Energy patterns in twist-opening models of DNA with solvent interactions

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Abstract Energy localization, via modulation instability, is addressed in a modified twist-opening model of DNA with solvent interactions. The Fourier expansion method is used to reduce the complex roto-torsional equations of the system to a set of discrete coupled nonlinear Schrödinger equations, which are used to perform the analytical investigation of modulation instability. We find that the instability criterion is highly influenced by the solvent parameters. Direct numerical simulations, performed on the generic model, further confirm our analytical predictions, as solvent interactions bring about highly localized energy patterns. These patterns are also shown to be robust under thermal fluctuations.

Keywords DNA · Solvent interaction · Modulational instability · Energy localization

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1 Introduction

DNA is fundamental in the life of all organisms, as it encodes the information needed for life and reproduction. To fully ensure its functions, DNA undergoes complex dynamical processes, which involve important structural deformations of its double helix. During the last decades, deep investigations have been carried out to effectively establish the relationship between these deformations and solitonic structures, the starting point being the seminal work by Englander et al. [1]. Thereafter, simplified models were proposed to describe the angular distortion of DNA [2–4] on the one hand while, on the other hand, all the evidence was brought to rather show the deep importance of radial displacements of bases during the processes of replication and transcription [5–7], via micromanipulation experiments of real DNA molecules. Indeed, the Peyrard–Bishop (PB) model has gained popularity in that direction, as it has successfully been used to analyze experiments on short DNA sequences [8]. Besides, the PB model has been adopted to evaluate the effects of inhomogeneities for the sharp staircase spectrum of the melting curve to be observed [9]. In recent years, more refined experiments of DNA micromechanics have revealed the involvement of various structural degrees of freedom in the dynamics of DNA, thus calling for more elaborated mathematical models including torsional and radial degrees of freedom. The PB model has been improved in that direction to efficiently model real DNA molecules [10–12], with insistence on the cooperative effects of unwinding and hydrogen bond oscillations in the process of transcription. Along with various enzymatic processes, *in vivo* helix-to-coil denaturation transition in DNA, via ultraviolet light absorption spectroscopy and small-angle neutron scattering, has been shown to be significantly influenced by the solvent surrounding the molecule in its environment [13]. In the same context, molecular dynamics simulations of DNA melting were performed [14, 15], indicating to sharp transition under solvent interaction effects. Similar arguments have been raised in the harmonic PB model, where a sharp transition for DNA melting was reproduced [16]. In this regard, a better understanding of some key biological phenomena in DNA dynamics requires the inclusion of such effects in more realistic models such as the twist-opening effect. This is addressed in this work, with a particular interest on energy localization. A direct mechanism leading to spontaneous energy localization in nonlinear systems is modulational instability (MI), which is the result of the interplay between nonlinear and dispersive effects, inherent to DNA and protein nonlinear models [17–20]. The way solvent interactions affect the emergence of energy patterns, under the activation of MI, in the twist-opening model of DNA is the main focus of the present contribution. In Section 2, we present the modified twist-opening model of DNA dynamics and the Fourier expansion method is used to show that angular and radial deformations can reduce to a set of discrete coupled nonlinear Schrödinger (DCNLS) equations. In Section 3, the linear stability analysis of plane waves, and solutions of the DCNLS equations, is obtained and confirmed by direct numerical simulations on the full DNA model. Patterns of energy are obtained and their robustness against thermal fluctuations is addressed. Some conclusions are drawn in Section 4.

2 Model and mathematical background

2.1 The model

The twist-opening model of DNA combines radial and torsional effects to reproduce the Watson–Crick B-DNA form. Taking n as the base index, the spatial structure of the molecule

Fig. 1 Schematic representation of the fixed-planes DNA anharmonic twist-opening model. r_n and ϕ_n are radial and torsional degrees of freedom, whose equilibrium values are R_0 and θ_0 . L is the length of the backbone segment connecting the attachment point of the bases along each strand and h is the fixed distance between two base planes in the B-DNA configuration

is described by a polar coordinate system in the plane perpendicular to the helical axis, where r_n is the radius and ϕ_n the angle of the n th base pair [10–12] as depicted in Fig. 1. The bonds that make the sugar-phosphate backbone are assumed to have an equilibrium length L , and the distance h between base planes is taken as constant. The Lagrangian describing the dynamics of such a complex system can be written as

$$\mathcal{L}_{BCP} = \sum_{n=0}^N T(\dot{r}_n, \dot{\phi}_n) - V_M(r_n) - V_s(\phi_n, \phi_{n-1}) - V_b(r_n, r_{n-1}), \quad (1)$$

where the first term, $T(\dot{r}_n, \dot{\phi}_n) = (m\dot{r}_n^2 + m\dot{\phi}_n^2)$, is the kinetic energy, with m being the reduced mass of a base pair. The hydrogen bond interactions between two bases in a pair are described by the Morse potential $V_M(r_n) = D[e^{-a(r_n - R_0)} - 1]^2$, where D is the dissociation energy and a the width of the Morse well. The term $V_s(\phi_n, \phi_{n-1}) = G_0(\phi_{n+1} + \phi_{n-1} - 2\phi_n)^2$ prevents the molecule from adopting a zigzag behavior by constraining each twist angle to have almost the same value as that of the previous one. The last term in expression (1) represents the stacking energy, $V_b(r_n, r_{n-1}) = K(\ell_n - L)^2$, between adjacent base pairs, where K stands for the coupling constant. The distance between planes of successive base pairs is denoted by h , while ℓ_n gives the length of the phosphodiester chain linking base pairs at sites n and $n + 1$ on the same chain. It is given as

$$\ell_n = \sqrt{h^2 + r_{n-1}^2 + r_n^2 - 2r_{n-1}r_n \cos(\phi_n - \phi_{n-1})}, \quad (2)$$

and its equilibrium value L is

$$L = \sqrt{h^2 + 4R_0^2 \sin^2\left(\frac{\theta_0}{2}\right)} > h. \quad (3)$$

In Eq. 3, θ_0 is the equilibrium twist angle between two consecutive base pairs.

Fig. 2 The Morse-solvent potential for two values of the solvent barrier factor f_s : (a) $f_s = 0.1$, and (b) $f_s = 0.3$. l_s sets the range of the potential V_{sol} so that, when $(r_n - R_0) < l_s$, the base pairs undergo large oscillations until the hydrogen bonds are broken and linked to solvent molecules. The plateau that appears for $(r_n - R_0) > l_s$ represents a situation where the unstacked regions are stabilized by free solvent molecules, which prevents them from re-closing

In order to introduce solvent effects in the above-described model, we modify the Morse potential as in Ref. [16] to obtain

$$\begin{aligned} V(r_n - R_0) &= D \left(e^{-a(r_n - R_0)} - 1 \right)^2 - D f_s \left[\tanh \left(\frac{r_n - R_0}{l_s} \right) - 1 \right] \\ &= V_M(r_n - R_0) + V_{sol}(r_n - R_0). \end{aligned} \quad (4)$$

The first term in Eq. 4 is the celebrated Morse potential, and the second one brings about solvent interactions between the unstacked bases and the environmental solvent. Comparisons between the Morse and “Morse-solvent” potential are made in Fig. 2. l_s sets the range of the potential $V_{sol}(r_n - R_0)$ so that, when $(r_n - R_0) < l_s$, the base pairs undergo large oscillations until the hydrogen bonds are broken and linked to solvent molecules. The plateau that appears for $(r_n - R_0) > l_s$ represents a situation where the unstacked bases are stabilized by free solvent molecules that prevent them from re-closing. The potential V_{sol} introduces a potential barrier in the Morse potential, characterized by the factor $f_s D$, which prevents unstacked bases from re-closing after the hydrogen bonds have been broken. For the original twist-opening model, values of parameters are given in Table 1 [10], while we discuss the suitable values for the parameters l_s and f_s . The unit system adopted in the table defines a time unit (t.u.), which corresponds to 0.01021 ps. Furthermore, to simplify the problem, we introduce the following dimensionless parameters

$$\begin{aligned} u_n &\rightarrow a(r_n - R_0), \quad \phi_n \rightarrow a R_0 (\phi_n - n \theta_0), \quad R_0 \rightarrow a R_0 \\ G_0 &\rightarrow \frac{G_0}{D}, \quad t \rightarrow \sqrt{\frac{D a^2}{m}} t, \quad K \rightarrow \frac{K}{D a^2}, \quad L_s \rightarrow a l_s \end{aligned} \quad (5)$$

Fig. 3 The optical (blue line) and acoustical (red line) frequencies for different values of the factor l_s . For the optical branch, the lower cut-off value, i.e., $\omega_+(q = 0)$, changes with l_s , compared to the no-solvent (NS) situation. For the acoustical frequency, it is rather its upper cut-off, i.e., $\omega_-(q = \pi)$, which increases with l_s

and we expand the stacking energy up to the second order

$$K \left(\sqrt{h^2 + r_{n-1}^2 + r_n^2 - 2r_{n-1}r_n \cos(\phi_n - \phi_{n-1})} - L \right)^2 \simeq K \frac{R_0^2}{L^2} \left[(\phi_n - \phi_{n-1}) \sin \theta_0 + (y_n + y_{n-1})(1 - \cos \theta_0) \right]^2. \quad (6)$$

With all these assumptions, the Lagrangian (1) reduces to

$$\mathcal{L}_{MBCP} = \sum_n \left\{ \left[\dot{u}_n^2 + \frac{1}{R_0^2} (u_n + R_0)^2 \dot{\phi}_n^2 \right] - G(\phi_{n+1} + \phi_{n-1} - 2\phi_n)^2 - (e^{-u_n} - 1)^2 + f_s \left[\tanh \left(\frac{u_n}{L_s} \right) - 1 \right] - \frac{K R_0^2}{L^2} \left[(\phi_n - \phi_{n-1}) \sin \theta_0 + 2(u_n + u_{n-1}) \sin^2 \frac{\theta_0}{2} \right]^2 \right\}. \quad (7)$$

From the above, we obtain the following set of equations for the radial and torsional dynamics of the DNA double helix

$$\ddot{u}_n = \frac{1}{R_0^2} (u_n + R_0) \dot{\phi}_n^2 - \frac{K_{u\phi}}{2} (\phi_{n+1} - \phi_{n-1}) - K_{uu} (u_{n+1} + u_{n-1} + 2u_n) + (e^{-2u_n} - e^{-u_n}) - \frac{f_s}{2L_s} \operatorname{sech}^2 \left(\frac{u_n}{L_s} \right) \quad (8)$$

$$\ddot{\phi}_n = K_{\phi\phi} (\phi_{n+1} + \phi_{n-1} - 2\phi_n) + \frac{1}{2} K_{u\phi} (u_{n+1} - u_{n-1}) - \frac{2}{R_0} \dot{u}_n \dot{\phi}_n - G(\phi_{n+2} + \phi_{n-2} - 4\phi_{n+1} - 4\phi_{n-1} + 6\phi_n) - \frac{2}{R_0^2} u_n \dot{u}_n \dot{\phi}_n - \frac{1}{R_0^2} u_n^2 \ddot{\phi}_n - \frac{2}{R_0^2} u_n \ddot{\phi}_n,$$

where

$$K_{\phi\phi} = \frac{4K R_0^2}{L^2} \sin(\theta_0) \sin^2 \left(\frac{\theta_0}{2} \right), \quad K_{uu} = \frac{4K R_0^2}{L^2} \sin^4 \left(\frac{\theta_0}{2} \right), \quad \text{and} \quad K_{u\phi} = \frac{K R_0^2}{L^2} \sin^2(\theta_0).$$

For mathematical manipulations, we expand the terms in exponential and sech around the minimum of the Morse-solvent potential, up to the third order, and Eq. (8) become

Fig. 4 The instability gain is plotted versus the barrier factor f_s . In *a*, we have fixed $Q = 0.25\pi$, while in panel *b* the perturbation wavenumber is fixed as $Q = 0.75\pi$. Solvent and no-solvent (NS) cases are compared. The dashed blue line indicates the reference for the NS case

$$\ddot{u}_n = \frac{1}{R_0} \left(1 + \frac{u_n}{R_0} \right) \dot{\phi}_n^2 - K_{uu}(u_{n+1} + u_{n-1} + 2u_n) + \frac{1}{2} K_{u\phi}(\phi_{n+1} - \phi_{n-1}) + C_1 u_n + C_2 u_n^2 + C_3 u_n^3 + C_4, \quad (9)$$

$$\ddot{\phi}_n = K_{\phi\phi}(\phi_{n+1} + \phi_{n-1} - 2\phi_n) + \frac{1}{2} K_{u\phi}(u_{n+1} - u_{n-1}) - \frac{2}{R_0} \dot{u}_n \dot{\phi}_n - \frac{2}{R_0^2} u_n \dot{u}_n \dot{\phi}_n - \frac{1}{R_0^2} u_n^2 \ddot{\phi}_n - \frac{2}{R_0^2} u_n \ddot{\phi}_n - G(\phi_{n+2} + \phi_{n-2} - 4\phi_{n+1} - 4\phi_{n-1} + 6\phi_n),$$

where the different coefficients of Eq. 9 are as follows

$$\begin{aligned} C_1 &= 4e^{-2u_0} - 2e^{-u_0} + \frac{2f_s \operatorname{sech}\left(\frac{u_0}{L_s}\right)^2 \tanh\left(\frac{u_0}{L_s}\right)}{L_s^2} \\ C_2 &= \frac{f_s \operatorname{sech}\left(\frac{u_0}{L_s}\right)^2 \tanh\left(\frac{u_0}{L_s}\right)}{L_s^3} + \frac{f_s \operatorname{sech}\left(\frac{u_0}{L_s}\right)^2 \tanh\left(\frac{u_0}{L_s}\right)^2}{L_s^3} - 4e^{-2u_0} + e^{-u_0}, \\ C_3 &= -\frac{8f_s \operatorname{sech}\left(\frac{u_0}{L_s}\right)^2 \tanh\left(\frac{u_0}{L_s}\right)}{3L_s^4} + \frac{4f_s \operatorname{sech}\left(\frac{u_0}{L_s}\right)^2 \tanh\left(\frac{u_0}{L_s}\right)^3}{L_s^4} + \frac{8e^{-2u_0} - e^{-u_0}}{3} \\ C_4 &= -2e^{-2u_0} + 2e^{-u_0} - \frac{f_s \operatorname{sech}\left(\frac{u_0}{L_s}\right)^2}{L_s}, \quad G = \frac{G_0}{R_0^2}. \end{aligned}$$

The linear dispersion relation of the studied model is obtained by keeping only linear terms in Eq. 9, and assuming solutions in the form of plane waves, i.e., $u_n(t) = D_1 e^{i(qn - \omega t)} + c.c.$ and $\phi_n(t) = D_2 e^{i(qn - \omega t)} + c.c..$ The frequency ω and the wave number q are then related by the linear dispersion relation

$$\omega_{\pm}^2 = \frac{1}{2} \left[d_1 + d_3 \pm \sqrt{(d_2 + d_3)^2 + 4|d_2|^2 - 4d_1 d_3} \right], \quad (10)$$

Fig. 5 Plots of the instability gain versus Q for $q = 0.25\pi$ (a) and $q = 0.75\pi$ (b). In panel a, the comparison is clearly made between the no-solvent case, i.e., $f_s = 0$ and when the solvent is taken into account, i.e., $f_s \neq 0$. In panel b, the two regions of instability progressively come together with increasing l_s to form only one region of instability

with $d_1 = -4K_{uu} \cos^2(\frac{q}{2}) + C_1$, $d_2 = iK_{u\phi} \sin(q)$, and $d_3 = -4 \sin^2(\frac{q}{2}) [K_{\phi\phi} + 4G \sin^2(\frac{q}{2})]$. The (+) and (−) signs stand for the optical and acoustical branches, respectively. The optical and acoustical frequencies, versus the wavenumber q , are displayed in Fig. 3, where the important effects of solvent interactions are obvious. For the optical branch, the lower cut-off value, i.e., $\omega_+(q = 0)$, changes with l_s , compared to the no-solvent (NS) situation. For the acoustical frequency, it is rather its upper cut-off, i.e., $\omega_-(q = \pi)$, which increases with l_s .

2.2 Amplitude equations

Equation (9) is discrete with strong nonlinearity, and cannot be solved easily. As many other systems, these equations can be reduced to more manipulable expressions without losing their characteristics. Among the methods generally used to handle such problems, we have the multiple scale expansion [18, 21, 22], the semi-discrete approximation [22, 23], and the method proposed by Johansson et al. [24], just to cite a few. These methods generally lead to nonlinear Schrödinger equations, in the continuum or discrete approximation. However, the method of Ref. [11, 12, 24] has been extensively used in the study of DNA nonlinear

Table 1 Typical parameter values for the modified twist-opening model of DNA nonlinear dynamics [10]

Parameter	M	D	a	K	θ_0	R_0	G_0
Value	300 amu	0.01 – 0.1 eV	$4.45 \text{ \AA}^{-1}$	$0.025 - 1.0 \text{ eV} \cdot \text{ \AA}^{-2}$	$\pi/5$	$10 \text{ \AA}$	$\frac{KR_0^2}{2}$

In general, some parameters like D , a and K can be chosen in an interval, which depends on the base sequence of the DNA portion

Fig. 6 Stability/instability diagrams are depicted with their corresponding gain of instability. We have fixed $f_s = 0.3$, $x_0 = 0.5$ and: (a1)-(a2) $l_s = 1$; (b1)-(b2) $l_s = 3$; (c1)-(c2) $l_s = 6$ and (d1)-(d2) $l_s = 8$. *Black regions* in stability/instability diagrams are regions of instability, the plane wave solutions are expected to break into trains of localized structures. White regions are where the plane waves are expected to remain stable under modulation. The instability gains display the same features as their corresponding diagrams. In general, increasing l_s obviously reduces instability regions as only one region remains for higher values of l_s

Fig. 7 Energy patterns generated by stable plane-wave oscillations. The wavenumber q and Q have been chosen in the *white regions* of diagrams of Fig. 6, i.e., $q = 0.75\pi$ and $Q = 0.45\pi$. We have also fixed $x_0 = 0.5$, $f_s = 0.3$ and: (a) $l_s = 1$; (b) $l_s = 6$. *Red patterns* indicate highest energy densities, where for $l_s = 1$, $E_n = 1.09 \times 10^{-3} \simeq 4.36 \times 10^{-5}$ eV, and $E_n = 7.8 \times 10^{-3} \simeq 3.12 \times 10^{-4}$ eV for $l_s = 6$

dynamics [11, 12], as it introduces important nonlinear effects. As we adopt it in this work, solutions for Eq. 9 are introduced as Fourier series, i.e.,

$$u_n(t) = \sum_{p=-\infty}^{\infty} a_n^{(p)} e^{ip\omega_b t} \quad \text{and} \quad \phi_n(t) = \sum_{p=-\infty}^{\infty} b_n^{(p)} e^{ip\omega_b t}, \quad (11)$$

where ω_b is close to some linear oscillation frequency and the Fourier coefficients $a_n^{(p)}(\epsilon^2 t)$ and $b_n^{(p)}(\epsilon^2 t)$ are time-dependent. Due to exponential decay of the Fourier coefficients in p , these Fourier coefficients must satisfy $a_n^{(p)} \sim \epsilon^p$ and $b_n^{(p)} \sim \epsilon^p$ for $p > 0$, while $a_n^{(0)} \sim \epsilon^2$ and $b_n^{(0)} \sim \epsilon^2$. Moreover, $a_n^{(p)} = (a_n^{(-p)})^*$ and $b_n^{(p)} = (b_n^{(-p)})^*$ since u_n and ϕ_n are real.

Reporting these trial solutions into Eq. 9 yields the set of equations

$$\begin{aligned} & - \sum_{p=-\infty}^{\infty} \left(\frac{d^2 a_n^{(p)}}{dt^2} + 2ip\omega_b \frac{da_n^{(p)}}{dt} - p^2 \omega_b^2 a_n^{(p)} \right) e^{ip\omega_b t} - \frac{1}{R_0} \left(1 + \frac{1}{R_0} \sum_{p=-\infty}^{\infty} a_n^{(p)} e^{ip\omega_b t} \right) \\ & \times \left\{ \sum_{p=-\infty}^{\infty} \left(\frac{da_n^{(p)}}{dt} + ip\omega_b a_n^{(p)} \right) e^{ip\omega_b t} \right\}^2 + \left(C_1 \sum_{p=-\infty}^{\infty} a_n^{(p)} e^{ip\omega_b t} \right) + \\ & C_2 \left(\sum_{p=-\infty}^{\infty} a_n^{(p)} e^{ip\omega_b t} \right)^2 \\ & + C_3 \left(\sum_{p=-\infty}^{\infty} a_n^{(p)} e^{ip\omega_b t} \right)^3 - K_{uu} \sum_{p=-\infty}^{\infty} \left(a_{n+1}^{(p)} + a_{n-1}^{(p)} + 2a_n^{(p)} \right) e^{ip\omega_b t} \frac{1}{2} K_{u\phi} \\ & \sum_{p=-\infty}^{\infty} \left(b_{n+1}^{(p)} - b_{n-1}^{(p)} \right) e^{ip\omega_b t} = 0. \end{aligned} \quad (12a)$$

$$\begin{aligned}
& - \sum_{p=-\infty}^{\infty} \left(\frac{d^2 b_n^{(p)}}{dt^2} + 2i\omega_b \frac{db_n^{(p)}}{dt} - p^2 \omega_b^2 b_n^{(p)} \right) e^{ip\omega_b t} + K_{\phi\phi} \\
& \sum_{p=-\infty}^{\infty} \left(b_{n+1}^{(p)} + b_{n-1}^{(p)}, -2b_n^{(p)} \right) e^{ip\omega_b t} \\
& - \frac{2}{R_0} \left\{ \sum_{p=-\infty}^{\infty} \left(\frac{da_n^{(p)}}{dt} + i\omega_b a_n^{(p)} \right) e^{ip\omega_b t} \right\} \left\{ \sum_{p=-\infty}^{\infty} \left(\frac{db_n^{(p)}}{dt} + i\omega_b b_n^{(p)} \right) e^{ip\omega_b t} \right\} \\
& - \frac{2}{R_0^2} \left(\sum_{p=-\infty}^{\infty} a_n^{(p)} e^{ip\omega_b t} \right) \left\{ \sum_{p=-\infty}^{\infty} \left(\frac{da_n^{(p)}}{dt} + i\omega_b a_n^{(p)} \right) e^{ip\omega_b t} \right\} \\
& \left\{ \sum_{p=-\infty}^{\infty} \left(\frac{db_n^{(p)}}{dt} + i\omega_b b_n^{(p)} \right) e^{ip\omega_b t} \right\} \\
& - \frac{1}{R_0^2} \left(\sum_{p=-\infty}^{\infty} a_n^{(p)} e^{ip\omega_b t} \right)^2 \left\{ \sum_{p=-\infty}^{\infty} \left(\frac{d^2 b_n^{(p)}}{dt^2} + 2i\omega_b \frac{db_n^{(p)}}{dt} - p^2 \omega_b^2 b_n^{(p)} \right) e^{ip\omega_b t} \right\} \\
& - G \sum_{p=-\infty}^{\infty} \left(b_{n+2}^{(p)} + b_{n-2}^{(p)} - 4b_{n+1}^{(p)} - 4b_{n-1}^{(p)} + 6b_n^{(p)} \right) e^{ip\omega_b t} \\
& + \frac{1}{2} K_{uu} \sum_{p=-\infty}^{\infty} \left(a_{n+1}^{(p)} - a_{n-1}^{(p)} \right) e^{ip\omega_b t} = 0.
\end{aligned} \tag{12b}$$

In the above, we consider the fundamental harmonics, i.e., $l = 1$, and the following set of DCNLS equations is obtained

$$\begin{aligned}
& -i2\omega_b \frac{db_n^{(1)}}{dt} + \omega_b^2 b_n^{(1)} + \left(\frac{3\omega_b^2}{R_0^2} \right) |a_n^{(1)}|^2 b_n^{(1)} + K_{\phi\phi} \left(b_{n+1}^{(1)} + b_{n-1}^{(1)} - 2b_n^{(1)} \right) \\
& + \frac{1}{2} K_{uu} \left(a_{n+1}^{(1)} - a_{n-1}^{(1)} \right) - G \left(b_{n+2}^{(1)} + b_{n-2}^{(1)} - 4b_{n+1}^{(1)} - 4b_{n-1}^{(1)} + 6b_n^{(1)} \right) = 0.
\end{aligned} \tag{13a}$$

$$\begin{aligned}
& -2i\omega_b \frac{da_n^{(1)}}{dt} + (\omega_b^2 + C_1) a_n^{(1)} + \frac{\omega_b^2}{R_0^2} |b_n^{(1)}|^2 a_n^{(1)} + C_3 |a_n^{(1)}|^2 a_n^{(1)} \\
& - K_{uu} \left(a_{n+1}^{(1)} + a_{n-1}^{(1)} + 2a_n^{(1)} \right) - \frac{1}{2} K_{\phi\phi} \left(b_{n+1}^{(1)} - b_{n-1}^{(1)} \right) = 0.
\end{aligned} \tag{13b}$$

We further assume

$$a_n^{(1)}(t) = Ax_n e^{i \frac{(2K_{uu} - C_1 - \omega_b^2)}{2\omega_b} t}, \quad b_n^{(1)}(t) = (-1)^n B y_n e^{i \frac{(2K_{\phi\phi} + 6G - \omega_b^2)}{2\omega_b} t}, \tag{14}$$

where $A = \sqrt{\frac{2\omega_b}{C_3 + \omega_b^2}}$ and $B = \sqrt{\frac{2R_0^2}{3\omega_b}}$, and the system reduces to the following set of DCNLS equations

$$i \frac{dx_n}{dt} + P_1(x_{n+1} + x_{n-1}) - (\sigma_1 |x_n|^2 + \sigma_2 |y_n|^2) x_n = 0 \tag{15}$$

$$i \frac{dy_n}{dt} + P_2(y_{n+1} + y_{n-1}) + P_3(y_{n+2} + y_{n-2}) - \sigma_3 |x_n|^2 y_n = 0,$$

where

$$P_2 = \frac{K_{\phi\phi} + 4G}{2\omega_b}, \quad P_3 = \frac{G}{2\omega_b}, \quad \sigma_3 = -\frac{3\omega_b A^2}{2R_0^2}, \quad P_1 = \frac{K_{uu}}{2\omega_b}, \quad \sigma_1 = -\frac{C_3 A^2}{2\omega_b}, \quad \sigma_2 = \frac{\omega_b B^2}{2R_0^2}.$$

Fig. 8 Energy localization due to MI. The wavenumbers have been chosen in the black regions of Fig. 6, i.e., $q = 0.8\pi$ and $Q = 0.65\pi$. Parameters have been fixed to be $x_0 = 0.5$, $f_s = 0.3$ and: (a) $l_s = 1$, (b) $l_s = 3$, (c) $l_s = 4$, and (d) $l_s = 6$. In panels (a)–(d), red regions give the highest energy density. For $l_s = 1$, $E_n = 3.8 \times 10^{-2} \simeq 1.52 \times 10^{-3}$ eV, and for $l_s = 3, 4$ and 6 , $E_n = 0.22 \simeq 8.80 \times 10^{-3}$ eV, $0.24 \simeq 9.6 \times 10^{-3}$ eV, and $0.61 \simeq 2.44 \times 10^{-2}$ eV, respectively

Equation (15) is nonlinearly coupled via the coefficients σ_2 and σ_3 . While radial amplitude oscillations are restricted to nearest-neighbor interactions (15), there are competitive interactions between first and second neighbors in the torsional amplitude equation (15). With some systematic differences, these equations are commonly found in nonlinear optics, biophysics, Bose–Einstein condensates and plasma physics [11, 25–28, 30]. In the context of biomolecular dynamics, they have been shown to be of potential interest in the study of energy transfer and storage in DNA and proteins [11, 12, 29, 30]. Only the stability of their plane-wave solutions will be studied here, while Eq. (8) and Lagrangian (7) will be considered for the full numerical analysis.

3 Modulated energy patterns

3.1 Linear stability analysis

The plane waves $x_n = x_0 e^{i(q_1 n - \omega_1 t)}$ and $y_n = y_0 e^{i(q_2 n - \omega_2 t)}$ are assumed to be solutions for the set of Eq. 15, where the frequencies ω_j and the wavenumbers q_j ($j = 1, 2$) satisfy

Fig. 9 Energy localization via MI for $l_s = 8$ (a) and $l_s = 10$ (b). The values of the other parameters have been fixed as $x_0 = 0.5$, $f_s = 0.3$, $q = 0.8\pi$ and $Q = 0.65\pi$. Red regions in all panels give the values of the highest energy density, which are $E_n = 0.7 \simeq 2.8 \times 10^{-2}$ eV for $l_s = 8$ and $E_n = 0.87 \simeq 3.4 \times 10^{-2}$ eV for $l_s = 10$

the dispersion relations

$$\begin{aligned}\omega_1 &= -2P_1 \cos(q_1) - 2P_4 \cos(2q_1) - \sigma_1 |x_0|^2 + \sigma_2 |y_0|^2 \\ \omega_2 &= -2P_2 \cos(q_2) - 2P_3 \cos(2q_2) - \sigma_3 |x_0|^2,\end{aligned}\quad (16)$$

with x_0 and y_0 the being the complex amplitudes of the solutions. Assuming $\omega_1 = \omega_2 = \omega$ and $q_1 = q_2 = q$ will further simplify the problem as it will be possible to use the following expression relating y_0 and x_0

$$|y_0|^2 = \frac{1}{\sigma_2} \left[2(P_1 - P_2) \cos(q) + 2(P_3 - P_4) \cos(2q) + (\sigma_1 - \sigma_3) |x_0|^2 \right]. \quad (17)$$

The study of the stability of the plane-wave solutions implies the introduction of small perturbations in the amplitude or in the phase, or in both of them. In our context, we slightly perturb the amplitudes as follows

$$x_n = x_0 [1 + \eta_n(t)] e^{i(qn - \omega t)}, \quad y_n = y_0 [1 + \xi_n(t)] e^{i(qn - \omega t)}, \quad (18)$$

where the small perturbations $\eta_n(t)$ and $\xi_n(t)$ are governed by the equations

$$\begin{aligned}i \frac{d\eta_n}{dt} + P_1(\eta_{n+1} + \eta_{n-1} - 2\eta_n) \cos(q) + i P_1(\eta_{n+1} - \eta_{n-1}) \sin(q) \\ + \sigma_1(\eta_n + \eta_n^*) |x_0|^2 - \sigma_2(\eta_n + \xi_n^*) |y_0|^2 = 0.\end{aligned}\quad (19a)$$

$$\begin{aligned}i \frac{d\xi_n}{dt} + P_2(\xi_{n+1} + \xi_{n-1} - 2\xi_n) \cos(q) + i P_2(\xi_{n+1} - \xi_{n-1}) \sin(q) \\ + P_3(\xi_{n+2} + \xi_{n-2} - 2\xi_n) \cos(2q) + i P_3(\xi_{n+2} - \xi_{n-2}) \sin(2q) \\ - \sigma_3(\eta_n^* + \xi_n) |x_0|^2 = 0.\end{aligned}\quad (19b)$$

Trial solutions for these perturbation equations can be adopted in the form

$$\eta_n(t) = B_1 e^{i(Qn - \Omega t)} + B_2^* e^{-i(Qn - \Omega^* t)}, \quad \xi_n(t) = B_3 e^{i(Qn - \Omega t)} + B_4^* e^{-i(Qn - \Omega^* t)}, \quad (20)$$

where Q and Ω are the wavenumber and complex frequency of perturbation. We then obtain a homogeneous system of equations for B_1 , B_2 , B_3 and B_4 in the form

$$M \times (B_1, B_2, B_3, B_4)^T = 0, \quad (21)$$

where M , a 4×4 matrix of the system, is given by

$$M = \begin{bmatrix} (a_{11} + \Omega) & a_{12} & a_{13} & a_{14} \\ a_{21} & (a_{22} - \Omega) & a_{23} & a_{24} \\ a_{31} & a_{32} & (a_{33} + \Omega) & a_{34} \\ a_{41} & a_{42} & a_{43} & (a_{33} - \Omega) \end{bmatrix}. \quad (22)$$

Accordingly, the matrix elements a_{rs} , with $r, s = 1, 2, 3, 4$, are written as

$$\begin{aligned} a_{11} &= 2P_1(\cos(Q) - 1)\cos(q) - 2P_1\sin(Q)\sin(q) + \sigma_1|x_0|^2 - \sigma_2|y_0|^2, \\ a_{12} &= a_{21} = \sigma_1|x_0|^2, \quad a_{13} = a_{24} = a_{34} = a_{42} = a_{43} = a_{31} = 0, \quad a_{14} = a_{23} = -\sigma_2|y_0|^2 \\ a_{22} &= 2P_1(\cos(Q) - 1)\cos(q) + 2P_1\sin(Q)\sin(q) + \sigma_1|x_0|^2 - \sigma_2|y_0|^2, \quad a_{32} = \\ &\quad a_{41} = -\sigma_3|x_0|^2 \\ a_{33} &= 2P_2(\cos(Q) - 1)\cos(q) + 2P_3(\cos(2Q) - 1)\cos(2q) - 2P_2\sin(Q)\sin(q) - \\ &\quad 2P_3\sin(2Q)\sin(2q) \\ a_{44} &= 2P_2(\cos(Q) - 1)\cos(q) + 2P_3(\cos(2Q) - 1)\cos(2q) + 2P_2\sin(Q)\sin(q) + \\ &\quad 2P_3\sin(2Q)\sin(2q). \end{aligned} \quad (23)$$

For system (21) to have non-trivial solutions, its determinant should be null, which satisfies the nonlinear dispersion relation

$$\Omega^4 + r_3\Omega^3 + r_2\Omega^2 + r_1\Omega + r_0 = 0, \quad (24)$$

with the coefficients r_3 , r_2 , r_1 , and r_0 being given in the [Appendix](#). In order to find solutions for Eq. 24, symbolic computation has been used. Recall that, the instability gain is given by the imaginary part of the complex frequency Ω , i.e., $G = \text{Im}(\Omega)$. The main concern of this work being to observe the influence of the solvent factors on the instability domain, we have first plotted G versus the barrier factor f_s , for $Q = 0.25\pi$ [see Fig. 4(a)] and $Q = 0.75\pi$ [see Fig. 4(b)]. In general, the case $f_s = 0$ represents the NS situation, i.e., a fixed value of $G(f_s)$ for fixed Q and q . However, in Fig. 4(a) the highest value of the gain is obtained for $l_s = 1$. $G(f_s)$ progressively decreases with increasing l_s . The last two cases, i.e., $l_s = 5$ and $l_s = 6$, illustrate the way instability changes and progressively tends to the limit case where solvent effects are neglected (the blue line NS in panels (a) and (b)). In Fig. 4(b), the general view is that G is a decreasing function of l_s . The lowest value of G is obtained for $l_s = 1$. Further increasing l_s , the gain increases, but for the same value of l_s , the NS limit is not reached, and rather requires higher values of l_s to be attained. There are therefore two situations where solvent effects are differently felt by the BCP model. For lower values of the perturbation wavenumber Q , it is possible to observe NS effects, while for big values of Q , l_s needs to be higher for possible switching between from solvent to NS features. However, in these two cases, even for $f_s = 0$, there is no instability extinction, meaning that unstable waves could also be obtained in the NS context. This is confirmed by Fig. 5(a), where, for $f_s = 0$, the gain for different values of l_s is compared to the NS case. It is clear that increasing l_s tends to extinguish some regions of instability with some features of the NS situation. For $f_s = 0.5$, the instability persists and the two regions tend to couple so that the region of instability gets expanded. Besides, stability/instability diagrams, along with their corresponding instability gains, have been represented for different values of l_s . In these diagrams, the black regions are those where unstable and localized patterns are expected, while white regions are those where the plane waves remain stable under modulation (see Fig. 6). Clearly, for $l_s = 1$, there are two regions of instability, as indicated by Fig. 6 (a1–a2), denoted by 1 and 2. The region of instability (2) is mainly caused by the solvent terms and is annihilated with increasing l_s . In so doing, we have examples in the cases $l_s = 3$ [Figs. 6 (b1–b2)] and $l_s = 6$ [Figs. 6 (c1–c2)], where the area of region 2 has diminished. The perfect case, where there are similarities between the simple BCP

model and the present one is displayed in Figs. 6 (d1–d2), where the instability zone 2 has completely disappeared. This does not really imply the absence of solvent factors, but rather pictures the case where the two models adopt the same dynamical behaviors, for example the complete opening of the base pairs. However, this cannot be specifically pointed out here, as we have gone through some linearization around the unperturbed cases. However, from the linear stability analysis, we see that the presence of solvent interactions brings about new features in the DNA model. Otherwise, we expect solvent effects to remarkably modify the original BCP model by bringing out new dynamical behaviors. At this point, we cannot make a conclusion on the longtime evolution of localized structures and energy patterns.

3.2 Numerical analysis

The linear stability analysis can only give information about the onset of instability. Therefore, in order to have a view of the spatiotemporal evolution of the predicted unstable modes, one has to perform full numerical simulations on the full model. In this framework, we have integrated numerically the set of Eq. 8 through the Runge–Kutta computational scheme with a time step $\Delta t = 10^{-3}$. The main concern of the present work being to bring out the effect of solvent interactions on energy localization, it is possible to write the energy density from Eq. 1 as follows:

$$E_n = \left[\dot{u}_n^2 + \frac{1}{R_0^2} (u_n + R_0)^2 \dot{\phi}_n^2 \right] + G(\phi_{n+1} + \phi_{n-1} - 2\phi_n)^2 + (e^{-u_n} - 1)^2 - f_s \left[\tanh\left(\frac{u_n}{L_s}\right) - 1 \right] + \frac{KR_0^2}{L^2} \left[(\phi_n - \phi_{n-1}) \sin \theta_0 + 2(u_n + u_{n-1}) \sin^2 \frac{\theta_0}{2} \right]^2 + \frac{KR_0^2}{L^2} \left[(\phi_{n+1} - \phi_n) \sin \theta_0 + 2(u_{n+1} + u_n) \sin^2 \frac{\theta_0}{2} \right]^2, \quad (25)$$

where, at the input, we have applied the slightly modulated plane wave initial conditions

$$\begin{aligned} u_n(t=0) &= x_0[1 + \zeta \cos(Qn)] \cos(qn) \\ \phi_n(t=0) &= y_0[1 + \zeta \cos(Qn)] \cos(qn), \end{aligned} \quad (26)$$

with ζ being the perturbation strength fixed as $\zeta = 0.01$. Furthermore, for the purpose of our numerical calculations, we work with a lattice of $N = 300$ base pairs and the initial amplitudes $x_0 = 0.5$, y_0 being given by Eq. 17. For the whole analysis, we fix $f_s = 0.3$ and the impact of the parameter l_s is studied.

We start our numerical analysis by considering points inside the region of stability. From Fig. 6, a point common to all the diagrams is ($q = 0.75\pi$; $Q = 0.45\pi$), which, as expected, should lead to stable plane-wave patterns. The results for this case are given in Fig. 7, where, for panel (a), we have fixed $l_s = 1$ and $l_s = 10$ for panel (b). In general, plane waves are inherent to DNA dynamics and, in some contexts, describe slight oscillations of strands. Some evidence of their contribution to the initiation of the so-called “DNA breathing” has been obtained, and they also carry energy as depicted in Fig. 7(a) and (b). It is obvious that these energy patterns are sensitive to solvent interactions as they get more localized with increasing l_s . However, Tabi and coworkers [12, 17, 18] have shown that the energy that has a strong biological effect on DNA should be localized in specific regions of the DNA lattice, as enzymes such as RNA-polymerase contribute to the collection of the vibrational energy available in the molecule for a better initiation of the transcription process, for example. Other arguments may go towards the effectiveness of plane-wave patterns in twist deformations, as the latter should importantly take place before any local opening of a coding sequence for RNA-messenger to copy sequence instructions for protein synthesis. For

instance, patterns to describe such a scenario are expected to be obtained in regions where the plane waves are unstable, as they arise in such systems under the concomitant effects of nonlinearity and dispersion. On this background, we have considered regions of instability, mainly the point ($q = 0.8\pi$; $Q = 0.65\pi$), to obtain the spectrum of behaviors displayed. In Fig. 8. The breaking of the strong H-bonds, in general, depends not only on the density of energy but also on the localization time of that energy. When the energy necessary for RNAP to break H-bonds is released by the hydrolysis of ATP, it should be concentrated on specific coding regions for a long time. Of course, DNA is made of sequences of AT and GC pairs and it has been demonstrated via micromanipulation experiments that GC sequences require more energy to be opened. The present study suggests that many factors such as the cooperative radial and twisting motions, as well as the environment, are involved in the process of energy localization. Also, as it will be apparent in the present work, where attention is particularly paid to solvent interactions that, the more solvent factors are involved, the more energy is localized quantitatively and confined to specific DNA sequences. For example, if $l_s = 1$, patterns of energy are effective from the beginning of the simulations, but energy is highly localized around $t = 400 (\simeq 80\text{ps})$, as shown in Fig. 8(a), where red regions correspond to $E_n = 3.8 \times 10^{-2} (\simeq 1.52 \times 10^{-3} \text{ eV})$. This energy is small, but, as one may remark, it is higher than the one obtained from stable plane-wave patterns. At this stage, we can assume that the hydrogen bonds between bases are not broken, and that the molecule is experiencing the initiation of some enzymatic mechanisms. As mentioned, these factors will contribute not only to increase the energy density but also to reduce the localization time. As we fix $l_s = 3$, there is a significant energy increase, while the localization time is situated around $t = 350 (\simeq 70\text{ps})$, and patterns of energy are confined to specific sequences of base pairs with density $E_n = 0.22 (\simeq 8.8 \times 10^{-3} \text{ eV})$ (see Fig. 8(b)). Of course, there are small radiations that appear here, and that may be due to small vibrations around the vibrating sequences of base pairs. We can also attribute the increase of energy with l_s to the existence of the potential barrier brought by the solvent terms in the Morse potential. For the cases of Figs. 8(c) and (d), the energy density has increased again to reach the value $E_n = 0.61 (\simeq 2.44 \times 10^{-2} \text{ eV})$ for $l_s = 6$ in Fig. 8(d). Further increasing l_s has revealed another interesting feature, as patterns of energy can be localized over a long time, with long patterns, for highest values of l_s . This is portrayed in Fig. 9(a) and (b), for $l_s = 8$ and $l_s = 10$, respectively. In the first case, i.e., Fig. 9(a), energy localizes from $t = 200 (\simeq 40\text{ps})$ to $t = 300 (\simeq 60\text{ps})$, while, in the second case, energy localization takes place from $t = 200 (\simeq 40\text{ps})$ to $t = 400 (\simeq 80\text{ps})$. Accordingly, the highest energy density for $l_s = 8$ is $E_n = 0.7 (\simeq 2.8 \times 10^{-2} \text{ eV})$ and $E_n = 0.87 (\simeq 3.4 \times 10^{-2} \text{ eV})$ for $l_s = 10$. These results suggest that the solvent interaction factor may consequently enhance the amplitude of the hydrogen bond oscillations, where the action of RNA-polymerase becomes efficient due to the progressive interactions between bases and solvent molecules. This also implies that, due to thermal fluctuations, solvent molecules can collide and bring about additional energy, which is once more collected by RNA-polymerase. This can explain why energy localizes for a long time when l_s gradually increases and why energy is high at that step. However, we cannot say anything about the robustness of these energy patterns if environmental factors such as thermal noise have not been considered. In fact, thermal fluctuations originate from the physiological temperature and have been pointed out to be the suitable pathway to energy localization and emergence of localized structures [34]. For this purpose, the random force $f_n(t)$, with the statistical properties

$$\langle f_n(t) \rangle = 0 \quad \text{and} \quad \langle f_n(t) f_{n'}(t') \rangle = 2T\gamma\delta_{n,n'}\delta(t - t'), \quad (26)$$

Fig. 10 Robustness of the energy patterns tested via thermal fluctuations. At the temperature $T = 30$ K, energy density has been plotted for $x_0 = 0.5$, $f_s = 0.3$, $q = 0.8\pi$, $Q = 0.65\pi$ and: $l_s = 1$ (a) and $l_s = 10$ (b). The highest energy densities for the respective cases are $E_n = 9.2 \times 10^{-2} \simeq 3.6 \times 10^{-3}$ eV and $E_n = 0.48 \simeq 1.92 \times 10^{-2}$ eV

has been introduced, where T is the temperature, and γ is the dimensionless friction coefficient with the value $\gamma = 0.01$. We have fixed the temperature as $T = 30$ K, and changing the values of l_s has led to the features of Fig 10. An interesting remark is that the energy that is localized in the DNA model spreads in small radiations for $l_s = 1$, with density $E_n = 9.2 \times 10^{-2} (\simeq 3.6 \times 10^{-3}$ eV), albeit it is not highly localized. Nevertheless, thermal fluctuations bring about selective energy localization, since some patterns present in Fig. 9(b) have disappeared for $l_s = 10$, where $E_n = 0.48 (\simeq 1.93 \times 10^{-2}$ eV). Quantitatively, energy is not localized as in the first case (i.e., Fig. 8(d)), but the molecule is sensitive to the strong effect of solvent interactions and experiences energy enhancement due to the subsequent binding of solvent molecules to the free bases. This analysis, which has not been made for high temperatures, satisfactorily shows that energy in DNA key dynamical processes is a robust phenomenon, regardless of thermal noise or base sequence distribution. Interestingly, thermal fluctuations themselves are expected to give rise to spontaneous energy bands and could be at the origin of the narrow bands served in Fig. 10(b). However, the localized modes due to thermal noise are not the focus of the present work and will be addressed in a forthcoming work with more emphasis on the thermal denaturation of DNA.

4 Conclusions

The nonlinear dynamics and energy localization in DNA have been addressed. We have modified the twist-opening model of DNA by introducing interactions with solvent. The system has been shown to be modeled by two DCNLS equations on which the linear stability analysis has been performed. Solvent effects have been shown to bring about new regions of instability. Increasing the solvent factor, we have observed that the instability features were similar to those of the classical twist-opening model. Through direct numerical simulations, we have obtained patterns of energy in agreement with our analytical predictions. Increasing the value of l_s has given rise to highly localized and narrow energy patterns. The robustness of these patterns has been tested under thermal fluctuations and the same behaviors have been observed. Further investigations will include cooperative effects in the new model and

real DNA sequences will be introduced. In the same way, we intend to study DNA thermal denaturation through the proposed modified model.

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Appendix

$$\begin{aligned}
 r_3 &= 4[(P_1 + P_2) \sin(q) \sin(Q) + P_3 \sin(2q) \sin(2Q)] \\
 r_2 &= -2\sigma_2 |y_0|^2 \sigma_3 |x_0|^2 + 4\sigma_1 |x_0|^2 P_1 \cos(q) - 4P_1^2 \cos(q)^2 - 4\sigma_1 |x_0|^2 P_1 \cos(q) \cos(Q) \\
 &\quad + 8P_1^2 \cos^2(q) \cos(Q) - 4P_1^2 \cos^2(q) \cos^2(Q) + 16(P_2 + 2P_3 \cos(q) + 2P_3 \cos(q - Q)) \sin\left(q - \frac{Q}{2}\right) \\
 &\quad \times \left\{ P_1 \sin\left(q - \frac{Q}{2}\right) + (P_1 + P_2 + 2P_3 \cos(q) + 2P_3 \cos(q + Q)) \sin\left(q + \frac{Q}{2}\right) \right\} \sin^2\left(\frac{Q}{2}\right) \\
 &\quad + 4P_1^2 \sin^2(q) \sin^2(Q) + 16P_1(P_2 + 2P_3 \cos(q) + 2P_3 \cos(q + Q)) \sin(q) \sin^2\left(\frac{Q}{2}\right) \\
 &\quad (\sin(q) + \sin(q + Q)) \\
 r_1 &= -4\sigma_2 |y_0|^2 \sigma_3 |x_0|^2 P_1 \cos(q) + 4\sigma_2 |y_0|^2 \sigma_3 |x_0|^2 P_1 \cos(q) \cos(Q) \\
 &\quad + 2\sigma_2 |y_0|^2 \sigma_3 |x_0|^2 [\sigma_1 |x_0|^2 + (P_2 - P_1) \cos(q) + P_3 \cos(2q) + P_1 \cos(q - Q) \\
 &\quad - P_2 \cos(q + Q) - P_3 \cos(2(q + Q))] - 2\sigma_2 |y_0|^2 \sigma_3 |x_0|^2 [\sigma_1 |x_0|^2 - (P_1 + P_2) \cos(q) - P_3 \cos(2q) \\
 &\quad + P_1 \cos(q + Q) + P_2 \cos(q + Q) + P_3 \cos(2(q + Q))] + 32P_1(P_2 + 2P_3 \cos(q) + 2P_3 \cos(q - Q)) \\
 &\quad \times \left[-P_2 - (\sigma_1 |x_0|^2 + P_3) \cos(q) + (P_1 + P_2) \cos(2q) + P_3 \cos(3q) - P_1 \cos(Q) - P_2 \cos(Q) \right. \\
 &\quad \left. - 2P_3 \cos(q + Q) + P_2 \cos(2q + Q) + 2P_3 \cos(3q + Q) - P_3 \cos(q + 2Q) + P_3 \cos(3q + 2Q) \right] \\
 &\quad \times \sin\left(q - \frac{Q}{2}\right) \sin^3\left(\frac{Q}{2}\right) - 32P_1 [\sigma_1 |x_0|^2 \cos(q) + P_1 (\cos(Q) - \cos(2q))] \\
 &\quad \times (P_2 + 2P_3 \cos(q) + 2P_3 \cos(q + Q)) \sin\left(q + \frac{Q}{2}\right) \sin^3\left(\frac{Q}{2}\right) \\
 r_0 &= \sigma_3 |x_0|^2 \left[-2(\sigma_2 |y_0|^2)^2 \sigma_3 |x_0|^2 - 8\sigma_2 |y_0|^2 (\sigma_1 |x_0|^2 - P_1 \cos(q) + P_1 \cos(q - Q)) \right. \\
 &\quad \times (P_2 + 2P_3 \cos(q) + 2P_3 \cos(q + Q)) \sin\left(q + \frac{Q}{2}\right) \sin\left(\frac{Q}{2}\right) \left. \right] + 2\sigma_2 |y_0|^2 \sigma_3 |x_0|^2 \\
 &\quad \times \left(\sigma_2 |y_0|^2 \sigma_3 |x_0|^2 + 4(\sigma_1 |x_0|^2 - P_1 \cos(q) + P_1 \cos(q + Q))(P_2 + 2P_3 \cos(q) + 2P_3 \cos(q + Q)) \right. \\
 &\quad \times \sin\left(q + \frac{Q}{2}\right) \sin\left(\frac{Q}{2}\right) \left. \right) + 16P_1(P_2 + 2P_3 \cos(q) + 2P_3 \cos(q - Q)) \sin\left(q - \frac{Q}{2}\right) \sin\left(\frac{Q}{2}\right) \\
 &\quad \times \left(\sigma_2 |y_0|^2 \sigma_3 |x_0|^2 \cos(q) - \sigma_2 |y_0|^2 \sigma_3 |x_0|^2 \cos(q) \cos(Q) + 8(\sigma_1 |x_0|^2 \cos(q) P_1 (\cos(Q) - \cos(2q))) \right. \\
 &\quad \times (P_2 + 2P_3 \cos(q) + 2P_3 \cos(q + Q)) \sin\left(q + \frac{Q}{2}\right) \sin^3\left(\frac{Q}{2}\right) \left. \right)
 \end{aligned}$$

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