gamma_j = \delta_j = 0$ for $j \geq 3$, and substituting these values in Eqs.(36d) and (36e), we obtain

$$\gamma_2 = 0, \quad \delta_2 = -i\frac{\delta_1}{k}. \quad (37)$$

On substituting the results given in Eq.(37) in Eqs. (36b) and (36c) we get

$$\gamma_1 = \delta_1 = -\frac{2ik\gamma_0}{(1 - k^2)}, \quad \delta_2 = -\frac{2\gamma_0}{(1 - k^2)}. \quad (38)$$

For our convenience we choose $\gamma_0 = \delta_0 = c(1 - k^2)$ and on substituting this in the above equations, we obtain the coefficients as follows.

$$\gamma_0 = \delta_0 = c(1 - k^2), \quad (39a)$$

$$\gamma_1 = \delta_1 = -2ik, \quad \gamma_2 = 0, \quad \delta_2 = -2c. \quad (39b)$$

Here c is an arbitrary constant which will be determined. Using the above values in Eqs. (35a) and (35b), and then in Eqs.(32a) and (32b), we finally obtain

$$X(\zeta, k) = c(1 - k^2 - 2ik \tanh \zeta)e^{ik\zeta}, \quad (40a)$$

$$\tilde{X}(\zeta, k) = c(1 - k^2 - 2ik \tanh \zeta - 2\text{sech}^2 \zeta)e^{ik\zeta}. \quad (40b)$$

On comparing Eqs. (40a) and (40b) we can write

$$\tilde{X}(\zeta, k) = \frac{X_\zeta(\zeta, k)}{ik}. \quad (41)$$

Using Eq.(41) in the right-hand side of Eq.(29) and comparing the resultant equation with (28a), we can write down the eigen value λ_0 as

$$\lambda_0 = i \frac{(1 + k^2)}{k}. \quad (42)$$

Now to determine the constant c we use the orthonormality relation between $X(\zeta, k)$ and $\tilde{X}(\zeta, k)$ given by

$$\int_{-\infty}^{\infty} X(\zeta, k) \tilde{X}^*(\zeta, k') d\zeta = \delta(k - k'). \quad (43)$$

On substituting the eigen functions $X(\zeta, k)$ and $\tilde{X}(\zeta, k)$ given in Eqs. (40a) and (40b) respectively in Eq.(43) and after evaluating the integral we obtain

$$2\pi c^2 [(1 - k^2)(1 - k'^2) + 4kk'] \delta(k - k') = \delta(k - k'), \quad (44)$$

which gives $c^2 = \frac{1}{2\pi}(1 + k^2)^{-2}$. The correct form of the eigen functions $X(\zeta, k)$ and $\tilde{X}(\zeta, k)$ is written down after using the above value of c in Eqs. (40a) and (40b).

$$X(\zeta, k) = \frac{(1 - k^2 - 2ik \tanh \zeta)}{\sqrt{2\pi}(1 + k^2)} e^{ik\zeta}, \quad (45a)$$

$$\tilde{X}(\zeta, k) = \frac{(1 - k^2 - 2ik \tanh \zeta - 2\text{sech}^2 \zeta)}{\sqrt{2\pi}(1 + k^2)} e^{ik\zeta}. \quad (45b)$$

It can be verified that the operator L_2 also has the following two discrete eigen functions.

$$\tilde{X}_0(\zeta) = (1 - \zeta \tanh \zeta) \text{sech} \zeta, \quad (46a)$$

$$\tilde{X}_1(\zeta) = \text{sech} \zeta \tanh \zeta. \quad (46b)$$

It may be further noted that the eigen function \tilde{X}_1 corresponds to the discrete eigen value $\lambda = 0$. That is

$$L_2 \tilde{X}_1(\zeta) = 0. \quad (47)$$

D. Complete set of orthonormal bases

Having found the eigen functions $X(\zeta, k)$ and $\tilde{X}(\zeta, k)$, we now check the completeness of them by writing

$$\int_{-\infty}^{\infty} X(\zeta, k)\tilde{X}^*(\zeta', k)dk + f(\zeta) = \delta(\zeta - \zeta'), \quad (48)$$

where $f(\zeta)$ is an arbitrary function to be determined. First we evaluate the integral in the left-hand side of Eq. (48) after substituting the values of the eigen functions $X(\zeta, k)$ and $\tilde{X}(\zeta, k)$ given in Eqs. (45a) and (45b). Thus we have the following integrals to evaluate.

$$\begin{aligned} \int_{-\infty}^{\infty} X(\zeta, k)\tilde{X}^*(\zeta', k)dk &= \delta(\zeta - \zeta') \\ &- \frac{1}{\pi} \left[\int_{-\infty}^{\infty} \frac{dk}{(1+k^2)} e^{ik(\zeta-\zeta')} \right. \\ &\quad \times \{2 - ik(\tanh \zeta - \tanh \zeta') \\ &\quad \left. - \operatorname{sech}^2 \zeta'\} - 2 \int_{-\infty}^{\infty} \frac{dk}{(1+k^2)^2} \right. \\ &\quad \times e^{ik(\zeta-\zeta')}(1 - ik \tanh \zeta) \\ &\quad \left. \times (ik + \tanh \zeta') \tanh \zeta' \right]. \end{aligned} \quad (49)$$

The integrals in the right-hand side of Eq.(49) are evaluated by the aid of residue theorem. It may be noted that the integrands in these two integrals as functions of the complex variable k are analytic everywhere in the complex k -plane except at the two poles $k = \pm i$ of first and second order respectively. Let R_1 and R_2 be the residues corresponding to the functions $\frac{1}{(1+k^2)}e^{ik(\zeta-\zeta')}\{2 - ik(\tanh \zeta - \tanh \zeta') - \operatorname{sech}^2 \zeta'\}$ and $\frac{1}{(1+k^2)^2}e^{ik(\zeta-\zeta')}(1 - ik \tanh \zeta)(ik + \tanh \zeta') \tanh \zeta'$ in Eq. (49) at the pole $k = i$ of first and second order respectively. On calculating the residues using standard procedure we obtain

$$R_1 = \frac{-i}{2} [2 + \tanh \zeta - \tanh \zeta' - \operatorname{sech}^2 \zeta] e^{(\zeta-\zeta')}, \quad (50a)$$

$$\begin{aligned} R_2 &= \frac{-i}{4} [(1 - \zeta + \zeta')(\tanh \zeta - \tanh \zeta') - (\zeta - \zeta') \\ &\quad \times (1 - \tanh \zeta \tanh \zeta')] e^{(\zeta-\zeta')}. \end{aligned} \quad (50b)$$

On summing up the above results Eq. (49) becomes

$$\begin{aligned} \int_{-\infty}^{\infty} X(\zeta, k)\tilde{X}^*(\zeta', k)dk &= \delta(\zeta - \zeta') \\ &- [\operatorname{sech} \zeta \operatorname{sech} \zeta' (1 - \zeta' \tanh \zeta') \\ &\quad + \zeta \operatorname{sech} \zeta \operatorname{sech} \zeta' \tanh \zeta'], \end{aligned} \quad (51)$$

which can be identified as

$$\begin{aligned} \int_{-\infty}^{\infty} X(\zeta, k)\tilde{X}^*(\zeta', k)dk &= \delta(\zeta - \zeta') \\ &- [X_0(\zeta)\tilde{X}_0(\zeta') + X_1(\zeta)\tilde{X}_1(\zeta')], \end{aligned} \quad (52)$$

upon using the values of $\tilde{X}_0(\zeta)$ and $\tilde{X}_1(\zeta)$ as given in Eqs.(46a) and (46b). By substituting Eq.(52) in Eq.(48), we can evaluate the following value of $f(\zeta)$ in terms of the discrete orthogonal states.

$$f(\zeta) = \sum_{j=0,1} X_j(\zeta)\tilde{X}_j(\zeta). \quad (53)$$

Thus, by comparing Eqs.(51) and (52), we can write two additional orthogonal discrete states given by

$$X_0(\zeta) = \operatorname{sech}\zeta, \quad (54a)$$

$$X_1(\zeta) = \zeta \operatorname{sech}\zeta. \quad (54b)$$

It may be checked that the following relations exist between the discrete states $X_0(\zeta)$, $\tilde{X}_0(\zeta)$, $X_1(\zeta)$ and $\tilde{X}_1(\zeta)$.

$$L_1 X_0 = 0, \quad L_1 X_1(\zeta) = -2\tilde{X}_1(\zeta), \quad L_2 \tilde{X}_0(\zeta) = 2X_0(\zeta), \quad (55)$$

in addition to the relation given in Eq.(47). In conclusion, we have a set of two complete orthonormal bases $\{X\}$ and $\{\tilde{X}\}$ given by $\{X(\zeta, k), X_0(\zeta), X_1(\zeta)\}$ and $\{\tilde{X}(\zeta, k), \tilde{X}_0(\zeta), \tilde{X}_1(\zeta)\}$ respectively. These set of orthonormal basis functions will be used to construct the perturbed soliton solution.

E. Evaluation of $T(\zeta)$

Having solved Eq.(28a) by finding $X(\zeta)$, in order to construct $\psi^{(1)}(\zeta, \tau)$, we now find $T(\tau)$ by solving Eq. (28b). For this first we rewrite Eq. (28b) by replacing the function $H(\tau)$ in the right-hand side using Eqs. (26b) and (38).

$$T_\tau - \lambda_0 T = \frac{F^{(1)}(\zeta, \tau)}{ik\tilde{X}(\zeta, k)}. \quad (56)$$

On multiplying and dividing the right-hand side of Eq. (56) by $X^*(\zeta, k)$ and on integrating with respect to ζ between the limits $-\infty$ to $+\infty$ we obtain due to orthonormality of the functions X and \tilde{X} (see Eq.(43)) the following equation.

$$T_\tau - \lambda_0 T = \frac{1}{ik} \int_{-\infty}^{\infty} F^{(1)}(\zeta, \tau) X^*(\zeta, k) d\zeta, \quad (57)$$

which can be explicitly written after substituting the values of $F^{(1)}(\zeta, \tau)$ and $X^*(\zeta, k)$ from Eqs. (24b) and (45a) respectively as

$$\begin{aligned} T_\tau - \lambda_0 T = & \frac{2}{i\sqrt{2\pi}k(1+k^2)} \int_{-\infty}^{\infty} d\zeta \left([g(\zeta)\operatorname{sech}\zeta]_\zeta \right. \\ & \left. + 2v_0 \operatorname{sech}\zeta [m_{t_1} + (m^2\xi_{t_1} - \zeta m_{t_1}) \tanh \zeta] \right) \\ & \times (1 - k^2 + 2ik \tanh \zeta) e^{-ik\zeta}. \end{aligned} \quad (58)$$

On solving the above equation using standard procedure, we obtain

$$T(\tau, k) = C(k)e^{\lambda_0\tau} - \frac{2}{i\sqrt{2\pi}\lambda_0k(1+k^2)} \int_{-\infty}^{\infty} d\zeta \left([g(\zeta)\text{sech}\zeta]_{\zeta} + 2v_0 \text{sech}\zeta [m_{t_1} + (m^2\xi_{t_1} - \zeta m_{t_1}) \times \tanh \zeta] \right) (1 - k^2 + 2ik \tanh \zeta) e^{-ik\zeta}, \quad (59)$$

where $C(k)$ is a constant which can be found by using the initial condition $T(\tau, k) = 0$ when $\tau \rightarrow -\frac{(1+v)\zeta}{2}$. Thus we obtain

$$C(k) = \frac{2}{i\sqrt{2\pi}\lambda_0k(1+k^2)} \int_{-\infty}^{\infty} d\zeta \left([g(\zeta)\text{sech}\zeta]_{\zeta} + 2v_0 \text{sech}\zeta [m_{t_1} + (m^2\xi_{t_1} - \zeta m_{t_1}) \tanh \zeta] \right) \times (1 - k^2 + 2ik \tanh \zeta) e^{\lambda_0(1+v_0)\frac{\zeta}{2} - ik\zeta}, \quad (60)$$

and hence

$$T(\tau, k) = \frac{2}{\sqrt{2\pi}i\lambda_0k(1+k^2)} \int_{-\infty}^{\infty} d\zeta' \left([g(\zeta')\text{sech}\zeta']_{\zeta'} + 2v_0 \text{sech}\zeta' [m_{t_1} + (m^2\xi_{t_1} - \zeta' m_{t_1}) \tanh \zeta'] \right) \times (1 - k^2 + 2ik \tanh \zeta') e^{-ik\zeta'} \left(e^{\lambda_0[\tau - \frac{(1+v_0)\zeta'}{2}]} - 1 \right). \quad (61)$$

The allowed discrete values of T will be determined in the next section while constructing the perturbed part of the soliton $\psi^{(1)}(\zeta, \tau)$ using the values of $X(\zeta)$ and $T(\tau)$.

F. Perturbation of soliton

As mentioned, we now write down the first order perturbation correction $\Psi^{(1)}(\zeta, \tau)$ in terms of the basis functions $\{X\} \equiv \{X(\zeta, k), X_0(\zeta), X_1(\zeta)\}$ and $\{\tau\} \equiv \{T(\tau, k), T_0(\tau), T_1(\tau)\}$. As per Eq.(26a), in terms of the basis functions the perturbed part of the soliton can be written as

$$\Psi^{(1)}(\zeta, k) = \int_{-\infty}^{\infty} X(\zeta, k)T(\tau, k)dk + \sum_{j=0,1} X_j(\zeta)T_j(\tau). \quad (62)$$

However, it should be noted that in the basis $\{T\}$, $T_0(\tau)$ and $T_1(\tau)$ are yet to be determined. Therefore before evaluating the values of $\Psi^{(1)}(\zeta, k)$, we determine $T_0(\tau)$ and $T_1(\tau)$. This is carried out by substituting Eq.(62) in Eq.(25) which finally becomes

$$\int_{-\infty}^{\infty} ik [T_{\tau}(\tau, k) - \lambda_0 T(\tau, k)] \tilde{X}(\zeta, k) dk + T_{1\tau}(\tau) \tilde{X}_0(\zeta) - [T_{0\tau}(\tau) - 2T_1(\tau)] \tilde{X}_1(\zeta) = F^{(1)}(\zeta, \tau), \quad (63)$$

upon using Eqs.(29),(42),(47) and (55). Now multiplying Eq.(61) by $X^*(\zeta, k)$, $X_0(\zeta)$ and $X_1(\zeta)$ separately and using the orthonormal relations such as $\int_{-\infty}^{\infty} \tilde{X}(\zeta, k)X^*(\zeta, k)dk =$

1, $\int_{-\infty}^{\infty} \tilde{X}(\zeta, k) X_j(\zeta) d\zeta \equiv \int_{-\infty}^{\infty} X(\zeta, k) \tilde{X}_j(\zeta) d\zeta = 0$, $\int_{-\infty}^{\infty} X_j(\zeta) \tilde{X}_l(\zeta) d\zeta = \delta_{jl}$, $j, l = 0, 1$, we get

$$T_\tau(\tau, k) - \lambda_0 T(\tau, k) = \frac{1}{ik} \int_{-\infty}^{\infty} F^{(1)}(\zeta, \tau) X^*(\zeta, k) d\zeta, \quad (64a)$$

$$T_{1\tau}(\tau) = \int_{-\infty}^{\infty} F^{(1)}(\zeta, \tau) X_0(\zeta) d\zeta, \quad (64b)$$

$$T_{0\tau}(\tau) - 2T_1(\tau) = - \int_{-\infty}^{\infty} F^{(1)}(\zeta, \tau) X_1(\zeta) d\zeta. \quad (64c)$$

As $F^{(1)}(\zeta, \tau)$ given in Eq. (24b) does not contain time ' τ ' explicitly, the right-hand side of Eqs. (64a-c) also should be independent of time. Then it is easy to verify that for the values of $F^{(1)}(\zeta, \tau)$, $X^*(\zeta, k)$, $T(\tau, k)$ and λ_0 given respectively in Eqs. (24b), (45a), (61) and (42), Eq. (64a) satisfies identically. As the right-hand sides of Eqs. (64b) and (64c) are also independent of time, they give rise to secularities and hence the nonsecular conditions can be written as

$$\int_{-\infty}^{\infty} F^{(1)}(\zeta, \tau) X_0(\zeta) d\zeta = 0, \quad (65a)$$

$$\int_{-\infty}^{\infty} F^{(1)}(\zeta, \tau) X_1(\zeta) d\zeta = 0. \quad (65b)$$

Using Eqs. (65a) and (65b) back in Eqs. (64b) and (64c), we obtain $T_1(\tau) = 0$ and $T_0(\tau) = C_1$ which has to be determined. For this, we substitute $T_1(\tau) = 0$ in Eq. (64c) and integrate with respect to τ to obtain

$$T_0(\tau) \equiv C_1 = (1 + v) \int_{-\infty}^{\infty} d\zeta \left([g(\zeta) \operatorname{sech}\zeta]_\zeta + 2v_0 \operatorname{sech}\zeta \right) \times [m_{t_1} + (m^2 \xi_{t_1} - \zeta m_{t_1}) \tanh \zeta] \zeta^2 \operatorname{sech}\zeta. \quad (66)$$

G. Variation of soliton parameters

We now estimate the nonsecularity conditions (65a) and (65b) by evaluating the integrals after substituting the values of $F^{(1)}(\zeta, \tau)$, $X_0(\zeta)$ and $X_1(\zeta)$ respectively from Eqs.(24b), (54a) and (54b). The results give

$$m_{t_1} = -\frac{1}{2v_0} \int_{-\infty}^{\infty} [g(\zeta) \operatorname{sech}\zeta]_\zeta \operatorname{sech}\zeta d\zeta, \quad (67a)$$

$$\xi_{t_1} = -\frac{1}{2m^2 v_0} \int_{-\infty}^{\infty} [g(\zeta) \operatorname{sech}\zeta]_\zeta \zeta \operatorname{sech}\zeta d\zeta. \quad (67b)$$

Eq. (67a) describes the time evolution of the inverse of the width of the soliton and Eq. (67b) gives the velocity of the soliton. $g(\zeta)$ that appears in the above nonsecularity relation is related to the stacking energy of DNA. In order to evaluate the integrals in Eqs. (67a) and (67b) explicitly we have to substitute specific value for $g(\zeta)$. We consider the values of $g(\zeta)$ in the

form of localized and periodic functions. A localized $g(\zeta)$ corresponds to the intercalation of a compound between neighbouring base pairs without disturbing the base pairs and their sequence in the DNA double helical chain. The periodic nature of $g(\zeta)$ represents a periodic repetition of similar base pairs along the helical chain. We consider the localized form of $g(\zeta)$ as (i) $g(\zeta) = \text{sech}\zeta$ and (ii) $g(\zeta) = \tanh\zeta$ and the periodic form of $g(\zeta)$ as (iii) $g(\zeta) = \cos\zeta$. Therefore we substitute the above values of $g(\zeta)$ one by one in Eqs. (67a) and (67b) and evaluate the integrals in the right-hand side to understand the time evolution of the width of the soliton and its velocity. At this point it is worth mentioning that Dandoloff and Saxena [44] realized that in the case of XY-spin chains the model of which identifies with our plane-base rotator model, the ansatz $g(\zeta) = \text{sech}\zeta$ energetically favours the deformation of spin chains.

When we substitute $g(\zeta) = \text{sech}\zeta$ in Eqs. (67a) and (67b) and on evaluating the integrals, we obtain

$$m_{t_1} = 0, \quad \xi_{t_1} = \frac{\pi}{6m^2v_0}. \quad (68)$$

The above equations can be rewritten in terms of the original time variable \hat{t} by using the transformation $\frac{\partial}{\partial \hat{t}} = \frac{\partial}{\partial t_0} + \epsilon \frac{\partial}{\partial t_1}$ or in other words $m_{\hat{t}} = m_{t_0} + \epsilon m_{t_1}$ and $\xi_{\hat{t}} = \xi_{t_0} + \epsilon \xi_{t_1}$. As m is independent of t_0 ($m_{t_0} = 0$) and $\xi_{t_0} = v_0$, we can write

$$m = m_0, \quad \xi_{\hat{t}} \equiv v = v_0 + \frac{\epsilon\pi}{6m_0^2v_0}, \quad (69)$$

where $1/m_0$ is the initial width of the soliton. The first of Eq.(69) says that when $g(\zeta) = \text{sech}\zeta$ the width (m^{-1}) of the soliton remains constant. However from the second of Eq.(69), we find that the velocity of the soliton gets a correction. As the correction term is a definite positive quantity the velocity of the soliton increases in this case. Interestingly, the amount of increment in velocity depends on the width and velocity of the soliton. Wider the soliton, greater the increment in velocity due to inhomogeneity. Also slowly moving solitons gain more speed.

Next, we substitute $g(\zeta) = \tanh\zeta$ in Eqs. (67a) and (67b) and evaluate the integrals to obtain

$$m_{t_1} = -\frac{1}{3v_0}, \quad \xi_{t_1} = 0, \quad (70)$$

so that

$$m = m_0 - \frac{1}{3v_0}\hat{t}, \quad \xi_{\hat{t}} \equiv v = v_0. \quad (71)$$

From Eq. (71) we observe that the width(m^{-1}) of the kink-soliton in this case changes linearly with respect to time whereas the velocity of the soliton remains constant. In fact the width of the soliton increases due to the above inhomogeneity as time passes on. It may be noted that increment in the width is more for slow moving solitons.

We then substitute the periodic function $g(\zeta) = \cos \zeta$ in Eqs.(67a) and (67b) and evaluate the integrals to obtain

$$m_{t_1} = 0, \quad \xi_{t_1} = \frac{\pi^2}{16m^2v_0}. \quad (72)$$

From the above the parameters m and ξ can be written in terms of the original variable \hat{t} after solving Eq.(72) as

$$m = m_0, \quad \xi_{\hat{t}} \equiv v = v_0 + \frac{\epsilon\pi^2}{16m^2v_0}. \quad (73)$$

From Eq. (73) we find that the width of the soliton in this case remains constant and the soliton velocity increases similar to the case $g(\zeta) = \text{sech}\zeta$. On comparing Eqs. (69) and (73), we observe that the increases in velocity of the soliton is more in the case when $g(\zeta) = \text{sech}\zeta$.

H. First order perturbed soliton

Now, we explicitly construct the first order perturbation correction to the one soliton for the different cases of $g(\zeta)$ by substituting the values of the basis functions $\{X\} \equiv \{X(\zeta, k), X_0(\zeta), X_1(\zeta)\}$ and $\{T\} \equiv \{T(\tau, k), T_0(\tau), T_1(\tau)\}$ after using the values of $F^{(1)}(\zeta, \tau), m_{t_1}$ and ξ_{t_1} for the respective $g(\zeta)$ values in Eq. (62). Thus in the case of $g(\zeta) = \text{sech}\zeta$, we substitute the values of $X(\zeta, k), X_0(\zeta)$ and $X_1(\zeta)$ from Eqs. (45a), (54a) and (54b) and $T(\tau, k), T_0(\tau)$ from Eqs. (61) and (66) and $F^{(1)}(\zeta, \tau)$ from Eq. (24b) and use the values of m_{t_1} and ξ_{t_1} from Eqs. (68) in Eq. (62) to obtain

$$\begin{aligned} \Psi^{(1)}(\zeta, t_0) = & -\frac{1}{3\pi} \int_{-\infty}^{\infty} \frac{dk}{(1+k^2)^3} (1-k^2 - 2ik \tanh \zeta) \\ & \times e^{ik\zeta} \int_{-\infty}^{\infty} d\zeta (1-k^2 + 2ik \tanh \zeta) \\ & \times (\pi - 6\text{sech}\zeta) \text{sech}\zeta \tanh \zeta \\ & \times \left[e^{-ik\zeta} - e^{i\frac{(1+k^2)}{k}\alpha} e^{i\beta\zeta} \right]. \end{aligned} \quad (74)$$

where $\alpha = \frac{t_0 - m(1+v_0)\zeta}{2m}$ and $\beta = \frac{(1+v_0)(1+k^2)}{2k} - k$. While writing the above, we have also used $T_1(\tau) = 0, \tau = \frac{1}{2m}[t_0 - m(1+v_0)\zeta]$ and the eigen value $\lambda_0 = \frac{i(1+k^2)}{k}$. The integrals in the right-hand side of Eq.(74) can be evaluated using the standard residue theorem [58]. The details are given in Appendix-A. The final form of $\Psi^{(1)}(\zeta, t_0)$ after evaluating the integrals becomes

$$\begin{aligned} \Psi^{(1)}(\zeta, t_0) \approx & \frac{80}{27\sqrt{2}} \sqrt{\text{sech}\zeta} e^{-\frac{3\zeta}{2}} + \frac{64}{27\sqrt[3]{2}} \tanh \zeta \\ & \times \sqrt[3]{\text{sech}\zeta} e^{-\frac{5}{3}\zeta} + \frac{\pi}{6v^2} [2v(1+v)\zeta \\ & + v^2 + 4\alpha v - 1] \text{sech}\zeta. \end{aligned} \quad (75)$$

While constructing the above perturbed solution, we have used the values of m 's and ξ 's and of course the corresponding $F^{(1)}(\zeta, \tau)$ values. Finally, the perturbed one soliton solution that is

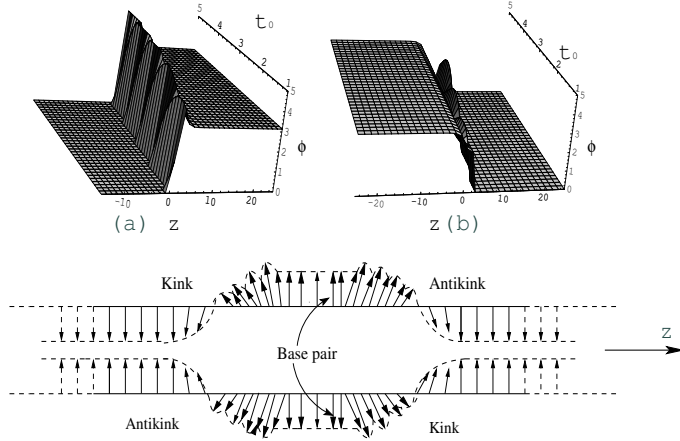


FIG. 4: (a) The perturbed kink-soliton and (b) the perturbed antikink-soliton for the inhomogeneity $g(z) = \text{sech}z$ and $v_0 = 0.4, m_0 = 1.1095$. (c) A sketch of the base pair opening in DNA double helix with fluctuation

$\Psi(z, t_0) = \Psi^{(0)}(z, t_0) + \Psi^{(1)}(z, t_0)$ (choosing $\epsilon = 1$) is written using Eqs. (22) and (75) as

$$\begin{aligned}
\Psi(z, t_0) \approx & 4 \arctan \exp[\pm m_0(z - v_0 t_0)] + \frac{80}{27\sqrt{2}} \\
& \times \sqrt{\text{sech}[\pm m(z - vt_0)]} e^{\mp \frac{3(m(z-vt_0))}{2}} + \frac{64}{27\sqrt[3]{2}} \\
& \times \tanh[\pm m(z - vt_0)] \sqrt[3]{\text{sech}[\pm m(z - vt_0)]} e^{\mp \frac{5}{3}m(z-vt_0)} \\
& + \frac{\pi}{6mv^2} [m(v^2 - 1) + 2t_0v] \text{sech}[\pm m(z - vt_0)]. \tag{76}
\end{aligned}$$

In Eq.(76) while the upper sign corresponds to perturbed kink soliton the lower sign represents the perturbed antikink soliton. The rotation of bases $\phi(z, t_0)$ can be immediately written down by using the relation $\phi = \frac{\Psi}{2}$. In Figs (4a,b) we plot $\phi(z, t_0)$ (rotation of bases under perturbation) for the parametric choices $v_0 = 0.4$ and $m_0 = 1.1095$. From the figure, we observe that there appears fluctuation in the form of a train pulses closely resembling the shape of the inhomogeneity profile in the width of the soliton as time progresses. Also, as time passes, the amplitude of the pulses generating this fluctuation increases. However in the asymptotic region of the soliton there is no change in the topological character and no fluctuation exists in that region. It shows that the localized inhomogeneity in stacking energy in DNA in the form of a pulse ($g(z) = \text{sech}z$) does not affect very much the opening of bases expect fluctuations in the form of train of pulses in the localized regions of the kink and antikink. We have schematically represented this in Fig.(4c)

We then repeat the procedure for constructing the perturbed one soliton solution $\Psi(\zeta, t_0)$ for the case $g(\zeta) = \tanh \zeta$. By substituting the above value of $g(\zeta)$ in Eq.(24b) and using the

corresponding m_{t1} and ξ_{t1} values from the Eq.(71), we get the perturbation correction as

$$\begin{aligned}
\Psi^{(1)}(\zeta, t_0) = & \frac{1}{3\pi} \int_{-\infty}^{\infty} \frac{dk}{(1+k^2)^3} (1-k^2 - 2ik \tanh \zeta) \\
& \times e^{ik\zeta} \int_{-\infty}^{\infty} d\zeta \left[(1-k^2 + 2ik \tanh \zeta) \right. \\
& \quad \times (6\operatorname{sech}^2 \zeta + 2\zeta \tanh \zeta - 5)\operatorname{sech} \zeta \\
& \quad \left. (e^{-ik\zeta} - e^{i\frac{(1+k^2)}{k}\alpha} e^{i\beta\zeta}) \right] + (1+v)\operatorname{sech} \zeta \\
& \times \int_{-\infty}^{\infty} d\zeta \zeta^2 (6\operatorname{sech}^2 \zeta + 2\zeta \tanh \zeta - 5)\operatorname{sech}^2 \zeta. \tag{77}
\end{aligned}$$

After evaluating the integrals in Eq.(77), the details of which are given in Appendix-B, we finally obtain the perturbed soliton $\Psi(z, t_0)$

$$\begin{aligned}
\Psi(z, t_0) \approx & 4\operatorname{arc tan} \exp[\pm m_0(z - v_0 t_0)] \\
& + \frac{1}{18v_0^4(t_0 - 3m_0 v_0)^2} \left([\pm 2v_0(t_0 - 3m_0 v_0)^2 \right. \\
& \times [3m_0 v_0(v_0^2 - 1) + (1 + 5v_0^2)t_0]z + a_1 + a_2 t_0 \\
& + a_3 t_0^2 \pm 18m_0 v_0^3(1 + 3v_0^2)t_0^3 \mp 2v_0^2(1 + 5v_0^2)t_0^4 \\
& \left. \operatorname{sech}[\pm \frac{(t_0 - 3m_0 v_0)}{3v_0}(z - v_0 t_0)] + 6v_0^2(v_0^2 - 1) \right. \\
& \times [2t_0^2 - 12v_0 m_0 t_0 + 9m_0^2 v_0^2] e^{\mp(m_0 - \frac{t_0}{3m_0})(z - v_0 t_0)} \\
& \quad \left. + \frac{135}{8} \left[\frac{1}{\sqrt{2}} e^{-\frac{1}{2}\mp(m_0 - \frac{t_0}{3m_0})(z - v_0 t_0)} \right. \right. \\
& \quad \times \sqrt{\operatorname{sech}[\pm(m_0 - \frac{t_0}{3m_0})(z - v_0 t_0)]} \\
& \quad \left. - \frac{1}{\sqrt[3]{2}} \sqrt[3]{\operatorname{sech}[\pm(m_0 - \frac{t_0}{3m_0})(z - v_0 t_0)]} \right. \\
& \quad \quad \left. \times e^{-\frac{2}{3}\mp(m_0 - \frac{t_0}{3m_0})(z - v_0 t_0)} \right. \\
& \quad \times (1 + \frac{1}{10} \tanh[\pm(m_0 - \frac{t_0}{3m_0})(z - v_0 t_0)] \\
& \quad \quad \left. \times e^{-2\mp(m_0 - \frac{t_0}{3m_0})(z - v_0 t_0)} \right) \Big]. \tag{78}
\end{aligned}$$

where $a_1 = 9m_0^2 v_0^2(1 + v_0)[-9 + 24v_0^2 + 24v_0^3 + (3\pi^2 - 15)v_0^4 + 2(\pi^2 - 12)v_0^5 - \pi^2 v_0^6]$, $a_2 = 6m_0 v_0[18 - 30v_0^2 - 48v_0^3 - (15 \mp 9m_0^2 + 6\pi^2)v_0^4 + 4(12 - \pi^2)v_0^5 + (2\pi^2 \mp 9m_0^2)]$ and $a_3 = \{-18 + 12v_0^2 + 48v_0^3 + 6(1 \mp 9m_0^2 + \pi^2)v_0^4 + 4(\pi^2 - 12)v_0^5 + (\mp 54m_0^2 - 2\pi^2)\}$. As in the previous case in Eq.(79) the upper and lower signs corresponds to perturbed kink and antikink solitons. After finding ϕ using the value of Ψ from Eq.(79), we plot the perturbed kink and antikink solitons for the rotation of bases in Figs. 5(a) and 5(b) by choosing the same parametric values for v_0 and m_0 as in the previous case. From Fig.(5), we observe that when the inhomogeneity appears in the form $g(z) = \tanh z$ it increases the width of the soliton there

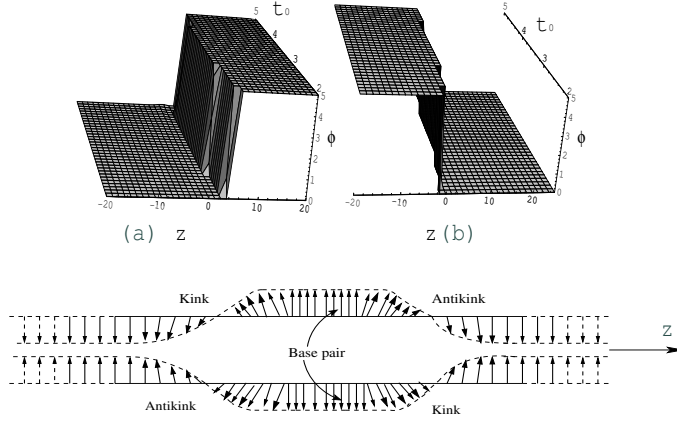


FIG. 5: The perturbed (a) kink-soliton and (b) antikink-soliton for the inhomogeneity $g(z) = \tanh z$ with $v_0 = 0.4$ and $m_0 = 1.1095$. (c) A sketch of the elongated base pair opening state.

by involving more number of bases to participate in the open state. This happens because, the topological character of the inhomogeneity is same as the kink-antikink soliton of the unperturbed system. Also as the profile of the inhomogeneity matches with the kink-antikink soliton only a small fluctuation is generated in the width of the soliton as shown in Figs.(5a,b). In Fig. (5c) we have given a sketch of the open state of base pairs with the small fluctuation during the opening process.

The first order correction in the case of $g(\zeta) = \cos \zeta$ is written as

$$\begin{aligned}
\Psi^{(1)}(\zeta, t_0) \approx & \frac{1}{\pi} \int_{-\infty}^{\infty} \frac{dk}{(1+k^2)^3} (1-k^2 - 2ik \tanh \zeta) \\
& \times e^{ik\zeta} \int_{-\infty}^{\infty} d\zeta (1-k^2 + 2ik \tanh \zeta) \\
& \times [\sin \zeta + (\cos \zeta - \frac{\pi^2}{8}) \tanh \zeta] \operatorname{sech} \zeta \\
& \times \{ e^{i\frac{(1+k^2)}{k}\alpha} e^{i\beta\zeta} - e^{-ik\zeta} \} + (1+v) \operatorname{sech} \zeta \\
& \times \int_{-\infty}^{\infty} d\zeta \zeta^2 [\sin \zeta + (\cos \zeta - \frac{\pi^2}{8}) \tanh \zeta] \\
& \times \operatorname{sech}^2 \zeta.
\end{aligned} \tag{79}$$

The details of values of the integrals in the above equation are given in Appendix-C. The perturbed kink (upper sign)-antikink (lower sign) one soliton solution in this case is finally

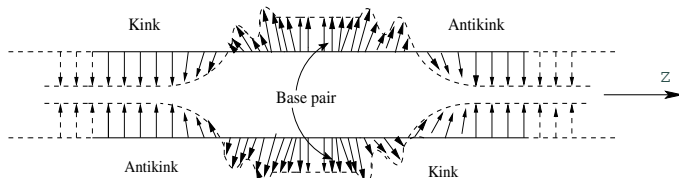
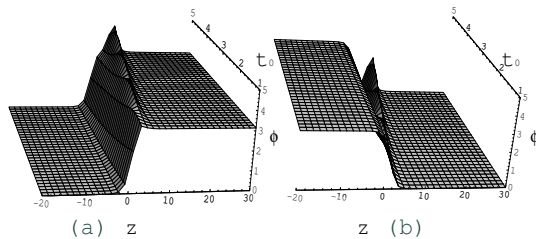


FIG. 6: The perturbed (a) kink-soliton and (b) antikink-soliton for the inhomogeneity $g(z) = \cos z$ with $v_0 = 0.4$ and $m_0 = 1.1095$. (c) A sketch of the open state configuration in DNA with small fluctuations

obtained as

$$\begin{aligned} \Psi(z, t_0) \approx & 4 \arctan \exp[\pm m_0(z - v_0 t_0)] \\ & + \frac{\pi^2}{16mv^2} [m + 2vt_0] \operatorname{sech}[m(z - vt_0)]. \end{aligned} \quad (80)$$

After finding $\phi(z, t_0)$ from the relation $\phi = \frac{\Psi}{2}$ we plot it in Figs. (6a,b) for the same values of the parameters as before. From the figures we observe that periodic oscillations appear as fluctuation in the width of the soliton without any change asymptotically.

IV. CONCLUSION

In this paper we studied the nonlinear dynamics of DNA double helix with stacking inhomogeneity by considering the dynamic plane-base rotator model. The dynamical equation which finally appeared in the form of a perturbed sine-Gordon equation was derived from a suitable Hamiltonian in analogy with Heisenberg model of inhomogeneous anisotropic coupled spin chains or spin ladder with ferromagnetic legs and antiferromagnetic rung coupling in the continuum limit. In the unperturbed limit which is also the homogeneous limit, the dynamics is governed by the kink-antikink soliton of the integrable sine-Gordon equation which represents the open state configuration of base pairs in DNA double helix. To understand the effect of stacking energy inhomogeneity on the open state configuration of base pairs we carry out a multiple scale soliton perturbation theory. For implementing this we linearized the perturbed sine-Gordon equation using multiple-scale expansion to obtain linearized equations in the form of eigen value problems. The perturbed kink-antikink soliton solutions were constructed for

different forms of inhomogeneities by solving the associated eigen value problem. By using the complete set of eigen functions thus obtained as the basis functions the perturbed solutions were constructed.

The perturbation not only modifies the shape of the soliton but also undergoes a slow time change of the soliton parameters namely the width and velocity. for the different forms of the inhomogeneity chosen. We, chose the inhomogeneity in the form of localized and periodic functions. The results show that when the inhomogeneity is either in the form $g(z) = sechz$ or $g(z) = \cos z$, the width of the soliton remains constant. However, in this case the speed of the soliton is increased by getting a correction that is proportional to the square of the width of the soliton and inversely proportional to it's initial velocity. On the other hand when the inhomogeneity is in the form $g(z) = \tanh z$, which coincides with the shape of the kink soliton of the unperturbed system, the inhomogeneity reduces the width of the soliton linearly with respect to time. However the velocity of the soliton remains the same in this case. From the perturbed solutions corresponding to different inhomogeneities (see Figs. 4,5,6)we observe that the perturbation due to inhomogeneity in stacking energy along the strands introduces fluctuations only in the width of the solitons. The nature of the fluctuation varies depending on the type of inhomogeneity. In particular, when the inhomogeneity is chosen as $g(z) = sechz$, we found that fluctuation in the form of pulse trains resembling the shape of the inhomogeneity is generated in the width of the soliton representing open state configuration, the amplitude of which increases as time passes on. In a similar way, when the inhomogeneity is of the form $g(z) = \cos z$, the fluctuation appears in the form of periodic oscillation in the width of the soliton. However when $g(z) = \tanh z$, since the shape of the inhomogeneity coincides with the profile of the soliton, only very small fluctuation occurs. In all these cases asymptotically the kink-antikink soliton shape is preserved. The results indicate that inhomogeneity in stacking energy in DNA double helix can introduce (i) small fluctuations in the process of opening and closing of base pairs (ii) increase or decrease the number of base pairs participating in the open state configuration and (iii) change the speed with which the open state configuration can travel along the double helical chain. It is also important to analyse the nonlinear dynamics of DNA double helix when the hydrogen bonding energy depends on the distance between the bases (inhomogeneity in hydrogen bonding) which is under progress.

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**APPENDIX A: EVALUATION OF INTEGRALS IN EQ.(74) USING RESIDUE
THEOREM**

In this appendix we evaluate the integrals found in Eq.(74) using standard residue theorem. Eq.(74) is of the form

$$\begin{aligned} \Psi^{(1)}(\zeta, t_0) = & -\frac{1}{3\pi} \int_{-\infty}^{\infty} \frac{dk}{(1+k^2)^3} (1-k^2-2ik \tanh \zeta) \\ & \times e^{ik\zeta} \int_{-\infty}^{\infty} d\zeta (1-k^2+2ik \tanh \zeta) \\ & \times (\pi-6\operatorname{sech}\zeta)\operatorname{sech}\zeta \tanh \zeta \\ & \times \left[e^{-ik\zeta} - e^{i\frac{(1+k^2)}{k}\alpha} e^{i\beta\zeta} \right]. \end{aligned} \quad (\text{A1})$$

The evaluation of various integrals in Eq. (A1) can be facilitated by first finding the values of the following two integrals [24].

$$I_1 = \int_{-\infty}^{\infty} \operatorname{sech}\zeta e^{i\chi\zeta} d\zeta, \quad (\text{A2})$$

$$I_2 = \int_{-\infty}^{\infty} \tanh \zeta e^{i\chi\zeta} d\zeta, \quad (\text{A3})$$

where χ can take values $-k$ and β . The integrand in I_1 is found to be analytic everywhere except at the pole $\zeta \rightarrow i(2n+1)\frac{\pi}{2}$, $n = 0, 1, 2, \dots$. The residue of the function $\operatorname{sech}\zeta e^{i\chi\zeta}$ can be written as

$$\operatorname{Res}(\zeta = i(2n+1)\frac{\pi}{2}) = \sum_{n=0}^{\infty} \lim_{\zeta \rightarrow i(2n+1)\frac{\pi}{2}} \frac{e^{i\chi\zeta}}{\frac{d}{d\zeta}(\cosh \zeta)}, \quad (\text{A4})$$

which can be simplified to give

$$\operatorname{Res}(\zeta = i(2n+1)\frac{\pi}{2}) = \frac{1}{2i \cosh \frac{\pi}{2}\chi}. \quad (\text{A5})$$

Thus the integral value of I_1 in Eq. (A2) is written as

$$I_1 \equiv \int_{-\infty}^{\infty} \operatorname{sech}\zeta e^{i\chi\zeta} d\zeta = \frac{\pi}{\cosh(\frac{\pi}{2}\chi)}. \quad (\text{A6})$$

Similarly, using the same procedure we evaluate the integral I_2 in which the integrand $\tanh \zeta e^{i\chi\zeta}$ contains poles at $\zeta \rightarrow i(2n+1)\frac{\pi}{2}$, $n = 0, 1, 2, \dots$ and obtain

$$I_2 \equiv \int_{-\infty}^{\infty} \tanh \zeta e^{i\chi\zeta} d\zeta = \frac{i\pi}{\sinh(\frac{\pi}{2}\chi)}. \quad (\text{A7})$$

Now using the value of the integral I_1 as given in Eq. (A6), we evaluate the following integrals found in Eq. (A1) by integrating them by parts successively to obtain

$$\int_{-\infty}^{\infty} \operatorname{sech}\zeta \tanh \zeta e^{i\chi\zeta} d\zeta = \frac{i\pi\chi}{\cosh(\frac{\pi}{2}\chi)}, \quad (\text{A8a})$$

$$\int_{-\infty}^{\infty} \operatorname{sech}\zeta \tanh^2 \zeta e^{i\chi\zeta} d\zeta = \frac{\pi(1-\chi^2)}{2 \cosh(\frac{\pi}{2}\chi)}. \quad (\text{A8b})$$

Similarly, using Eq. (A7) we evaluate the following integrals found in Eq. (A1) by making successive integrations by parts and obtain

$$\int_{-\infty}^{\infty} \operatorname{sech}^2 \zeta \tanh \zeta e^{i\chi\zeta} d\zeta = \frac{i\pi\chi^2}{2 \sinh(\frac{\pi}{2}\chi)}, \quad (\text{A9a})$$

$$\int_{-\infty}^{\infty} \operatorname{sech}^2 \zeta \tanh^2 \zeta e^{i\chi\zeta} d\zeta = \frac{\pi\chi(2 - \chi^2)}{6 \sinh(\frac{\pi}{2}\chi)}. \quad (\text{A9b})$$

Here also χ can take values $-k$ and β . Substituting the values of the integrals found in Eqs. (A8) and (A9) in Eq. (A1), we obtain

$$\begin{aligned} \Psi^{(1)}(\zeta, t_0) = & -\frac{i}{12} \left[\int_{-\infty}^{\infty} dk \frac{(1 - k^2 - 2ik \tanh \zeta)}{k^2(1 + k^2)^2} \right. \\ & \times \left(\pi(1 - v^2)k(1 + k^2) \operatorname{sech} \frac{\pi}{2} \beta \right. \\ & \left. - \{(2 - v)(1 + v)^2(1 + k^2)^2 - 4k^2 \right. \\ & \left. \times (1 + v + k^2)\} \operatorname{cosech} \frac{\pi}{2} \beta \right) e^{i\frac{(1+k^2)}{k}\alpha + ik\zeta} \\ & \left. + 4 \int_{-\infty}^{\infty} dk \frac{(k^2 - k^4 - 2ik^3 \tanh \zeta)}{(1 + k^2)^2 \sinh \frac{\pi}{2} k} e^{ik\zeta} \right]. \quad (\text{A10}) \end{aligned}$$

Now, before writing down the final form of $\psi^{(1)}(\zeta, t_0)$ we evaluate the integrals with respect to k in the right-hand side of the above equation. For this first we rearrange the integrand in Eq.(A10) by simple multiplication and call them I_3, I_4, I_5 and I_6 as given below.

$$I_3 = \int_{-\infty}^{\infty} dk \frac{(k^2 - k^4 - 2ik^3 \tanh \zeta)}{(1 + k^2)^2 \sinh \frac{\pi}{2} k} e^{ik\zeta}, \quad (\text{A11a})$$

$$\begin{aligned} I_4 = \int_{-\infty}^{\infty} dk \frac{(1 - k^2 - 2ik \tanh \zeta)}{(1 + k^2)^2 \sinh \frac{\pi}{2} \beta} (1 + v + k^2) \\ \times e^{i\frac{(1+k^2)}{k}\alpha + ik\zeta}, \quad (\text{A11b}) \end{aligned}$$

$$I_5 = \int_{-\infty}^{\infty} dk \frac{(1 - k^2 - 2ik \tanh \zeta)}{k^2 \sinh \frac{\pi}{2} \beta} e^{i\frac{(1+k^2)}{k}\alpha + ik\zeta}, \quad (\text{A11c})$$

$$I_6 = \int_{-\infty}^{\infty} dk \frac{(1 - k^2 - 2ik \tanh \zeta)}{k(1 + k^2) \cosh \frac{\pi}{2} \beta} e^{i\frac{(1+k^2)}{k}\alpha + ik\zeta}. \quad (\text{A11d})$$

The integral I_3 can be evaluated by finding the residue of the integrand $\frac{(k^2 - k^4 - 2ik^3 \tanh \zeta)}{(1 + k^2)^2 \sinh \frac{\pi}{2} k} e^{ik\zeta}$ at the poles $k = i$ of order two and at the simple pole $k = 2in$. The results are given by

$$\operatorname{Res}(k = i) = \frac{1}{2}(\zeta - 2) \operatorname{sech} \zeta, \quad (\text{A12a})$$

$$\begin{aligned} \operatorname{Res}(k = 2in) = & \frac{40}{9\sqrt{2}} \pi \sqrt{\operatorname{sech} \zeta} e^{-\frac{3\zeta}{2}} \\ & + \frac{32}{9\sqrt[3]{2}} \pi \tanh \zeta \sqrt[3]{\operatorname{sech} \zeta} e^{-\frac{5\zeta}{3}}. \quad (\text{A12b}) \end{aligned}$$

While writing the first term of Eq.(A12b), we have approximated the results obtained as a series in terms of suitable functions. Adding the above two residue values we obtain the value of the

integral I_3 as

$$I_3 = 2\pi i \left[\frac{1}{2}(\zeta - 2)\operatorname{sech}\zeta + \frac{40}{9\pi\sqrt{2}}\sqrt{\operatorname{sech}\zeta}e^{-\frac{3\zeta}{2}} + \frac{32}{9\sqrt[3]{2}}\frac{\tanh\zeta}{\pi}\sqrt[3]{\operatorname{sech}\zeta}e^{-\frac{5\zeta}{3}} \right]. \quad (\text{A13})$$

In the case of the integral I_4 , the integrand possesses a second order pole at $k = i$ and there is one more simple pole at $k = \frac{(2n+1)}{(1-v)}(-i \pm \sqrt{\frac{1-v^2}{(2n+1)^2} - 1})$ which is however out of the contour. Thus the residue for the integrand function $\frac{(1-k^2-2ik \tanh \zeta)}{(1+k^2)^2 \sinh \beta \frac{\pi}{2}}(1+v+k^2)e^{i\frac{(1+k^2)}{k}\alpha+ik\zeta}$ is obtained as

$$\operatorname{Res}(k = i) = \frac{1}{2}(2 + v\zeta + 2v\alpha)\operatorname{sech}\zeta, \quad (\text{A14})$$

and hence the right-hand side of Eq. (A14) represents the value of the integral I_4 .

The integrand of the integral I_5 namely $\frac{(1-k^2-2ik \tanh \zeta)}{k^2 \sinh \beta \frac{\pi}{2}}e^{i\frac{(1+k^2)}{k}\alpha+ik\zeta}$ admits an essential singularity at $k = 0$, in addition to a simple pole at $k = \frac{(2n+1)}{(1-v)}(-i \pm \sqrt{\frac{1-v^2}{(2n+1)^2} - 1})$ which is also out of the contour. The residue corresponding to the essential singularity is found by collecting the coefficient of $\frac{1}{k}$ after expanding the above function. Thus we obtain

$$\begin{aligned} \operatorname{Res}(k = 0) &= \sum_{n,n'=0}^{\infty} \frac{(-1)^{n+n'} \left(\frac{\pi}{2}\right)^{2n-1} b^{n-1} (b-1)^n \alpha^{n'}}{(n!)} \\ &\times (\zeta + \alpha)^{n'} \left[\frac{(2^{2n-1} - 1)B_n}{(n!)^2 (n!)} + \frac{\left(\frac{\pi}{2}\right)^2 b^2 B_{n+1}}{(n+1)!^2 (n!)} \right. \\ &\quad \times (2^{2n+1} - 1) \left[1 - 2 \tanh \zeta \frac{(\zeta + \alpha)}{(n' + 1)} \right. \\ &\quad \left. \left. + \frac{(\zeta + \alpha)^2}{(n' + 1)(n' + 2)} \right] + \frac{\left(\frac{\pi}{2}\right)^4 (n+1)b^4 B_{n+2}}{(n+2)!(n+3)!} \right. \\ &\quad \times \frac{(2^{2n+3} - 1)}{(n' + 2)!} \left[1 - 2 \tanh \zeta \frac{(\zeta + \alpha)}{(n' + 3)} \right. \\ &\quad \left. \left. \frac{(\zeta + \alpha)^2}{(n' + 3)(n' + 4)} \right] + \dots \right], \quad (\text{A15}) \end{aligned}$$

where B'_n s are Bernoulli numbers and $b = \frac{(1+v)}{2}$. Thus the right-hand side of Eq. (A15) gives the value of the integral I_5 . In the case of the integral I_6 , the integrand $\frac{(1-k^2-2ik \tanh \zeta)}{k(1+k^2) \cosh \frac{\pi}{2}\beta}e^{i\frac{(1+k^2)}{k}\alpha+ik\zeta}$ possesses a second order pole at $k = i$ and an essential singularity at $k = 0$. In addition, we have a simple pole at $k = \frac{(2n+1)}{(1-v)}(-i \pm \sqrt{\frac{1-v^2}{(2n+1)^2} - 1})$ which is again out of the contour. The

residues at the poles $k = i$ and at the essential singularity $k = 0$ are respectively found to be

$$Res(k = i) = \frac{-1}{\pi v^2} (1 - 2v\zeta - 4v\alpha) sech\zeta, \quad (A16a)$$

$$Res(k = 0) = \sum_{m,n,n'=0}^{\infty} \sum_{j=0}^m \frac{(-1)^{n+n'} (b-1)^n E_{n+m}}{(n!)(n+2m)!} \\ \times \frac{(\frac{\pi}{2})^{2n+2m} b^{n+2m} \alpha^{n'} (\zeta + \alpha)^{n'+2j}}{(n')!(n'+2j)!} \\ \times \left[1 - \frac{\frac{\pi^2}{2} b^2}{(n+1+2m)(n+2+2m)} \right. \\ \left. - \frac{2(\frac{\pi}{2})^2 b^2 (\zeta + \alpha) \tanh \zeta}{(n+1+2m)(n+2+2m)(n'+1+2j)} \right], \quad (A16b)$$

where E'_n s are Euler numbers. We evaluated the value of the residue given in (A16a) using Mathematica. The value of the integral I_6 is the sum of the right-hand sides of Eqs. (A16a) and (A16b).

Now the value of $\psi^{(1)}(\zeta, t_0)$ is found by combining Eqs. (A13), (A14), (A15), (A16a) and (A16b) and the final form is written as

$$\Psi^{(1)}(\zeta, t_0) \approx \frac{80}{27\sqrt{2}} \sqrt{sech\zeta} e^{-\frac{3\zeta}{2}} + \frac{64}{27\sqrt[3]{2}} \tanh \zeta \\ \times \sqrt[3]{sech\zeta} e^{-\frac{5}{3}\zeta} + \frac{\pi}{6v^2} [2v(1+v)\zeta \\ + v^2 + 4\alpha v - 1] sech\zeta. \quad (A17)$$

While writing the above, we have dropped few higher order terms due to smallness in values that appeared in the residue of the essential singularity.

APPENDIX B: EVALUATION OF THE INTEGRALS IN EQ.(77) USING RESIDUE THEOREM

Here we evaluate the various integrals found in Eq. (77) using the standard residue theorem as carried out in the previous case in Appendix-A. Eq.(77) reads

$$\Psi^{(1)}(\zeta, t_0) = \frac{1}{3\pi} \int_{-\infty}^{\infty} \frac{dk}{(1+k^2)^3} (1 - k^2 - 2ik \tanh \zeta) \\ \times e^{ik\zeta} \int_{-\infty}^{\infty} d\zeta (1 - k^2 + 2ik \tanh \zeta) \\ \times (6sech^2\zeta + 2\zeta \tanh \zeta - 5) sech\zeta \\ \left[e^{-ik\zeta} - e^{i\frac{(1+k^2)}{k}\alpha} e^{i\beta\zeta} \right] + \frac{(1+v)}{3} sech\zeta \\ \times \int_{-\infty}^{\infty} d\zeta \zeta^2 (6sech^2\zeta + 2\zeta \tanh \zeta - 5) sech^2\zeta. \quad (B1)$$

The last integral in the right-hand side of Eq. (B1) can be evaluated straightaway to obtain

$$\int_{-\infty}^{\infty} d\zeta \zeta^2 (6 \operatorname{sech}^2 \zeta + 2\zeta \tanh \zeta - 5) \operatorname{sech}^2 \zeta = \frac{\pi^2}{3} - 4. \quad (\text{B2})$$

The evaluation of some of the integrals in Eq. (B1) can be made by using the integral values given in Eqs. (A6) and (A8a). For instance, the following two integrals after integration by parts successively give

$$\int_{-\infty}^{\infty} \operatorname{sech}^3 \zeta e^{i\chi\zeta} d\zeta = \frac{(1 + \chi^2)\pi}{2 \cosh(\frac{\pi}{2}\chi)}, \quad (\text{B3a})$$

$$\int_{-\infty}^{\infty} \operatorname{sech}^3 \zeta \tanh \zeta e^{i\chi\zeta} d\zeta = \frac{i(\chi + \chi^3)\pi}{6 \cosh(\frac{\pi}{2}\chi)}. \quad (\text{B3b})$$

To evaluate the other integrals, we need to find the value of the following integral.

$$I_7 = \int_{-\infty}^{\infty} \zeta \operatorname{sech} \zeta e^{i\chi\zeta} d\zeta. \quad (\text{B4})$$

The integrand in Eq. (B4) is found to be analytic everywhere except at the pole $\zeta = i(2n + 1)\frac{\pi}{2}$, $n=0,1,2,\dots$. The residue of the function $\zeta \operatorname{sech} \zeta e^{i\chi\zeta}$ at the above pole is found to be $\frac{\pi}{4 \cosh(\frac{\pi}{2}\chi)} \left[1 - \frac{e^{-\frac{\pi}{2}\chi}}{\cosh(\frac{\pi}{2}\chi)} \right]$ and therefore we have

$$I_7 \equiv \int_{-\infty}^{\infty} \zeta \operatorname{sech} \zeta e^{i\chi\zeta} d\zeta = \frac{i\pi^2}{2 \cosh(\frac{\pi}{2}\chi)} \left[1 - \frac{e^{-\frac{\pi}{2}\chi}}{\cosh(\frac{\pi}{2}\chi)} \right]. \quad (\text{B5})$$

Using Eq. (B5) we find the values of the following integrals found in Eq. (B1) by integrating them by parts successively.

$$\int_{-\infty}^{\infty} \zeta \operatorname{sech} \zeta \tanh \zeta e^{i\chi\zeta} d\zeta = \frac{\pi}{\cosh(\frac{\pi}{2}\chi)} \left[\left(1 - \frac{\pi}{2}\chi\right) + \frac{\pi^2 \chi e^{-\frac{\pi}{2}\chi}}{2 \cosh(\frac{\pi}{2}\chi)} \right], \quad (\text{B6a})$$

$$\int_{-\infty}^{\infty} \zeta \operatorname{sech} \zeta \tanh^2 \zeta e^{i\chi\zeta} d\zeta = \frac{i\pi}{\cosh(\frac{\pi}{2}\chi)} \left[\chi + \frac{\pi}{4} \times (1 - \chi^2) \tanh\left(\frac{\pi}{2}\chi\right) \right]. \quad (\text{B6b})$$

Substituting the values of the integrals from Eqs. (A6), (A8a), (B3) and (B6) in Eq. (B1), we obtain

$$\begin{aligned} \Psi^{(1)}(\zeta, t_0) = & \frac{1}{3} \left[\frac{(\pi^2 - 12)}{3} (1 + v) \operatorname{sech} \zeta \right. \\ & + \int_{-\infty}^{\infty} dk \frac{(1 - k^2 - 2ik \tanh \zeta)}{k^2 (1 + k^2)^2 \cosh(\frac{\pi}{2}\beta)} \\ & \times [b^2 (2b - 3) (1 + k^2)^2 + k^2 (2b + k^2) \\ & + \pi b (1 - b) k (1 + k^2) \tanh(\frac{\pi}{2}\beta)] e^{\frac{i\alpha(1+k^2)}{k} + ik\zeta} \\ & \left. - \int_{-\infty}^{\infty} dk \frac{k^2 (1 - k^2 - 2ik \tanh \zeta)}{(1 + k^2)^2 \cosh(\frac{\pi}{2}k)} e^{i\zeta k} \right]. \quad (\text{B7}) \end{aligned}$$

In order to evaluate the integrals in Eq.(B7), we first rewrite them approximately. While evaluating the integrals in Eq.(B7) using Mathematica it is noticed that the residues at $k=0$ have unwieldy form. Hence we drop the residues at $k=0$ and evaluate the intergrals for the rest of the singularities. The last integral in the right-hand side of Eq. (B7) is evaluated by finding the residue of the function $\frac{k^2(1-k^2-2ik \tanh \zeta)}{(1+k^2)^2 \cosh(\frac{\pi}{2}k)} e^{ik\zeta}$ at the second order pole $k = i$ and at the simple pole $k = i(2n + 1)$.

$$\text{Res}[k = i] = \frac{i}{24\pi} [12 + (12\zeta^2 - 48\zeta + \pi^2 + 18) \times (1 + \tanh \zeta)] e^{-\zeta}, \quad (\text{B8a})$$

$$\begin{aligned} \text{Res}[k = i(2n + 1)] &= \frac{135i}{8\pi} \left[\frac{1}{\sqrt{2}} \sqrt{\text{sech}\zeta} e^{-\frac{1}{2}\zeta} \right. \\ &\quad \left. - \frac{1}{\sqrt[3]{2}} \sqrt[3]{\text{sech}\zeta} e^{-\frac{2}{3}\zeta} \left(1 + \frac{1}{10} \tanh \zeta e^{-2\zeta}\right) \right]. \end{aligned} \quad (\text{B8b})$$

While writing the final form of Eq.(B8b), we have approximated the results obtained in terms of a series as the functions given in Eq.(B8b). We then calculate the residue for the integrand function $\frac{(1-k^2-2ik \tanh \zeta)(2b+k^2)}{(1+k^2)^2 \cosh(\beta\frac{\pi}{2})} e^{\frac{i(1+k^2)\alpha}{k} + ik\zeta}$ at the second order pole $k = i$ and at the simple pole $k = \frac{(2n+1)}{(1-v)} (-i \pm \sqrt{\frac{1-v^2}{(2n+1)^2} - 1})$. However, as the latter one is out of contour we drop it. Thus the residue at the second order pole $k=i$ is written as

$$\begin{aligned} \text{Res}[k = i] &= \frac{i}{24(2b-1)^4\pi} [12(1-2b)^2 \\ &\quad + [12(1-2b)^2\zeta^2 + 24\{(2b-1) \\ &\quad \times (2-2\alpha + b(4\alpha-1))\}\zeta + \pi^2(1-2b)^4 \\ &\quad + 48(2b-1)^2\alpha^2 + 72(2b-1)\alpha \\ &\quad + 18 - 48b(1+b)] (1 + \tanh \zeta)] e^{-\zeta}. \end{aligned} \quad (\text{B9})$$

The integrand function $\frac{(1-k^2-2ik \tanh \zeta) \tanh(\beta\frac{\pi}{2})}{k(1+k^2) \cosh(\beta\frac{\pi}{2})} e^{\frac{i(1+k^2)\alpha}{k} + ik\zeta}$ admits the following residue at the pole $k = i$ of order two. Thus we have

$$\begin{aligned} \text{Res}(k = i) &= \frac{i}{6(2b-1)^4\pi^2} [12(2b-1)^2 \\ &\quad + [12(1-2b)^2\zeta^2 - 12\{(2b-1)(1+4\alpha \\ &\quad - b(8\alpha-2))\}\zeta + 48(2b-1)^2\alpha^2 \\ &\quad - 48(2b-1)\alpha - (2b-1)^4\pi^2 + 6 \\ &\quad + 48(1-b)b] (1 + \tanh \zeta)] e^{-\zeta}. \end{aligned} \quad (\text{B10})$$

However, the simple pole at $k = \frac{(2n+1)}{(1-v)} (-i \pm \sqrt{\frac{1-v^2}{(2n+1)^2} - 1})$ is out of contour. Summing up the results given in Eqs.(B8), (B9) and (B10) , the first order correction to the soliton in the case

of $g(\zeta) = \tanh \zeta$ is written as

$$\begin{aligned}
\Psi^{(1)}(\zeta, t_0) \approx & \frac{1}{9(1-2b)^4} [12b(b-1)(1-2b)^2 \\
& + [12b(b-1)(1-2b)^2\zeta^2 - 6(2b-1) \\
& \times \{-2\alpha + b[1+2b(-7+8b)+4\alpha]\}\zeta \\
& - 12(1-2b)^2\alpha^2 - 6(2b-1)[3+20(b-1)b]\alpha \\
& - 2b(b-2)(1-2b)^4\pi^2 \\
& + 12b(2b-1)\{3-2b[7+b(16b-19)]\} \\
& \times (1+\tanh\zeta)] e^{-\zeta} \Big] + \frac{135}{8} \left[\frac{1}{\sqrt{2}} e^{-\frac{1}{2}\zeta} \sqrt{\operatorname{sech}\zeta} \right. \\
& \left. - \frac{1}{\sqrt[3]{2}} \sqrt[3]{\operatorname{sech}\zeta} e^{-\frac{2}{3}\zeta} \left(1 + \frac{1}{10} \tanh \zeta e^{-2\zeta}\right) \right]. \tag{B11}
\end{aligned}$$

APPENDIX C: EVALUATION OF THE INTERGRALS IN EQ. (79) USING RESIDUE THEOREM

In this appendix, we evaluate the integrals found in Eq. (79) using the standard residue theorem as done in the previous two cases. Eq.(79) is written as

$$\begin{aligned}
\Psi^{(1)}(\zeta, t_0) = & \frac{1}{\pi} \int_{-\infty}^{\infty} \frac{dk}{(1+k^2)^3} (1-k^2-2ik \tanh \zeta) \\
& \times e^{ik\zeta} \int_{-\infty}^{\infty} d\zeta (1-k^2+2ik \tanh \zeta) \\
& \times [\sin \zeta + (\cos \zeta - \frac{\pi^2}{8}) \tanh \zeta] \operatorname{sech} \zeta \\
& \times \{e^{i\frac{(1+k^2)}{k}\alpha} e^{i\beta\zeta} - e^{-ik\zeta}\} + (1+v) \operatorname{sech} \zeta \\
& \times \left[\int_{-\infty}^{\infty} d\zeta \zeta^2 [\sin \zeta + \cos \zeta] \operatorname{sech}^2 \zeta \right. \\
& \left. - \frac{\pi^2}{8} \int_{-\infty}^{\infty} d\zeta \tanh \zeta \operatorname{sech}^2 \zeta \right]. \tag{C1}
\end{aligned}$$

It may be verified that the last integral $\int_{-\infty}^{\infty} d\zeta \operatorname{sech}^2 \zeta \tanh \zeta$ in the right-hand side of Eq.(C1) on evaluation vanishes. For evaluating some of the integrals found in Eq. (C1) we use the values of the integrals given in Eqs. (A6), (A8a) and (A8b) and also the value of the following integral.

$$I_8 = \int_{-\infty}^{\infty} \zeta^2 \tanh \zeta e^{i\zeta} d\zeta. \tag{C2}$$

The integrand in Eq.(C2) is found to be analytic everywhere except at the pole $\zeta = i(2n+1)\frac{\pi}{2}$, $n=0,1,2,\dots$. The residue of the function $\zeta^2 \tanh \zeta e^{i\delta\zeta}$ is then found to be

$-\frac{\pi^2}{8 \sinh(\frac{\pi}{2})} \left[1 + 2 \frac{e^{-\frac{\pi}{2}}}{\sinh(\frac{\pi}{2})} + \frac{e^{\frac{\pi}{2}}(1-e^{-2\pi})}{2 \sinh^3(\frac{\pi}{2})} \right]$ and hence the value of the integral I_8 is written as

$$I_8 \equiv \int_{-\infty}^{\infty} \zeta^2 \tanh \zeta e^{i\zeta} d\zeta = -\frac{i\pi^3}{4 \sinh(\frac{\pi}{2})} \times \left[1 + 2 \frac{e^{-\frac{\pi}{2}}}{\sinh(\frac{\pi}{2})} + \frac{e^{\frac{\pi}{2}}(1-e^{-2\pi})}{2 \sinh^3(\frac{\pi}{2})} \right]. \quad (C3)$$

Now, using the value of the integral given in Eq. (C3), we evaluate the following integrals found in Eq. (C1) by integrating them by parts successively.

$$\int_{-\infty}^{\infty} d\zeta \zeta^2 \operatorname{sech}^2 \zeta e^{\pm i\zeta} = \frac{\pi^2}{\sinh \frac{\pi}{2}} \left[\pm (1 \mp \frac{\pi}{4}) + \frac{(1 \mp \frac{\pi}{2})e^{\mp \frac{\pi}{2}}}{\sinh \frac{\pi}{2}} \pm \frac{\pi e^{\pm \frac{\pi}{2}}(1-e^{\mp 2\pi})}{\sinh^3 \frac{\pi}{2}} \right], \quad (C4a)$$

$$\int_{-\infty}^{\infty} d\zeta \zeta^2 \operatorname{sech}^2 \zeta \tanh \zeta e^{\pm i\zeta} = \frac{i\pi}{\sinh \frac{\pi}{2}} \left[(\pi \mp 1 \mp \frac{\pi^2}{8}) \pm \frac{\pi(2 \mp \frac{\pi}{2})e^{\mp \frac{\pi}{2}}}{2 \sinh \frac{\pi}{2}} - \frac{i\pi^2 e^{\pm \frac{\pi}{2}}(1-e^{\mp 2\pi})}{16 \sinh^3 \frac{\pi}{2}} \right]. \quad (C4b)$$

On substituting Eqs. (C4a) and (C4b) in Eq. (C1) we obtain

$$\begin{aligned} \Psi^{(1)}(\zeta, t_0) &= \frac{(1+v)i\pi^3}{16 \sinh \frac{\pi}{2}} \left[\frac{\cosh \frac{3\pi}{2}}{\sinh^3 \frac{\pi}{2}} - \cosh \frac{\pi}{2} \left(\frac{4}{\sinh \frac{\pi}{2}} + 1 \right) \right] \operatorname{sech} \zeta \\ &+ \frac{i}{2} \int_{-\infty}^{\infty} dk \frac{(1-k^2-2ik \tanh \zeta)}{k(1+k^2)^3} \\ &\times e^{\frac{i(1+k^2)\alpha}{k} + ik\zeta} \left[\{k^2 + b(1-b)(1+k^2)^2\} \right. \\ &\times \left(\operatorname{sech} \frac{\pi}{2}(\beta+1) + \operatorname{sech} \frac{\pi}{2}(\beta-1) \right) \\ &\left. - \frac{\pi^2}{4} b(1-b)(1+k^2)^2 \operatorname{sech} \frac{\pi}{2} \beta \right] \\ &- \frac{i}{2} \int_{-\infty}^{\infty} dk \frac{k(1-k^2-2ik \tanh \zeta)}{(1+k^2)^3} e^{ik\zeta} \\ &\times \left(\operatorname{sech} \frac{\pi}{2}(1-k) + \operatorname{sech} \frac{\pi}{2}(1+k) \right). \quad (C5) \end{aligned}$$

Before evaluating the integrals in Eq.(C5) we rewrite the same appropriately. We then evaluate the integrals in Eq. (C5) one by one by finding the value of the residues at the pole ($k = i$) at different orders. The residue for the integrand function $(\operatorname{sech} \frac{\pi}{2}(\beta+1) + \operatorname{sech} \frac{\pi}{2}(\beta-1)) \frac{k(1-k^2-2ik \tanh \zeta)}{(1+k^2)^3} e^{\frac{i(1+k^2)\alpha}{k} + ik\zeta}$ at the pole $k=i$ of order three is found to be

$$\operatorname{Res}(k=i) = -\frac{\pi}{16} [2(2b-1)\zeta + 4(2b-1)\alpha + 1] \operatorname{sech} \zeta. \quad (C6)$$

Next, we find the residue for the function $e^{\frac{i(1+k^2)\alpha}{k} + ik\zeta} \frac{(1-k^2-2ik \tanh \zeta)}{k(1+k^2) \cosh \beta \frac{\pi}{2}}$ at the simple poles $k=i$ and $k = \frac{(2n+1)}{(1-v)}(-i \pm \sqrt{\frac{1-v^2}{(2n+1)^2} - 1})$ (which is out of contour). Further, at $k=0$ there is an essential singularity, the residue of which is not shown here due its unwieldy form. Thus the residue for the above function at the first order pole $k=i$ is given by

$$\begin{aligned} Res(k=i) &= \frac{1}{\pi(1-2b)^2} [2(2b-1)\zeta \\ &\quad + 4(2b-1)\alpha - 1] sech\zeta. \end{aligned} \quad (C7)$$

The residues for the function $(sech \frac{\pi}{2}(k-1) + sech \frac{\pi}{2}(k+1)) \frac{(k-k^3-2ik^2 \tanh \zeta)}{(1+k^2)^3} e^{ik\zeta}$ at the pole $k=i$ of order three and at the simple poles $k = i(2n+1) + 1$ and $k = i(2n+1) - 1$ are written as

$$Res(k=i) = \frac{\pi}{16} (2\zeta - 1) sech\zeta, \quad (C8a)$$

$$\begin{aligned} Res[k = i(2n+1) + 1] &= \frac{-2i}{\pi} e^{(i-1)\zeta} \sum_{n=0}^{\infty} (-1)^{-n} \\ &\quad \frac{[1 + i(2n+1)]e^{-2n\zeta}}{[2 - (2n+1)^2 + 2i(2n+1)]^3} \\ &\quad \times \{[(2n+1)^2 - 2i(2n+1)] \\ &\quad - 2i \tanh \zeta [1 + i(2n+1)]\}, \end{aligned} \quad (C8b)$$

$$\begin{aligned} Res[k = i(2n+1) - 1] &= \frac{2i}{\pi} e^{-(1+i)\zeta} \sum_{n=0}^{\infty} (-1)^{-n} \\ &\quad \frac{[-1 + i(2n+1)]e^{-2n\zeta}}{[(2n+1)^2 - 2 + 2i(2n+1)]^3} \\ &\quad \times \{[(2n+1)^2 + 2i(2n+1)] \\ &\quad - 2i \tanh \zeta [-1 + i(2n+1)]\}. \end{aligned} \quad (C8c)$$

It can be verified that the residue of the function $(sech \frac{\pi}{2}(\beta+1) + sech \frac{\pi}{2}(\beta-1)) \frac{(1-k^2-2ik \tanh \zeta)}{k(1+k^2)} e^{\frac{i(1+k^2)\alpha}{k} + ik\zeta}$ at $k=i$ vanishes. On summing up the values of the residues given in Eqs. (C6), (C7) and (C8) (dropping higher order terms in Eqs. (C8b) and (C8c) while adding) we obtain the following expression for $\psi^{(1)}(\zeta, t_0)$.

$$\begin{aligned} \Psi^{(1)}(\zeta, t_0) &\approx \frac{\pi^2}{4(1-2b)^2} [b(2b-1)\zeta \\ &\quad + \{b(2\alpha + b - 1) - \alpha\}] sech\zeta \\ &\quad + \frac{4}{122825} \{(\cosh 2\zeta - \sinh 2\zeta) \\ &\quad \times [25 \cosh 2\zeta (523 \cos \zeta - 1512 \sin \zeta) \\ &\quad + 289(19 \cos \zeta + 8 \sin \zeta) + 15(766 \cos \zeta \\ &\quad - 2393 \sin \zeta) \sinh 2\zeta\} sech\zeta. \end{aligned} \quad (C9)$$

As residues due to the singularities in the plane except along the imaginary axis, lead to secular terms in the solutions, we take into account only singularities along the imaginary axis that is at

$k=i$, dropping residues due to the other two singularities at $k = i(2n+1)+1$ and $k = i(2n+1)-1$. Thus the first order correction $\psi^{(1)}(\zeta, t_0)$ given in Eq.(C9) finally becomes

$$\Psi^{(1)}(\zeta, t_0) \approx \frac{\pi^2}{4(1-2b)^2} [b(2b-1)\zeta + \{b(2\alpha + b - 1) - \alpha\}] \operatorname{sech}\zeta. \quad (\text{C10})$$

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