Solitary waves in twist-opening models of DNA dynamics

Giuseppe Gaeta* and Laura Venier†
Dipartimento di Matematica, Università di Milano, via Saldini 50, 20133 Milano, Italy
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We analyze traveling solitary wave solutions in the Barbi-Cocco-Peyrard twist-opening model of nonlinear DNA dynamics. We identify conditions, involving an interplay of physical parameters and asymptotic behavior, for such solutions to exist, and provide first-order ordinary differential equations whose solutions give the required solitary waves; these are not solvable in analytical terms, but are easily integrated numerically. The conditions for existence of solitary waves are not satisfied for trivial asymptotic behavior and physical values of the parameters, i.e., the Barbi-Cocco-Peyrard model admits only solitary wave solutions that entail a global modification of the molecule; this is compared with the situation met in another recently formulated class of DNA models with two degrees of freedom per site.

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I. INTRODUCTION

When trying to model DNA dynamics, one is faced with an extremely complex molecule [1,2]; the nearly regular structure (a regular backbone with attached bases, themselves of four possible types with similar properties) suggests considering it as a homogeneous polymer, deferring to a later stage considerations involving inhomogeneities due to actual base sequences. Such a model can support solitary wave excitations; this is especially interesting since it is conjectured that solitonlike excitations could be present, and play a functional role, in DNA [3]. They could be relevant both for denaturation (relevant excitations would be breathers [4–6]) and for DNA transcription (relevant excitations would be traveling kink solitons [7,8]).

Such a polymer, albeit homogeneous, is still extremely complex. Several physical considerations lead to consideration of mainly two degrees of freedom, whose activation energies are similar to and lower than those of others [7]: radial openings of the double helix (dominant in denaturation), and rotations in a plane roughly orthogonal to the double helix axis (dominant in transcription).

It is thus natural, as a first approximation, to elaborate models taking into account either one of these two degrees of freedom, depending on the process one aims at modeling. In fact, early models for DNA denaturation—e.g., the Peyrard-Bishop (PB) model [9] and improvements thereof, in particular the Peyrard-Bishop-Dauxois (PBD) model [5,10]—consider a radial degree of freedom; while models dealing with the DNA structure modification met in the transcription process—like the Yakushevich (Y) model [11] and improvements thereof [8,12]—consider angular degrees of freedom. These simple DNA models are able to support relevant nonlinear excitations, and quite successful in describing several experimentally measurable quantities associated with the dynamics of the DNA molecule [4,5,8].

In more recent years, the advancement of experimental techniques to study the dynamics of a single DNA molecule (subject to exactly controlled external forces) called for more detailed models, and a rather natural first step in this direction was to formulate models able to consider both the radial and the torsional degrees of freedom mentioned above at the same time. The first of these models was proposed by Barbi, Cocco, and Peyrard (BCP) [13–15] and, together with the Poland-Scheraga model [16,17], is at the basis of most of the present-day DNA modeling [4–6,18–25], either in its original form or in the modified version elaborated soon afterwards by Cocco and Monasson [26]. These models were built as a development of the PB and PBD models, and hence mainly with the aim of studying DNA denaturation; thus the analysis of their nonlinear excitations focused on breathers (see [4,5] for the results of this analysis). On the other hand, these models also take into account torsional degrees of freedom, and could be relevant—as improvements on the Y model—in the context of DNA transcription; this calls for an analysis of traveling solitary waves solutions.

As far as we know, theoretical analysis of traveling solitary wave solutions (also called simply solitons in the following) of the BCP model is not present in the literature except for our recent work [27] (for traveling solitons in the PBD model, see [28]). In our previous work on the BCP model [27] we used the setting and coordinates traditionally employed in studying the BCP model; hence, in particular, we used a fixed spatial frame. These coordinates (well adapted to the study of spatially localized objects like breathers) introduce some unneeded difficulty in the computations, and also in the interpretation of results concerning traveling kinklike solitary waves. In this paper, we will use a different set of coordinates, describing deviations from equilibrium, obtaining a simpler description of traveling solitons and more complete results.

We will be able to identify conditions (on the parameters appearing in the model) which—if satisfied—ensure the existence of solitary wave solutions; the latter will be described by solutions to certain ordinary differential equations (ODEs) which cannot be solved exactly (due to the analytic form of the Morse potential) but are easily integrated numerically. It should be stressed that, in order to have physical significance, these solutions must have a certain limit behavior (discussed below); the existence of solutions with the

*gaeta@mat.unimi.it
†laura_venier@infinito.it

required limit behavior can be discussed in analytic terms, and again is subject to certain conditions on the parameters appearing in the model.

The conditions mentioned above are not satisfied when we take parameters in the physical range *and* require solutions to be asymptotic to the trivial equilibrium. Solitary wave solutions become possible within the BCP model and physically realistic values of the parameters if we allow asymptotic behavior corresponding to a *nontrivial equilibrium*; roughly speaking, this means allowing the double helix to have a slightly modified pitch (i.e., being overtwisted) far ahead and behind the "active" region (the region where the solitary wave differs substantially from equilibria). The precise meaning of these statements will become clearer in the following.

In the Appendix, we will also discuss how these results compare with those obtained for another class of models, recently formulated [29–32], which also describe the DNA double chain by means of two degrees of freedom per site, but with a different geometry (more precisely, considering purely torsional motions rather than torsional and rectilinear ones).

A. Preliminary discussion

Before entering into the detail of our analysis of solitons in the BCP model, it is appropriate to briefly discuss two general points, i.e., (a) how relevant or justified is DNA modeling by Hamiltonian or Lagrangian dynamics (see [4,5,8,12,33–35] for a wider discussion of the validity and role of conservative DNA modeling, in particular at the mesoscopic level); and (b) how strict is the relation of our analysis to physical DNA features.

As for (a), it is well known that DNA *in vivo* operates in a highly damping fluid, and is on the other hand subject to thermal noise; it may thus appear rather inappropriate to discuss its dynamics in terms of conservative dynamics. The reasons to study conservative models of DNA are manifold. First of all, a sound understanding of the dynamics of the molecule *per se* is by all means desirable before tackling the more involved theme of its dynamics in a realistic environment, and hence the interactions between DNA and the fluid cell environment at realistic temperature. In recent years, another reason arose: in fact, we are now able to perform detailed and highly controlled experiments [36–39] in which a single DNA molecule is manipulated, and these experiments can be conducted by putting the molecule in an environment and at a temperature which can (to a large extent) be chosen by the experimenter [40–47] (see also [48,49] for recent reviews of experimental techniques). These experiments have in particular been able to study in great detail the elastic behavior of DNA [50–54]. Thus, modeling of DNA without damping and/or thermal noise due to interaction with the real environment met in the living cell is actually appropriate to confront theory with the outcome of some laboratory experiments. A very recent proposal for measuring the speed of would-be DNA solitons [28] is in fact based on one of these conservative models (the PBD one), strictly related to the BCP model we consider here.

This discussion also anticipates considerations concerning point (b), i.e., the relation of our analysis to DNA physical features. It is rather obvious that our analysis is not relevant in the context of DNA denaturation (which, as recalled above, was the first motivation for the introduction of the Peyrard-Bishop model and its refinements [9,10]); this not only for the general considerations about the role of damping and thermal noise in the dynamics of DNA in living cells (for this, see, e.g., the discussion in [4,5]), but first and foremost because the excitations we consider here (traveling solitons) are not the kind of excitations (breathers [5]) which are thought to be relevant in the context of DNA denaturation.

On the other hand, the traveling solitons we study could be relevant in the context of DNA behavior in the course of the transcription process. In a more direct way, they can be searched for, and possibly observed if they exist, by means of single-molecule laboratory experiments (such as, concretely, the one proposed in [28]). A sound understanding of the traveling solitons' features and of the range of conditions allowing or not allowing their existence can be considered a significant test concerning the understanding of DNA features relevant to the dynamics of excitations traveling along the double chain in an orderly manner; these excitations could be studied in laboratory experiments and according to some authors [3,7,8,11,33,55] could be relevant (with all the necessary modification in the modeling to take into account the complex fluid environment in which this takes place) in the transcription process.

II. THE BCP MODEL

The Barbi-Cocco-Peyrard model [4,13,15] describes the DNA double chain in terms of an array of nucleotides at sites $n \in \mathbf{Z}$ on each chain $i = \pm 1$; their position as a whole is characterized by two coordinates in a fixed plane orthogonal to the double helix axis. Note that nucleotides are supposed to move only in these planes.

A. Discrete BCP model

The (polar) coordinates used by BCP are the distance $r_n^{(i)}$ from the double helix axis and an angle $\psi_n^{(i)}$ describing the orientation of the base with a given spatial direction. The equilibrium configuration for the chain is a regular double helix. The equilibrium configuration is, of course, defined up to a global rotation; this feature will show up again later, leading to a conservation law.

If one restricts consideration—as suggested by Barbi, Cocco, and Peyrard—to *symmetric motions* (note that the equilibrium configuration is symmetric), this implies $r_n^{(-1)} = r_n^{(1)}$, $\psi_n^{(-1)} = \psi_n^{(1)}$. We will from now on adopt this reduction, and write

$$r_n = r_n^{(1)} = r_n^{(-1)}, \quad \psi_n = \psi_n^{(1)} = \psi_n^{(-1)}. \tag{1}$$

We will also denote by m the mass of the nucleotides, by h the distance between planes of successive base pairs, by ℓ_n the length of the phosphodiester chain segment linking bases at sites n and $n+1$ on the same chain, by L the value of this length in the equilibrium configuration; note that by elemen-

tary geometrical constraints $L>h$, so we also write $L=sh$ with $s=1+\sigma>1$. Moreover, we denote by D and α the parameters appearing in the Morse potential

$$V(r_n) := D\{\exp[-\alpha(r_n - R_0)] - 1\}^2 \tag{2}$$

modeling the intrapair interactions mediated by hydrogen bonding, with R_0 the equilibrium distance between such bases, and finally by K the coupling constant for the harmonic elastic interaction between successive bases (this is the *stacking potential*); see [13,15] for details.

With these notation and variables, the BCP model is described by the Lagrangian

$$\mathcal{L} = \sum_n (m\dot{r}_n^2 + mr_n^2\dot{\psi}_n^2) - \sum_n D(e^{-\alpha(r_n - R_0)} - 1)^2 + - \sum_n K(\ell_n - L)^2 - \sum_n G_0(\psi_{n+1} - 2\psi_n + \psi_{n-1})^2. \tag{3}$$

The term with coupling constant G_0 was introduced by BCP in order to prevent some degenerate behavior allowed by the discrete nature of the model [13,15]; as in the following we will study the continuum version of the BCP model, it will be inessential and we will set $G_0=0$.

The values proposed in [13] for the parameters appearing in the model are

$$R_0 = 2 \text{ Å}, \quad h = 3.4 \text{ Å}, \quad \alpha = 4.45 \text{ Å}^{-1},$$

$$D = 0.04 \text{ eV}, \quad K = 1 \text{ eV Å}^{-2},$$

$$m = 300 \text{ amu} \simeq 5.0 \times 10^{-22} \text{ g} \simeq 2.8 \times 10^{11} \text{ eV}/c^2. \tag{4}$$

In our discussion we will accept these values as the physical ones. We stress that the distance $h_n=h$ between planes in which base pairs at sites n and $(n+1)$ move, measured along the double helix axis, is a constant in this model; in a variant of the model, due to Cocco and Monasson [26], this is not the case. As for the lengths ℓ_n, these are allowed to change. They can be expressed in terms of the coordinates $(r_n, r_{n+1}, \psi_n, \psi_{n+1})$ as

$$\ell_n = \sqrt{h^2 + r_{n-1}^2 + r_n^2 - 2r_{n-1}r_n \cos(\psi_n - \psi_{n-1})}; \tag{5}$$

the equilibrium distance is obtained from this for $h_n=h$, $r_n=r_{n-1}=r_0$, and $\psi_n - \psi_{n-1} = \delta\psi = 2\pi/P$ where Ph is the pitch of the helix. In B-DNA, $P=10$ [2]. Hence

$$L = 4.88 \text{ Å}, \quad s = 1.435, \quad \sigma = 0.435. \tag{6}$$

Using (5), the Lagrangian $\mathcal{L}$ defined in (3) is rewritten as (recall we set $G_0=0$)

$$\mathcal{L} = \sum_n (m\dot{r}_n^2 + mr_n^2\dot{\psi}_n^2) - \sum_n D(e^{-\alpha(r_n - R_0)} - 1)^2 - \sum_n K\{[h^2 + r_{n-1}^2 + r_n^2 + - 2r_{n-1}r_n \cos(\psi_n - \psi_{n-1})]^{1/2} - L\}^2. \tag{7}$$

B. Continuum BCP model

It is convenient to pass to the continuum approximation. That is, the arrays $r_n(t)$ and $\psi_n(t)$ will be replaced by (interpolating) fields $R(x,t)$ and $\Psi(x,t)$ such that, with δ the distance between neighboring nucleotide planes, $R(n\delta,t) \approx r_n(t)$, $\Psi(n\delta,t) \approx \psi_n(t)$. In this way

$$r_n(t) \approx R(n\delta,t), \quad \psi_n(t) \approx \Psi(n\delta,t),$$

$$r_{n\pm1}(t) \approx R((n \pm 1)\delta,t) \approx R(n\delta,t) \pm \delta R_x(n\delta,t) + O(\delta^2),$$

$$\psi_{n\pm1}(t) \approx \Psi((n \pm 1)\delta,t) \approx \Psi(n\delta,t) \pm \delta\Psi_x(n\delta,t) + O(\delta^2). \tag{8}$$

We stress that we are keeping a distinction between the parameter h, entering into the expression of ℓ_n and hence of the stacking energy, and the expansion parameter δ. This distinction is essential in obtaining the series expansions below.

Using (8) and omitting the curvature term, i.e., setting $G_0=0$ as anticipated (this is legitimate as we are now dealing with a continuum version of the model; see the discussion in [13,15] for details), and setting $L=(1+\sigma)h$, the BCP Lagrangian (7) is written, to second order in δ and omitting an inessential constant term $(-Kh^2\sigma^2)$, as

$$\mathcal{L} = m(R_t^2 + R^2\Psi_t^2) - V(R) + K\sigma(R_x^2 + R^2\Psi_x^2)\delta^2. \tag{9}$$

Note that the stacking term now enters in the Lagrangian with a plus sign.

It should now be remarked that ψ_n and hence Ψ represent angles with respect to a given fixed spatial direction. It is more convenient to measure angles with respect to the direction corresponding to the equilibrium configuration. This is given by a helix with pitch $p=10\delta$ (i.e., of ten bases); thus at equilibrium $\Psi(x,t)=\bar{\Psi}(x)=\beta x$ with $\beta=2\pi/p=\pi/(5\delta)$. In B-DNA, we have hence

$$\beta \approx 0.185 \text{ Å}^{-1}. \tag{10}$$

We will write $\Phi=\Psi-\bar{\Psi}$ and hence

$$\Psi = \Phi + \beta x, \quad \Psi_x = \Phi_x + \beta, \quad \Psi_t = \Phi_t. \tag{11}$$

We also write, for ease of notation,

$$\kappa := K\sigma\delta^2 > 0; \tag{12}$$

note for later reference that using (4) and (6) we get

$$\kappa_{\text{phys}} \approx 5.032 \text{ eV}. \tag{13}$$

With this notation the Lagrangian (9) reads

$$\mathcal{L} = m(R_t^2 + R^2\Phi_t^2) - V(R) + \kappa(\beta^2R^2 + 2\beta R^2\Phi_x + R^2\Phi_x^2 + R_x^2). \tag{14}$$

It should be stressed that $\mathcal{L}$ does not depend on Φ; it follows by the Noether theorem [56,57] that it admits a conservation law, which will show up as the Euler-Lagrange equation associated with the field Φ.

The Euler-Lagrange equations for (14) read

$$mR_{tt} = mR\Phi_t^2 - (1/2)V'(R) + \kappa(R\Phi_x^2 + \beta^2R + 2\beta R\Phi_x - R_{xx}),$$

$$mR^2\Phi_{tt} = -2mRR_t\Phi_t - \kappa[R^2\Phi_{xx} + 2(\beta + \Phi_x)RR_x]. \tag{15}$$

III. TRAVELING WAVE REDUCTION FOR THE BCP MODEL

Equations (15) are nonlinear, and we have therefore little hope of devising their general solution. We are especially interested in traveling wave solutions, i.e., in solution depending on x and t only through $z=(x-vt)$; thus we set

$$R(x,t) = R(x-vt), \quad \Phi(x,t) = \Phi(x-vt). \tag{16}$$

With the *traveling wave ansatz* (16) and (15) reduce to

$$\mu f'' = \mu f g'^2 - (1/2)V'(f) + \beta\kappa(\beta + 2g')f,$$

$$\mu f g'' = -2\mu f' g' - 2\beta\kappa f', \tag{17}$$

where for ease of writing we have defined the (positive, because $\kappa > 0$) constant

$$\mu = mv^2 + \kappa > 0. \tag{18}$$

With the physical values (4), we get (here and below c is the speed of light)

$$\mu_{\text{phys}} \approx 5.032 + 2.804(v^2/c^2) \times 10^{11} \text{ eV}. \tag{19}$$

Equations (17) are ordinary differential equations describing traveling wave solutions for (the continuum approximation of) the BCP model. Note that the second of (17) is rewritten as

$$\frac{d}{dz}[\mu(f^2 g') + \beta\kappa f^2] = 0, \tag{20}$$

stating that the quantity in square brackets is conserved along the flow: we have the integral of motion

$$J := (\mu g' + \beta\kappa)f^2. \tag{21}$$

This also follows from the fact that $\mathcal{L}$ does not depend on Φ (see above), J being just the momentum conjugate to Φ under the traveling wave ansatz.

The conservation law (20) allows us to write

$$g' = [(J/f^2) - \beta\kappa]/\mu, \quad g'' = -2Jf'/(\mu f^3) \tag{22}$$

as solutions to (17); the constant J depends on initial data (recall that g' has the dimension of inverse length; J has the physical dimensions of an energy times length, $[M][L]^3[T]^{-2}$). With the physical values (4) we have

$$J_{\text{phys}} \approx f_0^2\{0.93AA^{-1} + g_0'[5.032 + 2.804(v/c)^2]\} \text{ eV}. \tag{23}$$

The dynamics is thus reduced [up to the quadrature corresponding to the first of (22)] to the single equation

$$f'' = \frac{1}{\mu^2}\left(\frac{J^2}{f^3} + \gamma f\right) - \frac{1}{2\mu}V'(f); \tag{24}$$

here we have simplified the writing by defining

$$\gamma := \beta^2\kappa(\mu - \kappa) = \beta^2\kappa m \ v^2 > 0. \tag{25}$$

With the physical values (4), the result is

$$\gamma_{\text{phys}} \approx 4.82 \times 10^{10}(v^2/c^2) \ (\text{eV/ Å})^2. \tag{26}$$

IV. THE EFFECTIVE POTENTIAL

We will now focus on the task of determining traveling wave solutions to the BCP model, i.e., solutions to (24). This can be seen as the equation for a point particle of unit mass in the *effective potential*

$$W(f) := \frac{1}{2\mu^2}\left(\mu V(f) + \frac{J^2}{f^2} - \gamma f^2\right) + W_0; \tag{27}$$

here W_0 is an additive arbitrary constant. The (conserved) total energy for the motion in this effective potential is of course given by

$$H(f,f') = \frac{1}{2}(f')^2 + W(f). \tag{28}$$

The motion with total energy E is thus described by

$$\frac{df}{dz} = \pm\sqrt{2[E - W(z)]}. \tag{29}$$

The effective potential W defined in (27) depends on the parameters J and μ (n addition to the physical parameters appearing in the Morse potential, which we consider as given); note that J is arbitrary (with $J>0$ if and only if $g' > -\beta\kappa/\mu$) and is identified by the initial conditions, while μ depends on the speed of the traveling wave. The values of these parameters affect not only the quantitative features of W, but its qualitative behavior as well, as we discuss in the following.

It follows easily from (27), the properties of the Morse potential, and $\mu > 0$ that

$$\lim_{f\to 0} W(f) = \infty, \quad \lim_{f\to\infty} W(f) = -\infty. \tag{30}$$

The potential can have zero or two critical points depending on the values of the parameters. We are especially interested in the case where the potential admits nontrivial solutions $f(z)$ which go to stationary points for $z \to \pm\infty$ [these correspond to solutions for which $R(x,t)$ is asymptotically constant for large $|x|$; due to conservation of J, this implies g' is also constant for large $|x|$].

In view of the properties of W, such large-amplitude traveling waves can exist only if W has a maximum, to which the required solution $f(z)$ is doubly asymptotic for $z \to \pm\infty$; this solution represents a separatrix for the phase portrait of (28). We have thus to determine for which values of the parameters this separatrix can exist, or equivalently for which values the potential $W(f)$ has a local maximum. With this aim, we write $W'(f)$ in the form

$$W'(f) = -\frac{1}{2\mu}[w_1(f) - w_2(f)],$$

$$w_1(f) := \frac{2}{\mu}[(J^2/f^3) + \gamma f],$$

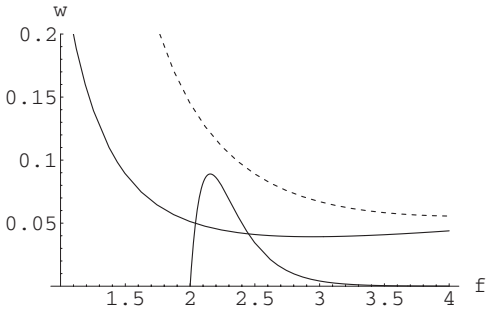

FIG. 1. Functions w_1 and w_2 defined in (31), with realistic values for the physical parameters [see (4)]. We plot the curve $w_2(f)$ (dotted) together with $w_1(f)$ for $J=1$, $\mu=2$, $\gamma=0.01$ (dashed) and for $J=0.5$, $\mu=2$, $\gamma=0.01$ (solid). This allows us to state that in the latter case traveling wave solutions are possible, while in the former they are not. See also Fig. 2.

$$w_2(f) := V'(f) = 2\alpha D e^{-\alpha(f-R_0)}(1 - e^{-\alpha(f-R_0)}) \tag{31}$$

(see Figs. 1–3). Points with $W'(f)=0$ correspond to crossing points for the graphs of w_1 and w_2. A sufficient condition to ensure these exist is provided by

$$w_2(f_0) \geq w_1(f_0), \tag{32}$$

where f_0 denotes the point where $w_2(f)$ attains its maximum. We have

$$f_0 = R_0 + \alpha^{-1} \ln(2), \tag{33}$$

so that $e^{-\alpha(f-R_0)}=1/2$; with the physical values (4) and (6) we get

$$(f_0)_{\text{phys}} \approx 2.156 \text{ Å}. \tag{34}$$

Using (33) together with (31), we immediately get

$$w_1(f_0) = [2(J^2 + \gamma f_0^4)](\mu f_0^3)^{-1},$$

$$w_2(f_0) = (D\alpha)/2. \tag{35}$$

The condition (32) then reads

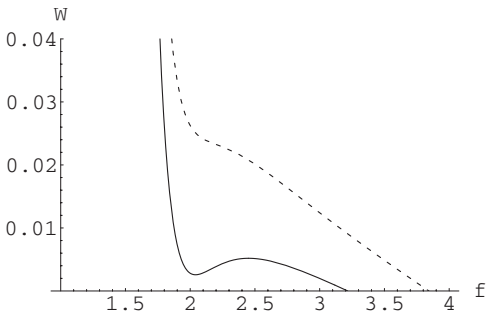

FIG. 2. Effective potential $W(f)$ for realistic values of the physical parameters [see (4)]. We plot the potential for $J=1$, $\mu=2$, $\gamma=0.01$ (dashed) and for $J=0.5$, $\mu=2$, $\gamma=0.01$ (solid). Note that in the latter case there is a local maximum—and solutions doubly asymptotic to it are possible—while in the former there is no critical point. This confirms the analysis based on the w_1 and w_2 functions; see Fig. 1.

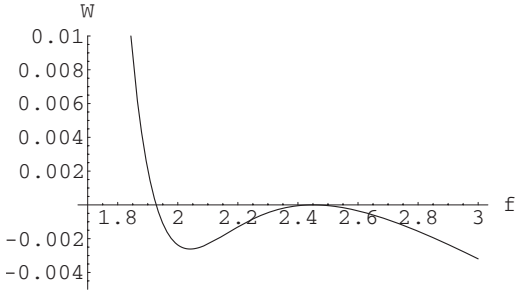

FIG. 3. Detail of the effective potential $W(f)$ in this case where (32) and (36) are satisfied and for the region of interest; the additive constant is chosen so that $E_0=0$. We have chosen realistic values of the physical parameters [see (4)], and $J=0.5$, $\mu=2$, $\gamma=0.01$.

$$4(J^2 + \gamma f_0^2) < (D\alpha)(\mu f_0^3). \tag{36}$$

Note that, while J is a free parameter, depending on initial conditions, γ can be expressed in terms of the physical parameters and v; doing this, (36) reads

$$\frac{v^2}{c^2} \leq \left(2.45 - 1.09\frac{J^2}{\text{eV}^2\ \text{Å}^2}\right) \times 10^{-12}. \tag{37}$$

This sets a limit on J to allow the existence of traveling wave solutions: it follows from (36) we should have $J^2 < [(D\alpha\mu f_0^3)/4 - \gamma f_0^2]$, and using physical values we get

$$J < J_0 \approx 1.5 \text{ eV Å}. \tag{38}$$

Finally, if crossing points exist we denote them by f_m and f_M, with $f_m < f_M$. We can immediately check that f_m (f_M) corresponds to the local minimum (local maximum) for $W(f)$.

V. TRAVELING WAVE SOLUTIONS AND ASYMPTOTIC BEHAVIOR

We assume from now on that (32) and (36) are satisfied, so that traveling solitary wave solutions exist; we discuss some features of these solutions.

A. Solutions

We denote again by f_M the point at which $W(f)$ has the local maximum, and by $E_0=W(f_M)$ the value of W at this point. Call, for ease of notation, f_1 the other point at which $W(f_1)=E_0$, and choose for definiteness $f(0)=f_1$. Then the solitary wave solution we are looking for is a solution to

$$\frac{df}{dz} = \pm\sqrt{-2[E_0 - W(f)]} \quad (\text{for } t = \pm|t|), \tag{39}$$

and is antisymmetric in t; by construction this satisfies $f_1 < f(z) < f_M$ for all z.

This is a separable equation, i.e., we can write

$$\int \frac{1}{\sqrt{-2[E_0 - V(f)]}} df = z. \tag{40}$$

Unfortunately, due to the functional form of the Morse potential, we are unable to perform the integral on the left-hand side; on the other hand, (39) is readily integrated numerically

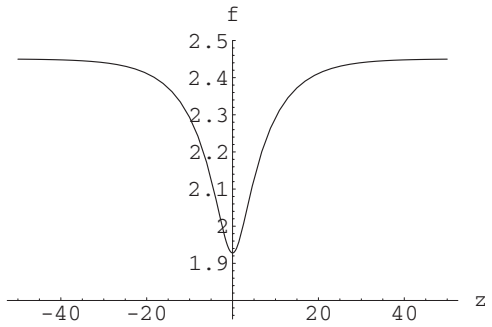

FIG. 4. Solitary wave solution $f(z)$ for W as in Fig. 3 (see caption there for values of the parameters); here f is given in angstroms. In this case $f_0 \simeq 2.4505$, $f_1 \simeq 1.9280$, and $E_0 \simeq 0.005185$.

(see Fig. 4). Once this $f(z)$ is known, the corresponding $g(z)$ is readily obtained from the integral of motion (21) (see Figs. 5 and 6).

B. Asymptotic behavior

We stress that the asymptotic behavior of the angle $g(z)$ for $z \to \pm\infty$ is given by

$$g(z) \approx c_{\pm} + \rho z; \tag{41}$$

correspondingly $f(z)$ is asymptotic to a constant value $f_\infty = f_M$ which is not exactly R_0, but slightly bigger. Obviously the constant of motion J can be evaluated on the asymptotic state; in this way we get

$$J = (\mu\rho + \beta\kappa) f_M^2. \tag{42}$$

The effective motion corresponds to an equilibrium between the restoring force due to the potential and the centrifugal force corresponding to the angular speed ρ.

In terms of the original system, the appearance of a traveling localized twist defect in the DNA double helix is accompanied by a long-range deformation consisting in the helix getting a slightly smaller pitch ahead of, and behind, the twist defect. It may be interesting to note that a connection between global twisting and existence of solitons was

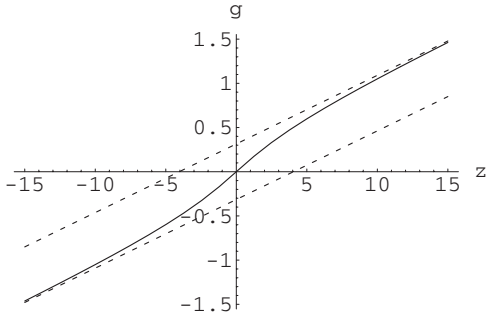

FIG. 5. Solution $g(z)$ corresponding to the $f(z)$ shown in Fig. 4. This is obtained making use of (21), with the values given in the caption to Fig. 3 for the constants J and μ; the value of σ is as in (6), and we plot, together with $g(z)$ (solid curve), also the solutions $g_{\pm}(z) = c_{\pm} + \rho z$ (dotted lines) to which it is asymptotic for $t \to \pm\infty$. These are obtained for $\rho \approx 0.077\,642\,2$, $c_{\pm} \approx \pm 0.314\,062$

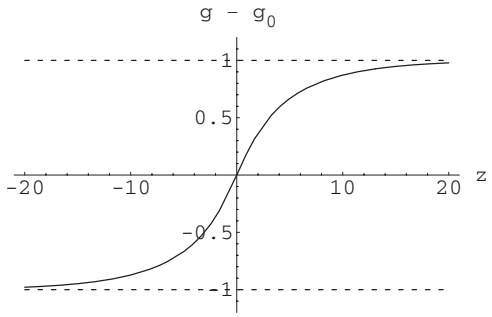

FIG. 6. $[g(z) - g_0(z)]/\pi$, with the definition $g_0(z) = \rho z$ with ρ as in the caption to Fig. 5, i.e., the angle shift with respect to a regular helix, measured in multiples of π.

also one of the conclusions reached by other authors [58] in their analysis of the Peyrard-Bishop-Dauxois model [10].

C. Standard helix as asymptotic condition

If we require that asymptotically (for $z \to \pm\infty$) $g'(z) \to 0$, then J is no longer a free parameter; it is instead determined as

$$J = \hat{J} := \beta\kappa f_M^2. \tag{43}$$

Note that f_M was defined as the local maximum for $W(f)$, which in turn depends on J. In this case we should define $\hat{W}(f)$ as $W(f)$ restricted to $J = \hat{J}$, that is,

$$\hat{W} = \frac{1}{2\mu^2}\left(\mu V(f) + \frac{\hat{J}^2}{f^2} - \gamma f^2\right). \tag{44}$$

This should satisfy a self-consistency condition, i.e., $\hat{W}'(f_M) = 0$; this reads explicitly

$$\alpha D e^{-\alpha(f_M - R_0)}(1 - e^{-\alpha(f_M - R_0)}) = \mu^{-1}(\beta^2\kappa^2 + \gamma) f_M = \beta^2\kappa f_M \tag{45}$$

(the last equality follows from the definition of γ). Note that in this condition no term depends explicitly on v; all parameters are fully determined in the physical case.

The condition (45) should be seen as an equation for f_M with given values of the physical parameters; this is a trascendental equation and hence cannot be solved in closed form. Moreover, we are not guaranteed a solution exists. When this is the case, the numerical solution for given values of the parameters is elementary.

When we set the parameters to their physical values, it turns out that (45) admits no solution. In order to have a solution, and keeping the experimental values for the geometrical parameters in the BCP model, we should set the ratio $D\alpha/K$ between coupling constants for different interactions to about four times its physical value (see Fig. 7). Thus we have shown that albeit traveling localized twist defects in the DNA double helix (as described by the BCP model) can exist, they cannot be asymptotic to the DNA double helix in its native (equilibrium) state for parameters in a physically acceptable range; in this range such solutions must instead be necessarily accompanied by an overtwisting of the helix in front of and behind them.

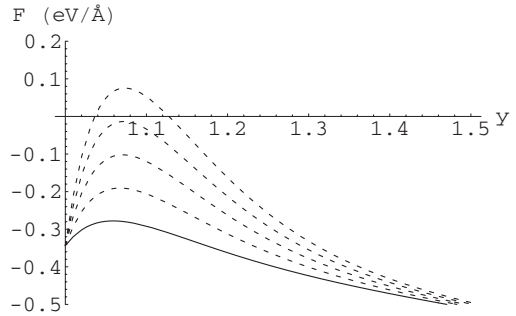

FIG. 7. Condition (45) expressed as $F(y)=0$, with $y=f_M/R_0$ and using the function $F(y)=\alpha De^{-\alpha R_0(y-1)}(1-e^{-\alpha R_0(y-1)})-\beta^2\kappa y R_0$. Here we plot $F(y)$ for physical values of all the parameters but D; the latter is set to q times its physical value ($D_0=0.04$ eV), and we plot $F(y)$ for $q=1$ (continuous line) as well as for $q=2,3,4,5$ (dashed lines, from below). The compatibility condition can first be satisfied when $q=q_0>4$, i.e., for a value of the coupling constant (actually, of the ratio between the coupling constants D and K, associated with the pairing and stacking interactions, respectively) which is more than four times the physical one.

VI. CONCLUSIONS AND DISCUSSION

We have considered the Barbi-Cocco-Peyrard twist-opening model for DNA dynamics [13–15], looking for traveling solitary wave excitations. We worked in a continuum approximation, so that the system is defined by the field Lagrangian (9), passing to a "helical" frame of reference by the simple change of coordinates (14). We noted that the Lagrangian does not depend on the field Φ and hence, by the Noether theorem [56,57], the model admits a conservation law.

With the traveling wave ansatz (16), the Euler-Lagrange field equations are reduced to the two ODEs (17); one of these is just stating that the quantity J defined in (21) is constant under the dynamics, so that we are reduced to the study of a single equation which depends parametrically on J. This equation can be seen as describing the motion of a particle of unit mass in the effective potential W.

The solitary wave solutions to the original partial differential equation (PDE) system we are looking for are represented by homoclinic solutions for this equation, doubly asymptotic to a local maximum of W; they exist only when the parameters entering into W are such that W itself admits a local maximum. We derived a condition for this to be the case, i.e., for the BCP model to admit traveling solitary wave (hence localized) solutions (32). This shows there will be a maximal allowed speed for such waves (36). The resulting equation cannot be solved exactly due to the specific form of the Morse potential, but we are guaranteed that solutions of the desired form exist—provided condition (32) is satisfied—and these are easily computed numerically.

Special attention should be given to the limiting conditions for this equation, inherited from boundary conditions for the Euler-Lagrange PDEs corresponding to the Lagrangian (14). In fact, solutions going asymptotically to the trivial equilibrium—identified by $R=R_0$ and $\Psi=2k\pi$—are possible only for a certain range of values of the parameters; this range does not include the physical values of parameters as identified by Barbi, Cocco, and Peyrard [5,13,15].

On the other hand, different limiting behaviors are also possible, corresponding to nontrivial equilibria. In terms of the resulting mechanical model for traveling wave solutions, these are obtained when the potential force produces the required centripetal acceleration to keep the mass in a circular motion. In terms of the DNA molecule, these correspond to a double helix with an untwisted region, a *twist defect*, which travels at constant speed and with a slight overtwisting in front of and behind the twist defect. The range of parameters for which these solutions are possible includes the physical range as identified in [5,13,15]. It should be stressed that checking a relation between the existence of solitons and a global overtwisting is within experimental reach, and actually goes in the same direction as the recent proposal by Zdravković and Satarić [28] of an experiment to check the existence and measure the speed of traveling solitons in DNA, based on their analysis in terms of the Peyrard-Bishop-Dauxois model [10].

We would like to make two final remarks concerning the relation of our work on the BCP model to parallel investigations on different DNA models. First, we note that our findings for the BCP model, and in particular the relation between traveling twist defects and overtwisting, could and should be compared with that arising from the study of other models also combining two degrees of freedom per nucleotide; in particular, those where both degrees of freedom are angular ones [29–31] (see the Appendix). In that case, traveling solitons (with physical values for the parameters appearing in the model) can exist with no need for the overtwisting needed in the BCP model. In this sense, an experiment of the type proposed by Zdravković and Satarić [28] could establish not only if traveling solitons are present in DNA in laboratory conditions, but also (in case they are found to exist) which one of the models analyzed in the literature—i.e., the Peyrad-Bishop-Dauxois [4,5,10], the Barbi-Cocco-Peyrard [4,5,13,15], the Cocco-Monasson [4,5,26], the Yakushevich [8,11], and the composite Yakushevich models [29,31,32]—better describes its features.

Second, we would like to mention that recent work [59] stressed the possible relevance of nonlinear stacking interaction—whose physical relevance was already pointed out by Peyrard and co-workers [4,5,10] (see also [26])—in the generation of traveling solitary waves with compact support; see also [60,61] in this respect. A different mechanism, based on a nonsmooth behavior of the on-site potential in elastic chains, was considered in separate work [62,63] (albeit not yet applied to DNA modeling). This might be relevant in the present context, as waves built by this mechanism would automatically have a limiting behavior corresponding to trivial equilibria (albeit carrying a nontrivial topological charge). It is thus natural to wonder if the BCP model, with modifications either in the stacking potential or in the pairing one, can carry twist defects with strictly compact support also within the physical range of parameters. If this was the case, one would like to investigate if an experiment such as the one proposed by Zdravković and Satarić [28] can discriminate between predictions by such models and those by fully smooth models; see above. This lies

well outside the limits of the present work, and we hope to be able to analyze this question in a later contribution.

ACKNOWLEDGMENTS

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APPENDIX: COMPARISON WITH DOUBLE-TWIST MODELS

As mentioned above, the BCP model [13–15] was the first to consider in precise mathematical terms a description of the DNA double chain associating with each nucleotide two degrees of freedom (a rectilinear and an angular one). A relevant extension of this model was provided by Cocco and Monasson [26], who considered the same topology—i.e., a phase manifold ($\mathbf{R}_+ \times S^1$) for each nucleotide—but a different geometry: in their model, the length of backbone units linking different sugars on DNA chains is fixed, but the distance between planes of subsequent base pairs can vary as a consequence of the backbone movements in space.

A different kind of model, still associating with each nucleotide two degrees of freedom, but in this case both angular (albeit one of them constrained to a finite region) was recently introduced in [29]. As in this case each nucleotide can change its state by exciting two rotation angles, we will refer to this class of models as *double twist* models. (Note that as one of the angle is restricted—to take into account steric hindrances related to the actual spatial conformation of the DNA molecule [1,2]—the phase manifold is in this case $I \times S^1$ for each nucleotide, where I is a finite interval.)

These models can be seen as an extension of the classical Yakushevich model [8,11,12] rather than of the Peyrard-Bishop one; it is thus not a surprise that they display a different behavior, especially concerning solitary wave solutions. In particular, it has been shown [29–32] that these support solitons that are deformations of standard sine-Gordon solitons [5,64] and in particular have speed near to that of the latter.

We recall in this respect that for the physical range of parameters the Y model admits soliton solutions (carrying an integer twist defect) with limiting solutions corresponding to trivial equilibria [5,7,8]. It should also be recalled that the Y model has a weak point in that it predicts an unphysical speed of transverse phonons with physical values of the parameters (or, seen from a different perspective, requires unphysical values of the parameters in order to fit the physical value of this speed) [65]; this is not the case with the double twist models [29–32].

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