Solitonic speed in DNA

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We propose a single molecule experiment that could be carried out in order to measure a solitonic wave speed in DNA. In addition, we discuss possible values of the speed according to the Peyrard-Bishop-Dauxois model of DNA dynamics.

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I. INTRODUCTION

A main goal of this paper is to justify the proposal of an experiment that, we believe, could be carried out in order to determine a speed of the solitonic wave in DNA. In that respect, we give a theoretical background relying on a well-known Peyrard-Bishop-Dauxois (PBD) model for DNA dynamics (Sec. II). This model is explained very briefly in this paper. As some undetermined parameters are involved in the model, we cannot calculate the wave speed precisely. However, we assesed reasonable intervals for these parameters and, consequently, are able to predict the interval of expected solitonic speed. In Sec. III we describe an experiment proposal to measure the wave speed. We suggest different initial deformations because we expect, relying on the PBD model, the solitonic wave to exist in DNA. Hence, if higher amplitude ensures higher velocity, which is typical for the solitons, then this will be a confirmation of the theoretical prediction that the existing wave is really the soliton. Finally, we give some concluding remarks in Sec. IV.

II. ESTIMATIONS ACCORDING TO THE PBD MODEL

Our theoretical calculations and predictions are based on the well-known (PBD) model of DNA [1]. This is an extended version of the Peyrard-Bishop model [2]. A key point is that the PBD model takes helicoidal structure of a DNA molecule into consideration. We assume that readers are familiar with the model. Hence, we only very briefly describe some basic points of the PBD model. Some more information and derivations can be found in Refs. [3,4].

According to the PBD model, the DNA chain is treated as a perfectly periodic structure with a period l. Only transversal motions are taken into consideration. The transversal hydrogen bonds between nucleotides of different strands are modeled by the Morse potential [1–4]. Suppose that u_n and v_n are the transversal displacements of the nucleotides of different strands at the site n from their equilibrium positions. Then, the Hamiltonian for the DNA chain has the form

$$H = \sum \left\{ \frac{m}{2}(\dot{u}_n^2 + \dot{v}_n^2) + \frac{k}{2}[(u_n - u_{n-1})^2 + (v_n - v_{n-1})^2] \right.$$
$$\left. + D[e^{-a(u_n - v_n)} - 1]^2 + \frac{K}{2}[(u_n - v_{n+h})^2 + (u_n - v_{n-h})^2] \right\}. \tag{1}$$

Parameters D and a are the depth and the inverse width of the Morse potential well and $k(K)$ is the harmonic constant of the longitudinal (helicoidal) spring.

It is convenient to introduce new coordinates x_n and y_n for the movement of the centre of mass of the nucleotide pair at the site n and the stretching of the pair, respectively. Hence, these coordinates describe the in-phase and the out-of-phase motions and are defined as

$$x_n = (u_n + v_n)/\sqrt{2}, \quad y_n = (u_n - v_n)/\sqrt{2}. \tag{2}$$

One can derive two decoupled dynamical equations of motion, linear for x_n and nonlinear for y_n [1,3,4],

$$m\ddot{x}_n = k(x_{n+1} + x_{n-1} - 2x_n) + K(x_{n+h} + x_{n-h} - 2x_n), \tag{3}$$

$$m\ddot{y}_n = k(y_{n+1} + y_{n-1} - 2y_n) - K(y_{n+h} + y_{n-h} + 2y_n)$$
$$+ 2\sqrt{2}aD(e^{-a\sqrt{2}y_n} - 1)e^{-a\sqrt{2}y_n}. \tag{4}$$

The solution $x_n(t)$ is a linear wave while the solution $y_n(t)$ represents a nonlinear solitonic wave [1,3,4]. Corresponding frequencies, e.g., the frequencies of the in-phase and the out-of-phase motions, usually called acoustical and optical, are [1,3,4]

$$\omega_x^2 \equiv \omega_a^2 = (4/m)[k \sin^2(ql/2) + K \sin^2(qhl/2)] \tag{5}$$

and

$$\omega_y^2 \equiv \omega_o^2 = (4/m)[a^2D + k \sin^2(ql/2) + K \cos^2(qhl/2)], \tag{6}$$

where $m = 5.1 \times 10^{-25}$ kg [3,4] is the nucleotide mass, $l = 0.34$ nm [1,2] is a distance between adjacent nucleotides of the same strand, and $h = 5$ [3,4]. The function $y_n(t)$ is a modulated solitonic wave [3–6], where $q = 2\pi/\lambda$ is the wave number of a carrier component of the wave. In this paper we use $ql = \pi/h$ [3,4].

Using a rather tedious procedure [1,3,4], one obtains the following expression for the function $y_n(t)$:

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$$y_n(t) = 2\varepsilon A \, \text{sech}\left(\frac{\varepsilon(nl - V_e t)}{L_e}\right)$$

$$\times \left\{ \cos(\Theta nl - \Omega t) + \varepsilon A \, \text{sech}\left(\frac{\varepsilon(nl - V_e t)}{L_e}\right) \right.$$

$$\left. \times \left[\frac{\mu}{2} + \delta \cos[2(\Theta nl - \Omega t)]\right]\right\} + O(\varepsilon^3), \quad (7)$$

where

$$\varepsilon A = \varepsilon \sqrt{\frac{u_e^2 - 2u_e u_c}{2PQ}}, \quad u_e > 2u_c, \quad (8)$$

$$\frac{L_e}{\varepsilon} = \frac{2P}{\varepsilon\sqrt{u_e^2 - 2u_e u_c}}, \quad (9)$$

$$P = \frac{1}{2\omega}\left\{\frac{l^2}{m}[k\cos(ql) - Kh^2\cos(qhl)] - V_g^2\right\}, \quad (10)$$

and the envelope velocity V_e is

$$V_e = V_g + \varepsilon u_e. \quad (11)$$

The speed V_g is a group velocity, defined as

$$V_g \equiv \frac{d\omega}{dq} = \frac{l}{m\omega}[k\sin(ql) - Kh\sin(qhl)], \quad (12)$$

where $\omega \equiv \omega_y$.

The meaning of the parameter $\varepsilon \ll 1$ is explained in the aforementioned references. Hence, we give only short explanation to make the paper self-contained. The essence of the model is that $y_n(t)$ is very small but big enough to be anharmonic. We introduce a function $\Phi_n(t)$, which, multiplied by $\varepsilon \ll 1$, gives small $y_n(t)$, e.g.,

$$y_n = \varepsilon \Phi_n, \quad \varepsilon \ll 1. \quad (13)$$

Then, we use the semidiscrete approximation and expect the solution to be a modulated solitonic wave [1–5]:

$$\Phi_n(t) = F_1(\varepsilon nl, \varepsilon t)e^{i\theta_n} + \varepsilon[F_0(\varepsilon nl, \varepsilon t) + F_2(\varepsilon nl, \varepsilon t)e^{i2\theta_n}] + \text{c.c.}$$

$$+ O(\varepsilon^2), \quad (14)$$

$$\theta_n = nql - \omega t, \quad (15)$$

where c.c. stands for conjugate complex and F_0 is real. The functions F_0 and F_2 can be expressed through the function F_1 [1–5], which is a solution of the nonlinear Schrödinger equation (NLSE) and all this brings about Eq. (7).

The expressions for all parameters in Eq. (7) that are not in this paper can be found in the cited references. One example for $k=8$ N/m, $K=0.1$ N/m, $a=0.9$ Å^{-1}, $D=0.06$ eV, and $n=300$ is shown in Fig. 1. It is obvious that the function $y_n(t)$ represents a modulated and localized wave. If such a localized wave is a function of $\xi = x - V_e t$ only then such function is a soliton, e.g., the solitonic wave. For $y_n(t)$, given by Eq. (7), this happens if velocities of the envelope and the carrier wave components are equal [5,6], e.g.,
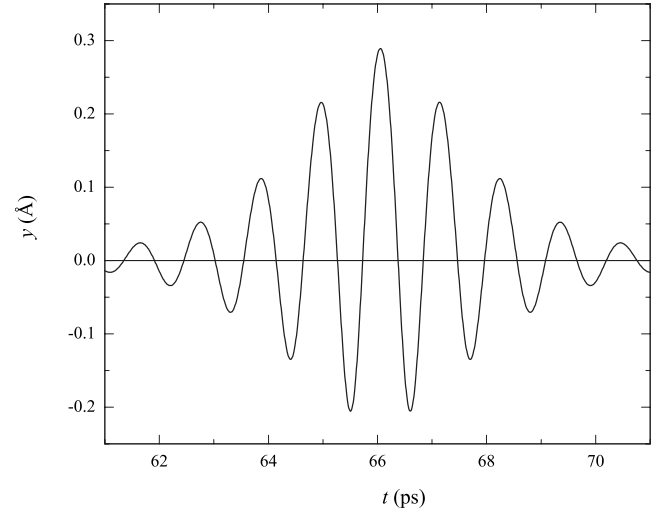

FIG. 1. Elongation of the out-of-phase motion as a function of time.

$$V_e = \Omega/\Theta. \quad (16)$$

This is what we call a coherent or a solitonic mode [5,6].

It is convenient to introduce a new dimensionless parameter η defined as

$$u_c = \eta u_e. \quad (17)$$

Figure 1 was carried out for $\eta = 0.47$ [6] while the value of the remaining parameter εu_e was obtained from the requirement for the solitonic mode. Namely, from Eq. (16) one can straightforwardly obtain a relation between the parameters u_e and u_c, e.g., a formula [6]

$$\varepsilon u_e = \frac{P}{1 - \eta}\left[-q + q\sqrt{1 + \frac{2(1-\eta)}{Pq^2}(\omega - qV_g)}\right]. \quad (18)$$

Note that the dispersion parameter P is positive and $\omega > qV_g$. The value of εu_e, for Fig. 1, is 643 m/s.

In order to justify the proposal for the appropriate experiment aimed to measure the speed of the above soliton we will make some estimations arising from the PBD model. As can be seen from Eqs. (11), (12), (6), (18), and (10), the speed V_e depends on the parameters $a^2 D$, k, K, and η. Unfortunately, the values of these parameters are not reliably known. In Ref. [5], we stated that a can probably not be above 1 Å^{-1}. For our estimations, we assume the interval $a \in [0.5 \text{ Å}^{-1}, 1 \text{ Å}^{-1}]$.

Regarding the parameter D, one can find the values from 0.03 eV [7] to 0.33 eV [2]. It is very likely that the values between 0.05 eV and 0.075 eV could be a good choice [8]. For our estimations, we assume the interval $D \in [0.04 \text{ eV}, 01 \text{ eV}]$. Hence, the chosen interval for $a^2 D$ becomes

$$a^2 D \in [0.2 \text{ N/m}, 1.6 \text{ N/m}]. \quad (19)$$

According to Eqs. (8) and (17), we know that η should be less than 0.5. We showed [6] that the values that are not far from its maximum are reasonable. For example, for Fig. 1, we picked up $\eta = 0.47$. Hence, we choose the interval
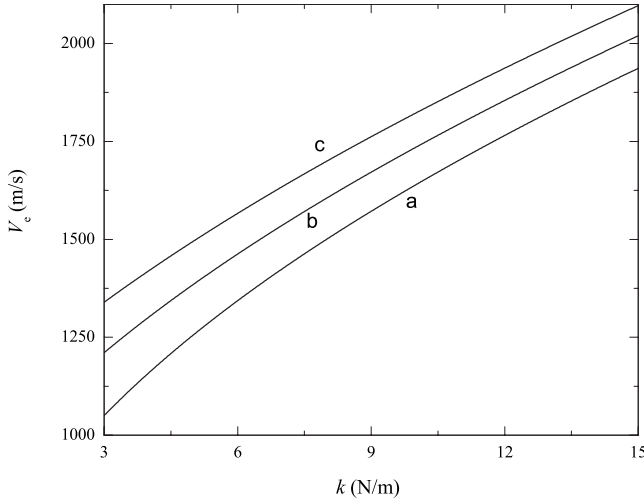
FIG. 2. Solitonic speed V_e as a function of the harmonic constant of the longitudinal spring k (a: $K=0.05$ N/m; b: $K=0.2$ N/m; c: $K=0.5$ N/m).

$$\eta \in [0.4, 0.48]. \tag{20}$$

The most uncertain parameters are k and K. Our choice for the pretty broad intervals of expected values are

$$k \in [3 \text{ N/m}, 20 \text{ N/m}] \tag{21}$$

and

$$K \in [0.05 \text{ N/m}, 1 \text{ N/m}]. \tag{22}$$

Note that all the combinations resulting from Eqs. (21) and (22) are not allowed. Studying a resonance mode in DNA, it was shown that there should be $k/K \leqslant 331$ [9] and $k/K \geqslant 70$ [10].

To calculate the smallest and the highest values of the solitonic speed we should know how V_e depends on these parameters. We start with the combination used for Fig. 1, that is $k=8$ N/m, $K=0.1$ N/m, $a^2D=0.78$ N/m, and $\eta=0.47$. One can easily plot the function V_e versus any of these parameters keeping the remaining three being fixed. For example, Fig. 2 shows how V_e depends on k for the three values of K and for $a^2D=0.78$ N/m and $\eta=0.47$. This figure, as well as the remaining three, shows that the solitonic speed V_e is the increasing function of all four parameters. Therefore, we can easily calculate the smallest V_e^s and the highest V_e^h values of V_e. These values are $V_e^s \approx 900$ m/s and $V_e^h \approx 2590$ m/s. The soliton shown in Fig. 1 moves with the speed of approximately 1544 m/s. If we pick up $k=15$ N/m and do not change the remaining three parameters we calculate the value $V_e \approx 1970$ m/s. Therefore, we can conclude that the solitonic speed is probably higher than 1000 m/s and is not too much above 2000 m/s.

A next step is to study how the variations of the four parameters affect V_e. For example, for $K=0.1$ N/m the solitonic speed V_e takes the values from $V_e^s \approx 1200$ m/s for $k=3$ N/m to $V_e^h \approx 2050$ m/s for $k=15$ N/m. Hence, one can say that the increase from V_e^s to V_e^h is about 71%. From the curve $V_e = V_e(K)$ we can see that these values are $V_e^s \approx 1550$ m/s and $V_e^h \approx 1950$ m/s, which means that the in-

crease is a little bit less than 26%. This is something we should not be surprised with. Namely, the wave speed depends on elasticity of the medium, e.g., of the DNA molecule in this case. This primarily depends on the parameter k, which describes strong covalent bonds. On the other hand, K describes weaker forces and, consequently, does not affect V_e as much as k. Note that we took into consideration the interval for k such that the ratio of the highest and the smallest k is about seven, which can be seen from Eq. (21). Even though the corresponding ratio for K is 20, the influence of K on V_e is smaller than the influence of the parameter k.

How about the parameter a^2D? It was explained above that a and D describe the transverse hydrogen bonds. Such interactions are soft as the forces between nucleotides at the same position belonging to different strand are pretty small. This means that we should expect smaller influence of a^2D on the speed V_e. Of course, we can plot the figure $V_e = V_e(a^2D)$ like $V_e = V_e(k)$ above. From such figure we can see that the smallest and the highest values of V_e are $V_e^s \approx 1440$ m/s and $V_e^h \approx 1650$ m/s, which means that the increase is about 14.5%.

We should keep in mind that the parameters k, K and a^2D describe geometry and chemistry, e.g., chemical interactions within DNA. However, η comes from the mathematical model. Namely, this parameter appears in a solution of the NLSE, which is not explained in this paper [1,3–5]. Of course, this model brings about the solution $y_n(t)$, given by Eq. (7). Hence, we expect very small or even almost negligible influence of this parameter on the solitonic speed V_e. Even if we took the highest possible interval from 0 to 0.5, the smallest and the highest values of V_e, e.g., V_e^s and V_e^h, would differ for less than 11%. However, for more reasonable interval for η, that is for Eq. (20), this influence is as small as about 2%.

As a conclusion, we can expect that the experimentally determined value of the solitonic speed would give us some closer informations about the aforementioned parameters k, K, and a^2D. We would be able to determine if not the precise value but at least the narrower interval for the parameter k, which would certainly improve our knowledge of the DNA dynamics.

III. EXPERIMENT PROPOSAL

The advent of novel methods of single biomolecule manipulation, visualization, and controlling have provided the opportunity to measure directly the forces holding molecular structures together and to make evidences of stress and strains generated in the course of chemical reactions. For example, DNA molecules under extreme tensional or torsional stress have been shown to exhibit new phases that may be relevant to cellular processes.

Smith *et al.* [11] published in 1992 the result of the first experiments in which a single DNA molecule was mechanically manipulated and stretched to determine its bending and extensional properties. This work was the bases of a number of assays of DNA dependent protein machines and laid the experimental and conceptual groundwork for studies of protein functions at the single-molecule level [12–18]. Those
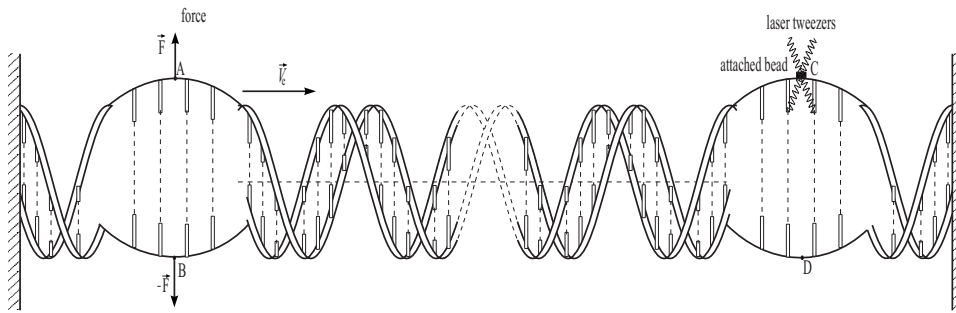
FIG. 3. Solitonic wave detection in DNA.

experiments were followed by theoretical research [19–23] and this research has been reviewed [7,24]. There were a couple of so-called unzipping experiments where mechanical strand separation was carried out [25–27]. Some papers report that interchain interaction was carried out in a different way. The complementary segments were covalently attached to opposing surfaces and force versus relative surface displacement was measured [28–30]. This helped us to estimate the highest value of the parameter a, which was mentioned above [5].

We now mention some of the most advanced tools designed to manipulate the single DNA molecule. These are optical or magnetic tweezers, atomic-force-microscope (AFM) cantilevers, or glass microfibers. In all of these techniques a DNA molecule has one and bound to a surface and the other to a force sensor. The force sensor is usually a micron-sized dielectric or magnetic bead or a cantilever, whose displacement could be measured in order to determine the force.

We believe that new single molecule experiments on DNA that yield the determination of the solitonic speed can be carried out. Figure 3 represents our suggestion for such an experiment. Nucleotide pair AB is stretched. This can be done using a cantilever, for example. In a certain moment, the force stretching the AB pair is released and the nucleotide pair AB begins to oscillate. Of course, this will affect the neighboring nucleotides and, after some time, the wave will reach the pair CD. This event could be detected using a laser tweezer, for example. Hence, one can detect the moment when the wave reaches the pair CD. As the distance AB-CD and the appropriate time are known, one can calculate V_e.

It is also possible that the cantilever, attached to the AB pair, is forced to oscillate with a certain frequency. After some time the pair CD will begin to oscillate, etc. For this variant of the experiment we suggest the frequency Ω from Eq. (7). For the values of the parameters η, a, D, k, and K chosen for Fig. 1, this frequency is $\Omega = 5.7$ rad/ps. According to the expression for the frequency Ω [3–5] one can easily show that Ω is the increasing function of η, a, D, and k and the decreasing function of K. Hence, the appropriate combinations of these parameters yield different possible values for the frequency Ω. According to the simple calculations this interval is between 3 rad/ps and 9 rad/ps. As was mentioned above, we take a very big interval of all the parameters into consideration. Therefore, a more realistic interval for Ω is probably between 4 rad/ps and 8 rad/ps.

In our proposed experiment, the double stranded DNA should be stretched and bound to the fixed surfaces. This must be performed in such a way that the chain of DNA be rigid enough to reduce the noise in measurements of transversal displacements of the nucleotide pairs. The length of stretched DNA chain should be long enough to be suitable for being bound transversally with two sensors distant enough to discriminate the time necessary for the breather soliton to travel the respective distance.

If the applied force F caused the examined DNA to be extended to the length L then the mean transversal fluctuations $\langle |\delta y| \rangle$ can be expressed as

$$\langle |\delta y| \rangle = \sqrt{\frac{k_B T L}{F}}. \qquad (23)$$

The nucleotide pair AB is being stretched by an AFM cantilever with an appropriate frequency, thus leading to excitation of a breather soliton in the AB region propagating along the DNA chain with corresponding velocity V_e. If this stable excitation reaches the position of the pair CD, where the second sensor was bound, the increased amplitude of the transversal oscillation should be detected. In our Fig. 3 the laser-tweezer was indicated just as an example. The sensor behaves like a noisy damped oscillator. The rout-mean-square noise δF in the force measurement depends solely on the dissipation due to the viscous friction as follows:

$$\delta F = \sqrt{4 k_B T \gamma \Delta f}, \qquad (24)$$

where γ is the viscous dissipation and Δf is the frequency bandwidth of the measurement. We hope that the AFM cantilever which can achieve angstrom-scale spatial resolution and estimates forces larger than 10 pN could be a proper candidate for sensing the breather reaching the position CD.

In what follows, we discuss possible evaluations of the initial deformation of the nucleotide pair AB required to excite the soliton. The amplitude of the solitonic wave is not known. In the example shown by Fig. 1 this value is $y_m = 0.29$ Å. Hence, we would suggest this value for the initial deformation. Note that the distance between the nucleotides belonging to the same pair is about 3 Å. As was explained above, we expect the nonlinear solitonic wave. It is well known that the velocity of the soliton depends on its amplitude. Higher amplitude means more localized wave and higher velocity. Therefore, we would suggest carrying out the experiments with the different initial deformations. To be more precise, higher initial deformation should ensure higher amplitude and, consequently, higher velocity. Hence, differ-

ent velocities corresponding to different initial deformations would be the confirmation of the theoretical prediction that the existing wave is really the solitonic one.

In what follows, we want to discuss one more important point. To carry out the proposed experiment the DNA molecule should be stretched. A crucial question is to what extent the molecule has to be stretched. Namely, it is possible to use small enough stretching force so that the helicoidal structure is preserved. On the other hand, if the applied force is much stronger, then the DNA can be completely stretched, e.g. the molecule becomes completely unwounded. In the first case, DNA is explained by the PBD model, as was explained above. For the second possibility one should use $K = 0$, which means that DNA would be described by the Peyrard-Bishop (PB) model. In other words, the PB model can be obtained from the PBD one by letting $K = 0$. To be more precise, the Hamiltonian (1), without the last term, represents the Hamiltonian of the PB model which does not take the helicoidal structure into consideration.

The advantage of the PBD over the PB model was shown in Ref. [3]. The soliton existing in DNA is the modulated wave, as was explained above. A density of internal oscillations (density of carrier wave oscillations) is larger for the bigger K [3]. This means that the modulation is better, e.g., more efficient, if the molecule is twisted, which means that $K > 0$. Also, the resonance mode [9] and an extremely high amplitude mode [31] cannot occur for $K = 0$. Therefore, we suggest that the experiment should be carried out over the helicoidal DNA. Such experiment might be more delicate but is certainly more realistic.

So far, we have explained the proposed experiment and have discussed some important points about it. It is the solitonic wave that we expect to be detected in DNA. However, one may ask if such wave really exists in the molecule. Hence, we want to explain why it is the soliton that we believe will be excited and probably detected in the experiment. This will be done according to both the basic theory, e.g., the PBD model, and numerical simulations.

First of all, DNA represents a system of mutually connected springs. According to the PBD model, there are three types of interactions and, consequently, three potential energy terms in the Hamiltonian (1). If only one spring is stretched then all the remaining springs will be affected after some time. In other words, if one nucleotide pair oscillates, like the pair AB in Fig. 1, then, after some time, the pair CD will also begin to oscillate. This means that a certain wave definitely exists in DNA as the wave is nothing but the movement of the disturbance along the molecule in time. We state that this wave is a solitonic one because Eq. (7) represents the true soliton providing Eq. (16) is satisfied. If Eq. (16) were not satisfied we would talk about an envelope soliton, which is completely irrelevant for the proposed experiment. A key point is that this wave does not depend on the initial conditions. Namely, Eq. (7) is a result of the Hamiltonian (1) and the applied procedure only. We should keep in mind that the function F_1 in Eq. (14) is the solution of the NLSE while $y_n(t)$ is obtained from Eqs. (13)–(15) and the applied procedure. Therefore, the function F_1, as well as $y_n(t)$, does not depend on the initial conditions, otherwise, it would not depend on the parameters ε, u_e and u_c. In other words, the initial conditions were not used to determine the values of these parameters! Therefore, the wave (7) is a result of the molecule itself, e.g., of the geometry and the chemistry determining it.

Of course, all this is still not the exact proof that the wave is really the soliton. We rely on the PBD model which may be wrong. So, either some experiments and/or numerical simulations are needed to support or deny our statements. We want to point out that the experiment proposed in this paper might be useful in this regard. Namely, as was explained above, the solitonic speed depends on its amplitude. The amplitude represents the initial stretching of the AB pair. Hence, if the wave speed depends on the amplitude, we can say that this is nothing but the confirmation that the wave is really the soliton.

In what follows, we discuss the results of some numerical simulations. It is worth noting that such simulations refer to the NLSE, e.g., the function F_1 in Eq. (14). This function, as well as the whole procedure, is explained in the aforementioned references. However, in simple words, one can say that F_1 is more or less Eq. (7) without the term with ε^2, as can be seen from Eq. (14). This "more or less" means that the solution of the NLSE if a function of different time and space coordinates but, basically, this is the first part of Eq. (7). The influence of the second part of Eq. (7) can be seen from Fig. 1. Namely, the figure has higher positive than negative amplitude but the figure would be basically the same without the term with ε^2.

In Ref. [32] authors studied the solutions of the NLSE for three initial conditions. One of them certainly corresponds to our proposal where the cantilever attached the pair AB would oscillate. To be more precise, this initial condition is a product of the exponential function and the secans hyperbolic component. This is, practically, our function F_1 for $t = 0$. It is shown [32] that this numerical simulation brought about the envelope solitonic wave. This is the wave like the one in Fig. 1 but without internal oscillations. The lack of the modulation is probably the result of some approximations in the numerical procedure. However, this is completely irrelevant from the point of view of the proposed experiment. Namely, the experiment will probably detect the envelope of the soliton in Fig. 1 and this is the same as was predicted by Ref. [32].

One more initial condition, relevant for the proposed experiment, was discussed in Ref. [32]. This is the function sech x. This initial condition corresponds to our proposal where the cantilever attached to the pair AB does not oscillate except the thermal vibrations. Namely, the shape of the DNA segment containing the stretched AB pair and, probably, a few more around them, is like this function or, at least, very similar.

The numerical simulations with this initial condition were studied in more details in Ref. [33]. Namely, the NLSE

$$iu_t + u_{xx} + \kappa |u|^2 u = 0 \qquad (25)$$

and the initial condition

$$u(x,0) = \operatorname{sech} x \qquad (26)$$

bring about the following three possible solutions (N is a positive integer). (1) If $\kappa = 2N^2$ then $u(x,t)$ is a "bound state of N solitons" [33,34]. (2) If $2N^2 < \kappa < 2(N+1)$ then the asymptotic solution comprises both such a bound state and an $O(t^{-1/2})$ oscillation [33]. (3) If $\kappa < 2$ then only the $O(t^{-1/2})$ oscillation is present [33].

The parameter existing in the PBD model, which correspond to κ is Q. This parameter depends on k, K, a and D. It was explained above that the values of these parameters are not known. However, reasonable values of them confirm that κ can not be less than two. For example, our choice for Fig. 1 brings about $\kappa \approx 4.4$. Therefore, we can conclude that the initial condition (26) yields a solitonic solution of the NLSE. To be more precise, the signal is like the envelope of the function $y_n(t)$ shown in Fig. 1. Therefore, we can conclude that these numerical simulations give support to our statements.

In the end, we should discuss one more important point. The solution of Eq. (4) is the nonlinear solitonic wave $y_n(t)$, given by Eq. (7). But, how about Eq. (3)? Obviously, this is the linear equation and its solution is an ordinary wave. Hence, introducing the continuous variable $nl \rightarrow z$, we can obtain the following wave equation:

$$\frac{\partial^2 x(z,t)}{\partial t^2} - V_x{}^2 \frac{\partial^2 x(z,t)}{\partial z^2} = 0, \qquad (27)$$

where

$$V_x{}^2 = \frac{l^2}{m}(k + h^2 K). \qquad (28)$$

Of course, its solution is of the form

$$x_n(t) = B \cos(\Theta_x nl - \Omega_x t), \quad \frac{\Omega_x}{\Theta_x} = V_x. \qquad (29)$$

Hence, according to Eqs. (2), (7), and (29), we can easily obtain the expressions for the displacements $u_n(t)$ and $v_n(t)$. It is important to keep in mind that the out-of-phase oscillations are determined by the weak hydrogen bonds, while the in-phase oscillations are bounded by the strong covalent forces. Therefore, the amplitude B should be much smaller than the amplitude A and, consequently, $x_n(t)$ can be neglected. This means that we do not expect a detection of both the optical and the acoustical waves. It is much more likely that the in-phase wave, represented by $x_n(t)$, will be just a noise.

However, we should not disregard a possibility for a more optimistic result of the experiment. Hence, in what follows, we compare the speeds of the nonlinear and the linear components of the wave. Note that the speed V_x depends on two parameters only, as can be seen from Eq. (28). Hence, if we knew the value of V_x we would have some very important information about the parameters k and K. In Fig. 4 we compare the speeds V_e and V_x. Namely, a ratio V_e/V_x as a function of k is showed. One can see that the speed V_e is higher
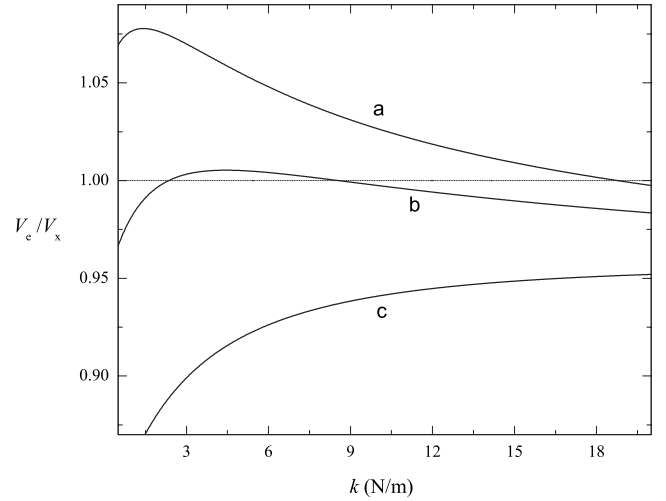

FIG. 4. Ratio V_e/V_x as a function of k (a: $K = 0.05$ N/m, b: $K = 0.1$ N/m, c: $K = 0.2$ N/m).

than V_x for K small enough. For example, line a shows that the ratio V_e/V_x is higher than one for $k < 18.8$ N/m. It is quite opposite for large K. For $K = 0.2$ N/m (line c) the linear wave is faster than the nonlinear one for any k. In Fig. 4(b), these speeds are equal for $k_1 = 2.4$ N/m and $k_2 = 8.6$ N/m.

IV. CONCLUDING REMARKS

In this paper, we suggested the single molecule experiment on the DNA molecule. The purpose of this experiment would be the attempt to measure the solitonic speed. At the same time that would confirm the existence of the nonlinear solitonic wave in the DNA molecule. Hence, such an experiment might be a support to a couple of models that describe the DNA dynamics and predict the existence of the nonlinear waves in DNA.

We also estimated the speed of the solitons relying on the PBD model. Of course, similar estimations can be done using some other models. We want to mention only one of them [35]. The PBD model describes the nucleotide pair oscillations using the displacements u_n and v_n, as was explained above. In Ref. [35], radial and angular displacements were used. The derivations are much more complicated and the partial differential equations for both variables are nonlinear. However, the conclusions are basically the same. Namely, according to the helicoidal model for DNA opening [35], the nonlinear localized wave is expected again. This can be the true soliton if Eq. (16) is satisfied, where V_e, Θ and Ω have the same meaning as in the PBD model. All this certainly means that the results of the proposed experiment could be compared with known theoretical models and justify or deny them.

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