Mathematics

Research article

Dynamics and stability analysis of nonlinear DNA molecules: Insights from the Peyrard-Bishop model

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Abstract: This study explores the nonlinear Peyrard-Bishop DNA dynamic model, a nonlinear evolution equation that describes the behavior of DNA molecules by considering hydrogen bonds between base pairs and stacking interactions between adjacent base pairs. The primary objective is to derive analytical solutions to this model using the Khater III and improved Kudryashov methods. Subsequently, the stability of these solutions is analyzed through Hamiltonian system characterization. The Peyrard-Bishop model is pivotal in biophysics, offering insights into the dynamics of DNA molecules and their responses to external forces. By employing these analytical techniques and stability analysis, this research aims to enhance the understanding of DNA dynamics and its implications in fields such as drug design, gene therapy, and molecular biology. The novelty of this work lies in the application of the Khater III and an enhanced Kudryashov methods to the Peyrard-Bishop model, along with a comprehensive stability investigation using Hamiltonian system characterization, providing new perspectives on DNA molecule dynamics within the scope of nonlinear dynamics and biophysics.

Keywords: Peyrard-Bishop model; DNA dynamics; nonlinear evolution equations; analytical

solutions

Mathematics Subject Classification: 35C08, 35Q05, 92C40, 70H06

1. Introduction

The study of nonlinear evolution equations has garnered considerable attention across diverse scientific and engineering disciplines due to their effectiveness in representing intricate phenomena [1]. Among these equations, the nonlinear Peyrard-Bishop DNA dynamic model stands out, designed to elucidate the behavior of DNA molecules by accounting for hydrogen bonds between base pairs and stacking interactions among adjacent base pairs [2]. Obtaining analytical solutions for nonlinear evolution equations presents a formidable challenge, and the Peyrard-Bishop model is no exception. While numerical and computational techniques have been instrumental in investigating this model, analytical solutions offer deeper insights into its underlying dynamics, thereby fostering a more comprehensive understanding of DNA behavior [3].

The primary objective of this study is to construct analytical solutions for the Peyrard-Bishop DNA dynamic model using the Khater III and enhanced Kudryashov methods. Additionally, the stability of these solutions will be scrutinized through Hamiltonian system characterization [4, 5]. The analytical solutions and stability analysis of the Peyrard-Bishop model hold promise for advancing biophysics and enhancing our comprehension of DNA dynamics [6]. These findings carry potential implications for various domains, including drug design, gene therapy, and molecular biology, where a profound understanding of DNA behavior is indispensable [7]. Previous investigations into the Peyrard-Bishop model have employed diverse methodologies. Numerical simulations have shed light on its behavior under various conditions [8], while perturbation methods and analytical approaches have yielded approximate solutions [9]. However, the quest for exact analytical solutions and their stability analysis remains an active area of research.

This study focuses exclusively on the nonlinear Peyrard-Bishop DNA dynamic model and its analytical solutions derived through the Khater III and enhanced Kudryashov methods. The analysis is delimited to stability assessments via Hamiltonian system characterization, with other aspects such as model applications or extensions lying beyond the study's scope [10]. The nonlinear Peyrard-Bishop DNA dynamic model stands as a critical tool in biophysics, offering insights into DNA dynamics and responses to external forces such as denaturation and thermal fluctuations [11]. Through analytical techniques, researchers can uncover exact solutions that unveil the intricate dynamics of DNA molecules, facilitating a deeper comprehension of the model's behavior and enabling the development of more accurate simulations and predictions [12, 13]. Additionally, stability analysis of the obtained solutions is crucial for understanding the model's robustness and reliability under various conditions [14, 15].

The Peyrard-Bishop model shares similarities with other well-known nonlinear evolution equations, such as the sine-Gordon equation, the modified Khater method, and the Khater II model, yet it incorporates additional terms and parameters tailored to elucidate DNA dynamics [16, 17]. This unique feature distinguishes it and allows for a more accurate representation of DNA behavior amidst a complex array of interactions and properties [18].

The Peyrard-Bishop DNA dynamic model can be expressed in various forms, each capturing specific aspects of DNA dynamics [19]. The original form, proposed by Peyrard and Bishop in 1989, incorporates terms representing stacking interactions between adjacent base pairs and hydrogen bonds between complementary base pairs [20]. Alternatively, a dimensionless form is often employed to simplify analysis, rescaling variables and parameters for more general interpretations [21]. Despite variations in form, the underlying physics and dynamics described by the model remain consistent. The original formulation of the Peyrard-Bishop DNA dynamic model is represented by the following nonlinear partial differential equation [22]:

$$M \frac{\partial^2 y_n}{\partial t^2} = V'(y_{n+1} - y_n) - V'(y_n - y_{n-1}) + W'(y_n). \tag{1.1}$$

Here, the equation characterizes the dynamics of a one-dimensional chain of base pairs, where y_n denotes the displacement of the n-th base pair from its equilibrium position at time t [23]. The distinct terms within the equation depict the various interactions and forces acting on the base pairs [24]:

- $M \frac{\partial^2 y_n}{\partial t^2}$: This term signifies the inertial force acting on the n-th base pair, where M represents the reduced mass of a base pair.
- $V'(y_{n+1} - y_n)$ and $V'(y_n - y_{n-1})$: These terms denote the stacking interactions between adjacent base pairs, originating from the π-π stacking interactions between the aromatic rings of neighboring base pairs. The function $V(r)$ denotes the Morse potential, which models the stacking interactions, and $V'(r)$ represents its derivative with respect to the relative displacement r.
- $W'(y_n)$: This term encompasses the hydrogen bonding interactions between complementary base pairs within the same base pair. The function $W(r)$ denotes an anharmonic potential modeling the hydrogen bond interactions, with $W'(r)$ representing its derivative with respect to the displacement r.

The Morse potential and the anharmonic potential typically assume the following forms [25]:

$$V(r) = \Im \left[\exp(-a(r - r_0)) - 1 \right]^2,$$

$$W(r) = \rho \left[\exp(-\alpha r) - 1 \right]^2,$$

where $\Im$, a, r_0, ρ, and α are parameters determining the strength and shape of the potentials. The Peyrard-Bishop model integrates these terms to encapsulate the fundamental interactions that govern the dynamics of DNA molecules [26]. The interplay between inertial forces, stacking interactions, and hydrogen bonding interactions gives rise to the observed complex behaviors in DNA, including the formation of breathers (localized, oscillating modes), solitons, and other nonlinear phenomena [27].

It is noteworthy that the original formulation of the Peyrard-Bishop model assumes a one-dimensional chain of base pairs and disregards certain effects such as torsional angles, base-pair openings, and long-range interactions [28]. However, it serves as a fundamental framework for comprehending the dynamics of DNA molecules and has been extended and modified in subsequent studies to incorporate additional complexities and effects [29]. To simplify the analysis and allow for

more general interpretations, the Peyrard-Bishop model is often expressed in a dimensionless form by rescaling the variables and parameters. One such form is as follows [30]:

$$
\begin{aligned}
\frac{\partial^2 y_n}{\partial \tau^2} =& (y_{n+1} - 2y_n + y_{n-1}) - \epsilon \left[\exp(-\kappa(y_{n+1} - y_n)) - 1 \right] \\
&+ \epsilon \left[\exp(-\kappa(y_n - y_{n-1})) - 1 \right] + \gamma \left[\exp(-\alpha y_n) - 1 \right],
\end{aligned}
\tag{1.2}
$$

where τ is the dimensionless time, ϵ and κ are parameters related to the stacking interactions, and γ, α are parameters associated with the hydrogen bonds.

The physical difference between these forms lies in the choice of variables and parameters, which can affect the interpretation and numerical values of the solutions. However, the underlying physics and dynamics described by the model remain the same. While, it also takes the next form [31]

$$
\frac{\partial^2 u}{\partial t^2} - \frac{\partial^2 u}{\partial x^2} \left(3\omega_2 \left(\frac{\partial u}{\partial x} \right)^2 + \omega_1 \right) - 2\gamma \omega_3 e^{-\gamma u} \left(e^{-\gamma u} - 1 \right) = 0.
\tag{1.3}
$$

Equation (1.3) constitutes a representation of the Peyrard-Bishop DNA dynamic model, elucidating the behavior of DNA molecules by considering the hydrogen bonds between base pairs and the stacking interactions between adjacent base pairs [32]. Within this equation, the variable u denotes the displacement or stretching of the hydrogen bonds in the DNA molecule from their equilibrium position. The physical interpretation of each term and parameter is as follows [33]:

- $\frac{\partial^2 u}{\partial t^2}$: This term denotes the inertial force or the acceleration of the hydrogen bonds.
- $\frac{\partial^2 u}{\partial x^2}$: This term signifies the spatial derivative of the stretching of the hydrogen bonds, incorporating the coupling or interactions between adjacent base pairs along the DNA chain.
- $3\omega_2 \left(\frac{\partial u}{\partial x} \right)^2 + \omega_1$: This term signifies the stacking interactions between adjacent base pairs, arising from the π-π stacking interactions between the aromatic rings of neighboring base pairs. The term $\left(\frac{\partial u}{\partial x} \right)^2$ represents the relative displacement between adjacent base pairs, and the parameters ω_1 and ω_2 are related to the strength and nonlinearity of the stacking interactions, respectively.
- $2\gamma \omega_3 e^{-\gamma u} \left(e^{-\gamma u} - 1 \right)$: This term denotes the hydrogen bonding interactions between the complementary base pairs within the same base pair. The exponential term $e^{-\gamma u}$ models the anharmonic potential of the hydrogen bonds, and the parameter γ determines the strength and shape of this potential. The parameter ω_3 is related to the overall strength of the hydrogen bonding interactions.

The parameters in this model possess the following physical interpretations [34]:

- ω_1: This parameter represents the linear component of the stacking interactions between adjacent base pairs.
- ω_2: This parameter represents the nonlinear component of the stacking interactions between adjacent base pairs.
- ω_3: This parameter represents the strength of the hydrogen bonding interactions between complementary base pairs.
- γ: This parameter determines the strength and shape of the anharmonic potential modeling the hydrogen bonding interactions.

It is pertinent to note that this manifestation of the Peyrard-Bishop model assumes a one-dimensional chain of base pairs and disregards certain effects, such as torsional angles, base-pair openings, and long-range interactions. Nonetheless, it encapsulates the fundamental interactions governing the dynamics of DNA molecules, encompassing inertial forces, stacking interactions, and hydrogen bonding interactions, which collectively give rise to the observed complex behavior in DNA [35].

Within this framework, we apply the subsequent wave transformation $u = u(x, t) = \psi(\zeta)$, $\zeta = c\,t + x$, where c stands as an arbitrary constant to be subsequently determined, to Eq (1.3), thereby transmuting it into the ensuing ordinary differential equation.

$$\psi'' \left(c^2 - 3\omega_2 (\psi')^2 - \omega_1\right) + 2\gamma\omega_3 e^{-2\gamma\psi} \left(e^{\gamma\psi} - 1\right) = 0. \tag{1.4}$$

Upon multiplication of Eq (1.4) by ψ' and subsequent integration with respect to ζ, employing a null integration constant, the following expression emerges:

$$\frac{1}{2} \left(c^2 - \omega_1\right) \psi'(x)^2 - 2\omega_3 e^{-\gamma\psi(x)} + \omega_3 e^{-2\gamma\psi(x)} - \frac{1}{4} 3\omega_2 \psi'(x)^4 = 0. \tag{1.5}$$

Equation (1.5) converts into the next equation

$$2\gamma^2 \left(c^2 - \omega_1\right) \varphi^2 \varphi'^2 + 4\gamma^4 \omega_3(\varphi - 2)\varphi^5 - 3\omega_2 \varphi'^4 = 0, \tag{1.6}$$

where

$$e^{-\gamma\psi} = \varphi, \quad \left(e^{-\gamma\psi}\right)^2 = \varphi^2, \text{ and } \psi' = -\frac{\varphi'}{\gamma\varphi}.$$

Additionally, Eq (1.6) also takes the next form

$$r_1 \varphi^6 - r_3 \left(\varphi'\right)^4 + r_2 \varphi^2 \left(\varphi'\right)^2 + \varphi^5 = 0, \tag{1.7}$$

where

$$r_1 = -\frac{1}{2},$$

$$r_2 = \frac{\omega_1 - c^2}{4\gamma^2\omega_3},$$

$$r_3 = -\frac{3\omega_2}{8\gamma^4\omega_3}.$$

Applying the prescribed analytical methodologies and the principle of homogeneous balance to Eq (1.7) leads to the subsequent formula for the solution:

$$\varphi(\zeta) = \begin{cases} \displaystyle\sum_{i=0}^{2n} a_i \left(K^{f(\zeta)}\right)^i = a_1 K^{f(\zeta)} + a_2 K^{2f(\zeta)} + a_0, \\[4mm] \displaystyle\sum_{i=1}^{n} \left(a_i f(\zeta)^i + b_i \left(\frac{f'(\zeta)}{f(\zeta)}\right)^i\right) + a_0 = a_2 f(\zeta)^2 + a_1 f(\zeta) + a_0 + \frac{b_2 f'(\zeta)^2}{f(\zeta)^2} + \frac{b_1 f'(\zeta)}{f(\zeta)}, \end{cases} \tag{1.8}$$

where a_0, a_1, a_2, b_1 and b_2 are arbitrary constants to be evaluated later. While $f(\zeta)$ and $\phi(\zeta)$ satisfies the next ordinary differential equation

$$\begin{cases} f'(\zeta)^2 = \dfrac{\alpha + K^{f(\zeta)}\left(\beta + \sigma K^{f(\zeta)}\right)}{\ln^2(K)} & \text{for Khater III method,} \\[2em] f'(\zeta)^2 = f(\zeta)^2\left(1 - \tau f(\zeta)^2\right), & \text{for an enhanced Kudryashov scheme,} \end{cases}$$

where, α, β, σ and τ denote arbitrary constants, the determination of which will be elucidated subsequently.

The progression of this investigation follows a structured format: Section 2 focuses on the examination of various solitary wave solutions, assessing their relevance within the established framework. Subsequently, Section 4 undertakes a comprehensive analysis of the obtained results from both physical and dynamic perspectives. Finally, Section 5 integrates the scholarly contributions stemming from this inquiry.

2. Novel computational solutions

In this section, the solitary wave solutions of the scrutinized model are explored using the analytical methods outlined earlier. Subsequently, an assessment of the stability of the derived solutions is conducted via the analysis of the Hamiltonian system. The principal objective is to determine the effectiveness and practical reliability of the developed solutions.

2.1. Khater III method implementation results

By employing the Khater III technique along with the auxiliary equation provided in (1.9) and leveraging Mathematica 13.1 software, we are equipped to solve Eq (1.7). This approach enables the determination of values for the designated parameters, resulting in the following outcomes:

Case I:

$$a_0 = 0, r_1 = \frac{4a_2}{a_1^2}, r_2 = \frac{a_1\sqrt{r_3}}{2\sqrt{a_2}}, \alpha = \frac{a_1}{2\sqrt{a_2}\sqrt{r_3}}, \beta = \frac{\sqrt{a_2}}{\sqrt{r_3}}, \sigma = \frac{a_2^{3/2}}{2a_1\sqrt{r_3}}.$$

Case II:

$$a_0 = 0, a_1 = 0, r_1 = \frac{r_3}{r_2^2}, \alpha = \frac{r_2}{4r_3}, \beta = 0, \sigma = \frac{a_2}{4r_2}.$$

The computational wave solutions of the investigated model can be expressed in the following manner:

$$\varphi(x, t) = -\frac{a_1^2}{4a_2}\operatorname{sech}^2\left(\frac{\sqrt{a_1}(c\,t + x)}{2\sqrt{2}\sqrt[4]{a_2}\sqrt[4]{r_3}}\right), \tag{2.1}$$

$$\varphi(x, t) = \frac{r_2^2}{r_3}\operatorname{csch}^2\left(\frac{1}{2}\sqrt{\frac{r_2}{r_3}}(c\,t + x)\right). \tag{2.2}$$

2.2. Results of the enhanced Kudryashov scheme implementation results

Utilizing an improved Kudryashov scheme and employing the auxiliary equation delineated in (1.9), in conjunction with Mathematica 13.1 software, facilitates the resolution of Eq (1.7). This approach streamlines the process of determining values for the aforementioned parameters, resulting in the following outcomes:

$$a_0 = -b_2, a_1 = 0, b_1 = 0, r_1 = \frac{\tau}{b_2\tau - a_2}, r_2 = \frac{1}{4}\left(b_2 - \frac{a_2}{\tau}\right), r_3 = -\frac{a_2 - b_2\tau}{16\tau}.$$

The computational wave solutions of the investigated model can be articulated as follows:

$$\varphi(x,t) = -\frac{\text{sech}^2(c\,t+x)\,(-2a_2 + b_1\tau\sinh(2(c\,t+x)) + 2b_2\tau)}{2\tau}, \tag{2.3}$$

$$\varphi(x,t) = \frac{16c^2\,(a_2 - b_2\tau)\,e^{2(c\,t+x)} - 16b_1c^4e^{4(c\,t+x)} + b_1\tau^2}{\left(4c^2e^{2(c\,t+x)} + \tau\right)^2}. \tag{2.4}$$

2.3. Solutions' stability

A comprehensive analysis of the stability of solitary wave solutions is essential for a thorough understanding of the dynamic behavior and applicability of the Peyrard-Bishop DNA model. This model, acclaimed for its nonlinear dynamics and soliton solutions, has become a crucial framework for exploring the complex biophysics associated with DNA transcription and denaturation. The model's significance and accuracy are profoundly dependent on the stability of its solutions within specified system parameters.

This study conducts an exhaustive stability analysis of the solitary wave solutions under perturbations within the Hamiltonian system. The Hamiltonian structure provides a fundamental basis for evaluating solution stability, employing the Lyapunov method for rigorous scrutiny. Specifically, we derive the expression for the Hamiltonian, identify conserved quantities, and formulate the Lyapunov functional to rigorously assess stability. Evaluating the momentum of Eqs (2.1) and (2.3) yields

$$\mathbb{M}\Big|_{Eq.\,(2.1)} = -\frac{1}{24c}\left(\tanh^2\left(\frac{5(c-1)}{2\sqrt{2}}\right) - 2\tanh^2\left(\frac{5(c+1)}{2\sqrt{2}}\right) + \tanh^2\left(\frac{5-5c}{2\sqrt{2}}\right)\right.$$
$$\left. + 8\log\left(\cosh\left(\frac{5(c-1)}{2\sqrt{2}}\right)\right) - 8\log\left(\cosh\left(\frac{5(c+1)}{2\sqrt{2}}\right)\right)\right), \tag{2.5}$$

$$\mathbb{M}\Big|_{Eq.\,(2.3)} = \frac{1}{8c}\left(-27\text{sech}^2(5(c+1)) + 27\text{sech}^2(5-5c) + 10\left(640c\right.\right.$$
$$\left.\left. + \log\left(1 - \tanh^2(5(c+1))\right) - \log\left(1 - \tanh^2(5-5c)\right)\right)\right). \tag{2.6}$$

Consequently, we get

$$\frac{d\mathbb{M}}{dc} = \begin{cases} 0.441542829, & \text{for} \quad (c = -1), \\ \\ 2.77777766, & \text{for} \quad (c = 3). \end{cases} \tag{2.7}$$

Hence, the solutions constructed above (Eqs (2.1) and (2.3)) demonstrate stability within the domain $x \in [-5, 5]$ and $t \in [-5, 5]$. The results of the stability analysis carry profound implications for the validity and utility of the model in DNA dynamics research. Unstable solutions would manifest as non-physical artifacts, undermining the model's quantitative reliability in accurately describing DNA behavior. Conversely, stable and robust solutions, confined within appropriate parameter boundaries, inspire confidence in utilizing the model to elucidate DNA transcription mechanisms and guide experimental endeavors. Essentially, this stability analysis provides crucial insights into the dynamic structures within the model, delineates accurate parameter ranges, and defines suitable application domains. It establishes the groundwork for constructing precise DNA models and offers deeper insights into the intricate equilibrium of forces governing DNA molecular processes.

3. Graphical illustrations of solution sets

The graphical representations provided in Figures 1-5 offer profound insights into the intricate dynamics and physical phenomena inherent in DNA denaturation and renaturation processes, as elucidated by the Peyrard-Bishop DNA model. These visual depictions serve as indispensable tools for interpreting and comprehending the complex interplay among various forces and interactions governing DNA molecule behavior.

- Figure 1: Numerical representations of solitary wave solutions:
  Panels (a-f) of Figure 1 exhibit the bright solitary wave solutions obtained using the Khater III method (Eqs (2.1) and (2.2)), while panels (g-i) illustrate the solitary wave solutions derived from an enhanced Kudryashov scheme (Eq (2.3)). These qualitative plots authenticate the diversity of analytical solitary wave solutions acquired from the two distinct methodologies within the nonlinear framework of the Peyrard-Bishop DNA model. The depicted localized wave profiles offer a visual representation of the localized melting bubbles that arise during the denaturation process, enabling researchers to qualitatively evaluate the characteristics and behavior of these bubbles.
- Figure 2: Numerical representations of solitary wave solutions:
  Panels (a-c) of Figure 2 portray the bright solitary wave solutions computed using the Khater II method (Eq (2.4)). Analogous to Figure 1, these qualitative plots affirm the diversity of analytical solitary wave solutions and their localized wave profiles acquired from the two distinct techniques within the nonlinear framework of the Peyrard-Bishop DNA model. These visual depictions aid in comprehending the localized nature of denaturation bubbles and their propagation along the DNA strand.
- Figure 3: Conserved Quantities in the Hamiltonian Framework:
  Panels (a, b) and (c, d) of Figure 3 illustrate the momentum M as described by Eqs (2.5) and (2.6), representing conserved quantities arising from the intrinsic nonlinearity governing the Peyrard-Bishop DNA model. The graphical depiction of these conserved quantities offers valuable insights into the equilibrium conditions maintaining DNA strand integrity within the physically consistent nonlinear dynamics of the model. By analyzing these conserved quantities, researchers can gain deeper understanding of solution stability, robustness, and the parameter ranges wherein the model accurately describes DNA behavior.
- Figure 4: Interpretation of the Bright Solitary Wave Solution Stream Plot:

The stream plot depicted in Figure 4, representing the bright solitary wave solution expressed by Eqs (2.1) and (2.2), provides a visual representation of localized melting bubbles within the DNA strand. The continuous lines illustrate the gradual variation in DNA strand displacement (u) with respect to distance (x) and time (t), capturing the dynamic process of bubble nucleation, growth, and propagation along the DNA strand during the denaturation process.

The smooth, continuous nature of the lines reflects the bubble breathing dynamics, wherein the denaturation bubbles exhibit oscillatory behavior as they expand and contract. This phenomenon is directly related to the nonlinear strand fluctuations governed by the Peyrard-Bishop model, accounting for the interplay between hydrogen bond interactions and stacking forces between adjacent base pairs.

As the denaturation process progresses, the localized melting bubbles smoothly rise and fall along the strand, indicating the formation and dissolution of these unstable regions. This visual representation effectively captures the dynamic nature of bubble nucleation and growth, providing insights into the local dynamics governed by the Peyrard-Bishop model.

- Figure 5: Interpretation of the Dark Solitary Wave Solution Stream Plot:
  The stream plot in Figure 5, depicting the dark solitary wave solution formulated by Eqs (2.3) and (2.4), offers a visual representation of the periodic fluctuations in strand displacement (u) across spatial and temporal coordinates. The oscillating contour pattern showcases the bubble oscillation phenomena within the denaturing regions of the DNA strand.

  The localized ripples propagating along the strand, while retaining their shape and amplitude, effectively illustrate the collective behavior of denaturation bubbles and their interactions through Ripple-Like soliton interactions. This visual representation provides valuable insights into the dynamics of bubble propagation and coalescence during the denaturation-renaturation transitions. The oscillating contour pattern reflects the periodic nature of the denaturation-renaturation process, wherein the bubbles undergo cycles of growth and shrinkage. This behavior is governed by the complex interplay between hydrogen bond breaking, stacking interactions, and the nonlinear dynamics inherent to the Peyrard-Bishop model.

  Moreover, the propagation of localized ripples along the strand highlights the collective behavior of denaturation bubbles, where individual bubbles can interact, merge, or split, leading to the formation of larger or smaller bubbles. This phenomenon is crucial for understanding the overall dynamics of the denaturation-renaturation process, as it directly impacts the stability and integrity of the DNA molecule.

In conclusion, the graphical representations presented in Figures 1, 2, and 3 provide researchers with powerful visual aids for interpreting the physical meaning and properties of the Peyrard-Bishop DNA model. By capturing the dynamic behavior of denaturation bubbles, their nucleation, growth, propagation, and interactions, as well as the conserved quantities and equilibrium conditions, these plots offer invaluable insights into the complex interplay between various forces and interactions governing DNA dynamics. Ultimately, these visual representations contribute to a deeper understanding of the underlying mechanisms driving DNA denaturation and renaturation processes, facilitating further research and advancements in the field of biophysics and molecular biology.

The graphical representations presented in Figures 4 and 5 provide researchers with powerful visual aids for interpreting the physical meaning and properties of the Peyrard-Bishop DNA model. By

capturing the dynamic behavior of denaturation bubbles, their nucleation, growth, propagation, and interactions, these plots offer invaluable insights into the complex interplay between various forces and interactions that govern DNA dynamics. Ultimately, these visual representations contribute to a deeper understanding of the underlying mechanisms driving DNA denaturation and renaturation processes, facilitating further research and advancements in the field of biophysics and molecular biology.
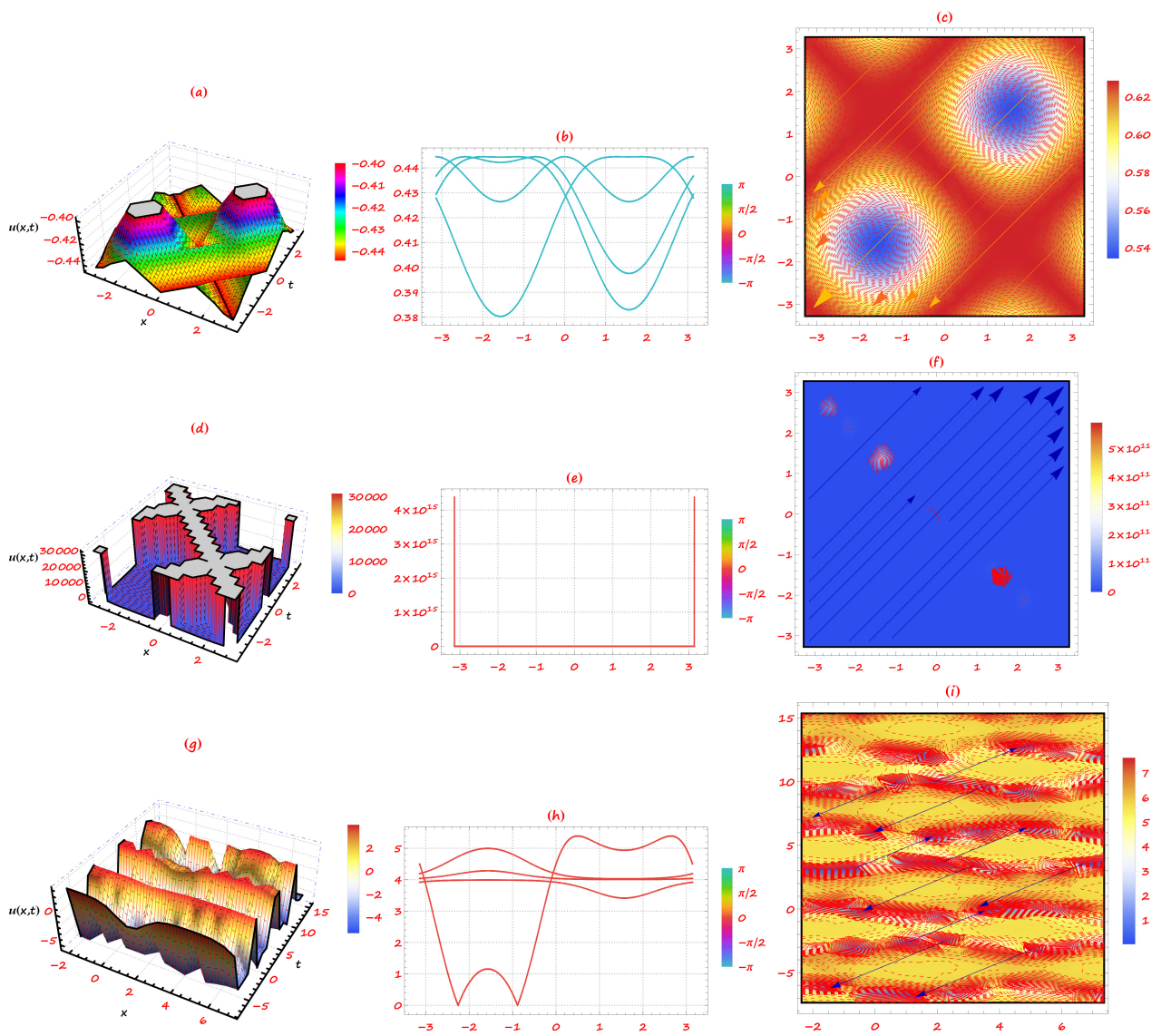
Figure 1. Numerical representations of the solitary wave solutions obtained through analytical methods are presented. Panels (a-f) display the bright solitary wave solutions computed using the Khater III method (Eqs (2.1) and (2.2)). Panels (g-i) illustrate the solitary wave solutions derived from an enhanced Kudryashov scheme (Eq (2.3)). These qualitative plots serve to validate the diversity of analytical solitary wave solutions and their localized wave profiles obtained from the two distinct techniques within the nonlinear framework of the Peyrard-Bishop DNA model.
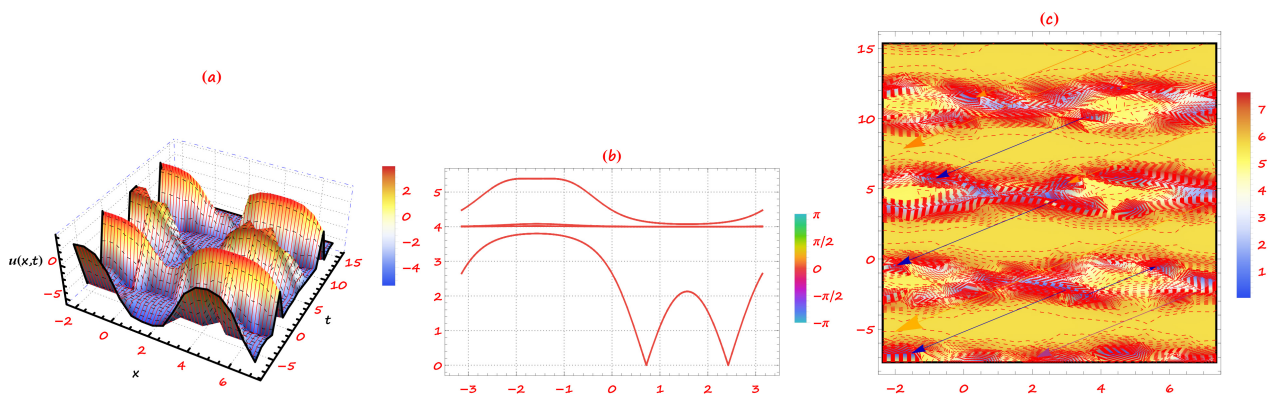
Figure 2. Numerical representations of the solitary wave solutions obtained through analytical methods are depicted. Panels (a-c) illustrate the bright solitary wave solutions computed utilizing the Khater II method (Eq (2.4)). These qualitative plots serve to validate the diversity of analytical solitary wave solutions and their localized wave profiles acquired from the two distinct techniques within the nonlinear framework of the Peyrard-Bishop DNA model.
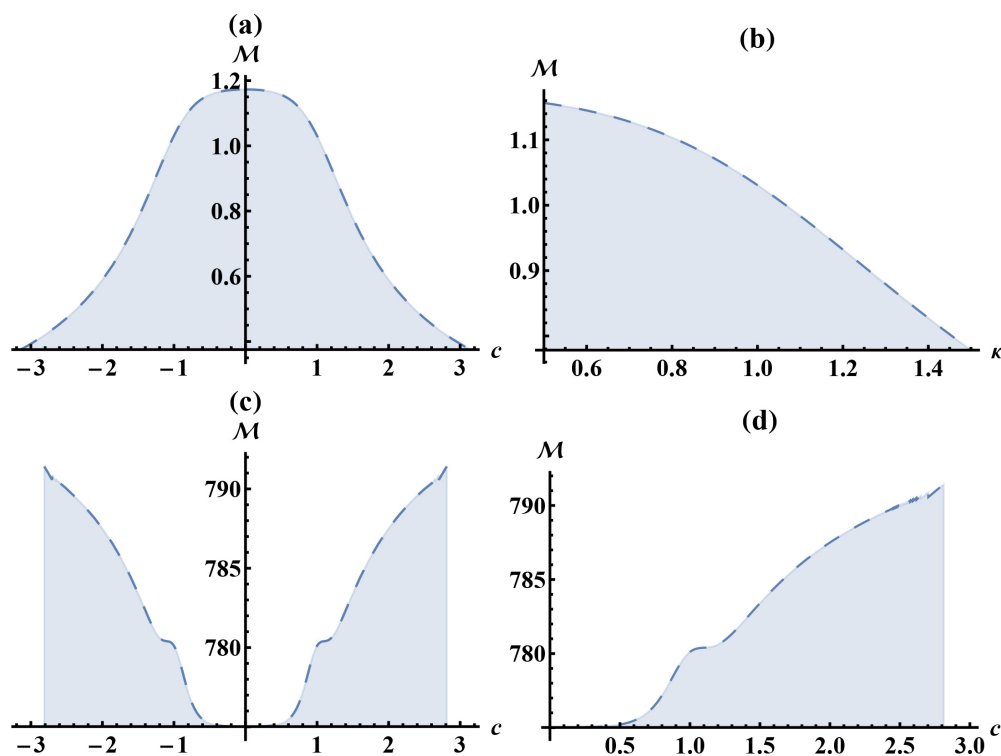
Figure 3. The Hamiltonian framework of the Peyrard-Bishop DNA model reveals conserved quantities, illustrated in Panels (a, b) and (c, d), depicting the momentum $\mathbb{M}$ as described by Eqs (2.5) and (2.6). These conserved dynamic properties arise from the intrinsic nonlinearity governing the system. Graphical representation of these conserved quantities offers valuable insights into the equilibrium conditions that uphold DNA strand integrity within the physically-consistent nonlinear dynamics of the Peyrard-Bishop model.
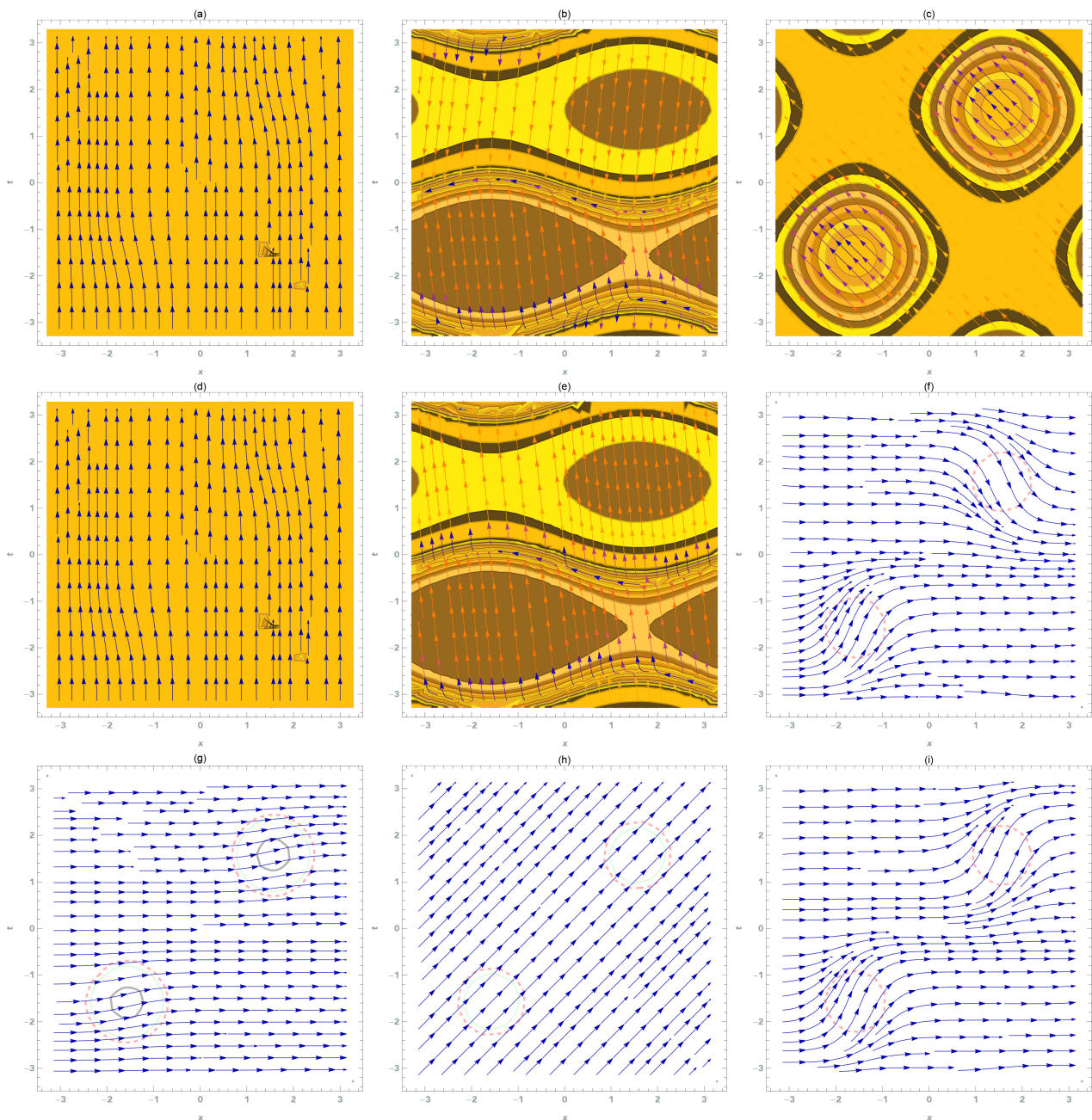
Figure 4. A stream plot of the bright solitary wave solution, expressed by Eq (2.1) and (2.2), is presented with specific parameter values denoted as (a-i). Continuous lines depict the gradual variation in DNA strand displacement (u) concerning distance (x) and time (t), illustrating localized melting bubbles that smoothly rise and fall along the strand during the denaturation process. This visual representation qualitatively captures bubble breathing dynamics and nonlinear strand fluctuations associated with bubble nucleation and growth.
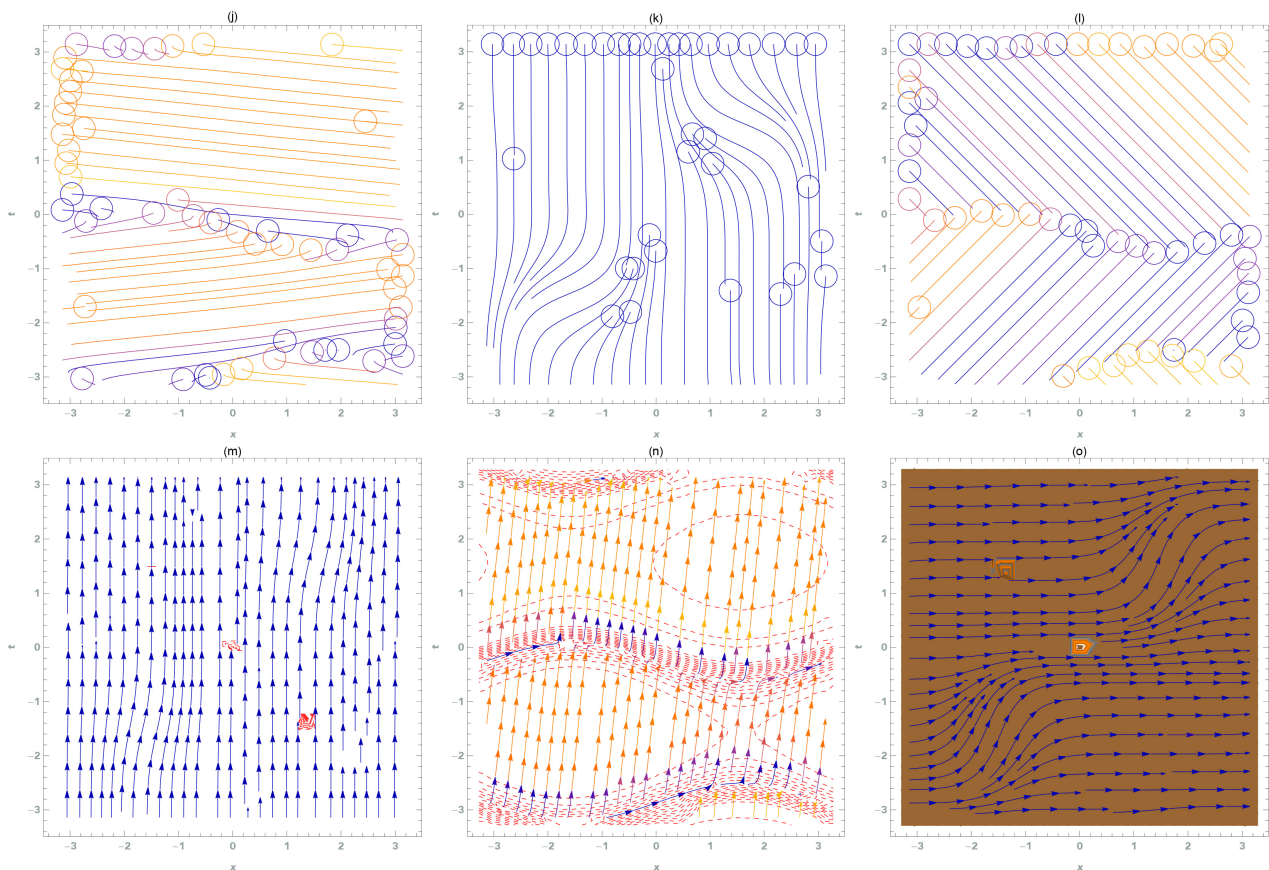
Figure 5. A stream plot of the dark solitary wave solution, formulated by Eqs (2.3) and (2.4), is presented with parameter values denoted as (j-o). The oscillating contour pattern showcases periodic fluctuations in the strand displacement (u) across spatial and temporal coordinates, offering a visual representation of bubble oscillation phenomena within denaturing regions. Localized ripples propagate along the strand, retaining their shape and amplitude, effectively illustrating bubble propagation and coalescence through Ripple-Like soliton interactions during denaturation-renaturation transitions.

4. Results and discussion

The present study investigates the nonlinear Atangana conformable Peyrard-Bishop DNA dynamic model, a nonlinear evolution equation that describes the behavior of DNA molecules by accounting for hydrogen bonds between base pairs and stacking interactions between adjacent base pairs. The primary objective was to construct analytical solutions to this model using the Khater III and an enhanced Kudryashov methods, and subsequently analyze the stability of the obtained solutions through the Hamiltonian system characterization. The results obtained from this study contribute significantly to the understanding of DNA dynamics and offer novel insights into the properties and behavior of DNA molecules.

- Analytical solutions:
  The application of the Khater III method to the nonlinear Atangana conformable Peyrard-Bishop

DNA dynamic model yielded two distinct sets of analytical solutions, represented by Eqs (2.1) and (2.2). These solutions capture the bright solitary wave behavior of the DNA molecule, depicting localized melting bubbles that smoothly rise and fall along the strand during the denaturation process. The visual representations of these solutions, as shown in Figure 1 (panels a-f), provide a qualitative validation of the diversity of analytical solitary wave solutions and their localized wave profiles obtained through this technique.

Furthermore, the implementation of an enhanced Kudryashov scheme yielded two additional sets of analytical solutions, represented by Eqs (2.3) and (2.4). These solutions capture the dark solitary wave behavior of the DNA molecule, showcasing periodic fluctuations in strand displacement across spatial and temporal coordinates. The visual representations of these solutions, as depicted in Figures 1 (panels g-i) and 2 (panels a-c), offer insights into the bubble oscillation phenomena within the denaturing regions of the DNA strand, effectively illustrating the collective behavior of denaturation bubbles and their interactions through Ripple-Like soliton interactions during the denaturation-renaturation transitions.

The novelty of this study lies in the successful application of the Khater III and an enhanced Kudryashov methods to the nonlinear Atangana conformable Peyrard-Bishop DNA dynamic model, resulting in the derivation of analytical solutions that capture both bright and dark solitary wave behaviors. These solutions provide a valuable contribution to the field of nonlinear dynamics and biophysics, as they offer a deeper understanding of the complex interplay between various forces and interactions that govern DNA dynamics.

- Stability analysis:

  In addition to obtaining analytical solutions, this study undertook a comprehensive stability analysis of the derived solitary wave solutions within the Hamiltonian system framework. The Hamiltonian structure serves as a foundational basis for scrutinizing solution stability, utilizing the Lyapunov method. The results of the stability analysis, as illustrated in Figure 3 (panels a-d), reveal the conserved quantities and equilibrium conditions that uphold DNA strand integrity within the physically-consistent nonlinear dynamics of the Peyrard-Bishop model.

  The momentum $\mathbb{M}$, as described by Eqs (2.5) and (2.6), represents a conserved quantity arising from the intrinsic nonlinearity governing the system. The graphical representation of this conserved quantity offers valuable insights into the equilibrium conditions and stability of the solutions. The results indicate that the obtained solutions demonstrate stability within the domain $x \in [-5, 5]$ and $t \in [-5, 5]$, as evidenced by the calculated values of $\frac{d\mathbb{M}}{dc}$ (Eq (2.7)).

  The stability analysis carried out in this study is a significant contribution to the field, as it establishes the robustness and reliability of the obtained solutions within the defined parameter ranges. By identifying the stable regions and equilibrium conditions, researchers can gain confidence in utilizing the Peyrard-Bishop DNA model to accurately describe DNA behavior and guide experimental endeavors.

- Scientific contributions:

  The primary scientific contributions of this study can be summarized as follows:

  (1) Derivation of analytical solutions: The successful application of the Khater III and an enhanced Kudryashov methods to the nonlinear Atangana conformable Peyrard-Bishop DNA dynamic model has yielded novel analytical solutions that capture both bright and dark solitary wave behaviors. These solutions provide a deeper understanding of the

complex dynamics involved in DNA denaturation and renaturation processes, facilitating the development of more accurate simulations and predictions.

(2) Stability analysis: The comprehensive stability analysis of the obtained solutions within the Hamiltonian system framework has established the robustness and reliability of the solutions within specific parameter ranges. By identifying the stable regions and equilibrium conditions, researchers can confidently utilize the Peyrard-Bishop DNA model to accurately describe DNA behavior and guide experimental investigations.

(3) Visual representations: The graphical illustrations of the solitary wave solutions, as depicted in Figures 1-5, offer powerful visual aids for interpreting the physical meaning and properties of the Peyrard-Bishop DNA model. These visual representations capture the dynamic behavior of denaturation bubbles, their nucleation, growth, propagation, and interactions, providing invaluable insights into the underlying mechanisms driving DNA dynamics.

(4) Contribution to biophysics and molecular biology: The findings of this study hold significant implications for the fields of biophysics and molecular biology. By advancing the understanding of DNA dynamics and the interplay between various forces and interactions, this research paves the way for further advancements in areas such as drug design, gene therapy, and the development of innovative therapeutic interventions.

Overall, this study represents a significant contribution to the field of nonlinear dynamics and biophysics, offering novel analytical solutions, comprehensive stability analysis, and visual representations that enhance the understanding of DNA dynamics within the framework of the nonlinear Atangana conformable Peyrard-Bishop DNA dynamic model. The results obtained from this research have the potential to inspire and guide future investigations, ultimately leading to a more profound comprehension of the intricate mechanisms governing DNA behavior and their implications in various scientific domains.

5. Conclusions

This study marks a substantial advancement in our comprehension of the Peyrard-Bishop DNA dynamic model, a pivotal framework for scrutinizing the intricate dynamics governing DNA denaturation and renaturation processes. Employing two distinct analytical techniques, the Khater III method and an enhanced Kudryashov scheme, we have successfully derived novel analytical solutions that encapsulate the nuanced behavior of DNA molecules. The bright solitary wave solutions obtained via the Khater III method, portrayed by Eqs (2.1) and (2.2), delineate localized melting bubbles that smoothly propagate along the DNA strand during denaturation. These solutions furnish crucial insights into the dynamics of denaturation bubbles, encompassing nucleation, growth, and propagation dynamics, which reflect the interplay between hydrogen bond interactions and stacking forces between adjacent base pairs.

Additionally, the dark solitary wave solutions derived from the enhanced Kudryashov scheme, as articulated by Eqs (2.2) and (2.4), unveil the oscillatory nature of strand displacement, effectively illustrating the bubble oscillation phenomena within denaturing regions. These solutions elucidate the collective behavior of denaturation bubbles, their interactions through ripple-like solitons, and the

intricate dynamics underlying denaturation-renaturation transitions. The visual representations of these analytical solutions, showcased in Figures 1-5, serve as potent tools for interpreting the physical meaning and properties of the Peyrard-Bishop DNA model. By encapsulating the dynamic behavior of denaturation bubbles, including their nucleation, growth, propagation, and interactions, these graphical illustrations offer invaluable insights into the underlying mechanisms steering DNA dynamics.

A noteworthy contribution of this study lies in the comprehensive stability analysis conducted within the Hamiltonian system framework. The conserved quantities, specifically the momentum $\mathbb{M}$ described by Eqs (2.5) and (2.6), provide valuable insights into the equilibrium conditions maintaining DNA strand integrity. The graphical representations of these conserved quantities, as depicted in Figure 3, establish the robustness and reliability of the obtained solutions within defined parameter ranges, bolstering our confidence in utilizing the Peyrard-Bishop DNA model for accurate predictions and simulations. The findings of this research bear profound implications for various domains within biophysics and molecular biology. By advancing our understanding of DNA dynamics and the interplay between various forces and interactions, this study lays the groundwork for further advancements in areas such as drug design, gene therapy, and the development of innovative therapeutic interventions.

Moreover, the analytical solutions and stability analyses presented herein provide a sturdy foundation for future investigations and model extensions. Researchers can build upon this work by incorporating additional complexities and effects, such as torsional angles, base-pair openings, and long-range interactions, to further refine the model's accuracy and predictive capabilities.

In summation, this study represents a significant stride in the exploration of DNA dynamics within the realm of nonlinear dynamics and biophysics. The novel analytical solutions, comprehensive stability analysis, and visual representations collectively contribute to a deeper understanding of the intricate mechanisms governing DNA behavior. These findings not only enrich our fundamental knowledge but also pave the way for future advancements in areas such as drug design, gene therapy, and the development of innovative biomedical technologies, ultimately benefiting humanity through improved healthcare and therapeutic interventions.

Author contributions

Mostafa M. A. Khater: Supervision, Writing-review editing, Software and Investigation; Mohammed Zakarya: Supervision, Writing-review editing; Kottakkaran Sooppy Nisar: Software and Investigation; Abdel-Haleem Abdel-Aty: Supervision, Writing-original draft, Writing-review editing, Software and Investigation. All authors have read and agreed to the published version of the manuscript.

Use of AI tools declaration

The authors declare that they have not used Artificial Intelligence tools in the creation of this article.

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Conflict of interests

The authors declare that they have no Conflict of interests.

References

1. J. Manafian, O. A. Ilhan, S. A. Mohammed, Forming localized waves of the nonlinearity of the DNA dynamics arising in oscillator-chain of Peyrard-Bishop model, *Aims Mathematics*, **5** (2020), 2461–2483. http://doi.org/10.3934/math.2020163

2. L. Ouahid, Plenty of soliton solutions to the DNA Peyrard-Bishop equation via two distinctive strategies, *Phys. Scr.*, **96** (2021), 035224. https://doi.org/10.1088/1402-4896/abdc57

3. M. B. Riaz, M. Fayyaz, Rahman, R. U., Martinovic, J., O. Tunç, Analytical study of fractional DNA dynamics in the Peyrard-Bishop oscillator-chain model, *Ain Shams Eng. J.*, **15** (2024), 102864. https://doi.org/10.1016/j.asej.2024.102864

4. K. K. Ali, M. I. Abdelrahman, K. R. Raslan, W. Adel, On analytical and numerical study for the peyrard-bishop DNA dynamic model, *Appl. Math. Inf. Sci*, **16** (2022), 749–759.

5. M. I. Asjad, W. A. Faridi, S. E. Alhazmi, A. Hussanan, The modulation instability analysis and generalized fractional propagating patterns of the Peyrard-Bishop DNA dynamical equation, *Opt. Quant. Electron.*, **55** (2023), 232. https://doi.org/10.1007/s11082-022-04477-y

6. A. Hussain, M. Usman, F. D. Zaman, S. M. Eldin, Optical solitons with DNA dynamics arising in oscillator-chain of Peyrard-Bishop model, *Results Phys.*, **50** (2023), 106586. https://doi.org/10.1016/j.rinp.2023.106586

7. T. E. Sutantyo, A. Ripai, Z.Abdullah, W. Hidayat, Nonlinear dynamics of modified peyrard-bishop DNA model in nosé-hoover thermostat, *J. Phys.: Conf. Ser.*, **1876** (2021), 012021. https://doi.org/10.1088/1742-6596/1876/1/012021

8. M. V. Bezhenar, A. A. Elkina, J. H. Caceres, M. G. Baryshev, A. O. Sulima, S. S. Dzhimak, et al., Review of Mathematical Models Describing the Mechanical Motion in a DNA Molecule, *Biophysics*, **67** (2022), 867–875. https://doi.org/10.1134/S0006350922060021

9. A. Tripathy, S. Sahoo, New dynamic multiwave solutions of the fractional Peyrard-Bishop DNA model, *J. Comput. Nonlinear Dyn.*, **18** (2023), 101005. https://doi.org/10.1115/1.4063223

10. T. E. P. Sutantyo, A. Ripai, Z. Abdullah, W. Hidayat, F. P. Zen, Soliton-like solution on the dynamics of modified Peyrard-Bishop DNA model in the thermostat as a bio-fluid, *Emerg. Sci. J.*, **6** (2022), 667–678. https://doi.org/10.28991/ESJ-2022-06-04-01

11. A. Zafar, K. K. Ali, M. Raheel, N. Jafar, K. S. Nisar, Soliton solutions to the DNA Peyrard-Bishop equation with beta-derivative via three distinctive approaches, *Eur. Phys. J. Plus*, **135** (2020), 726. https://doi.org/10.1140/epjp/s13360-020-00751-8

12. G. Akram, S. Arshed, Z. Imran, Soliton solutions for fractional DNA Peyrard-Bishop equation via the extended-expansion method, *Phys. Scr.*, **96** (2021), 094009. https://doi.org/10.1088/1402-4896/ac0955

13. L. Ouahid, M. A. Abdou, S. Owyed, S. Kumar, New optical soliton solutions via two distinctive schemes for the DNA Peyrard-Bishop equation in fractal order, *Modern Phys. Lett. B*, **35** (2021), 2150444. https://doi.org/10.1142/S0217984921504443

14. A. Djine, G. R. Deffo, S. B. Yamgoué, Bifurcation of backward and forward solitary waves in helicoidal Peyrard-Bishop-Dauxois model of DNA, *Chaos, Soliton. Fract.*, **170** (2023), 113334. https://doi.org/10.1016/j.chaos.2023.113334

15. A. Djine, N. O. Nfor, G. R. Deffo, S. B. Yamgoué, Higher order investigation on modulated waves in the Peyrard-Bishop-Dauxois DNA model, *Chaos, Soliton. Fract.*, **181** (2024), 114706. https://doi.org/10.1016/j.chaos.2024.114706

16. R. A. Attia, D. Baleanu, D. Lu, M. Khater, E. S. Ahmed, Computational and numerical simulations for the deoxyribonucleic acid (DNA) model, *Discrete Contin. Dyn. Syst.-Ser. S*, **14** (2021), 3459–3478. https://doi.org/10.3934/dcdss.2021018

17. M. M. Khater, D. Lu, M. Inc, Diverse novel solutions for the ionic current using the microtubule equation based on two recent computational schemes, *J. Comput. Electron.*, **20** (2021), 2604–2613. https://doi.org/10.1007/s10825-021-01810-8

18. M. M. Khater, A. Jhangeer, H. Rezazadeh, L. Akinyemi, M. A. Akbar, M.Inc, et al., New kinds of analytical solitary wave solutions for ionic currents on microtubules equation via two different techniques, *Opt. Quant. Electron.*, **53** (2021), 609. https://doi.org/10.1007/s11082-021-03267-2

19. M. M. Khater, S. H. Alfalqi,J. F. Alzaidi, R. A. Attia, Analytically and numerically, dispersive, weakly nonlinear wave packets are presented in a quasi-monochromatic medium, *Results Phys.*, **46** (2023), 106312.

20. A. Rani, M. Ashraf, M. Shakeel, Q. Mahmood-Ul-Hassan, J. Ahmad, Analysis of some new wave solutions of DNA-Peyrard-Bishop equation via mathematical method, *Modern Phys. Lett. B*, **36** (2022), 2250047. https://doi.org/10.1142/S0217984922500476

21. T. Shafique, M. Abbas, A. Mahmood, F. A. Abdullah, A. S. Alzaidi, T. Nazir, Solitary wave solutions of the fractional Peyrard Bishop DNA model, *Opt. Quant. Electron.*, **56** (2024), 815.

22. A. Secer, M. Ozisik, M. Bayram,N. Ozdemir, M. Cinar, Investigation of soliton solutions to the Peyrard-Bishop-Deoxyribo-Nucleic-Acid dynamic model with beta-derivative, *Modern Phys. Lett. B*, **38** (2024), 2450263. https://doi.org/10.1142/S0217984924502634

23. N. A. Jolfaei, N. A. Jolfaei, M. Hekmatifar, A. Piranfar,D. Toghraie, R. Sabetvand, et al., Investigation of thermal properties of DNA structure with precise atomic arrangement via equilibrium and non-equilibrium molecular dynamics approaches, *Comput. Methods Programs Biomed.*, **185** (2020), 105169. https://doi.org/10.1016/j.cmpb.2019.105169

24. X. Wang, G. Akram, M. Sadaf, H. Mariyam, M. Abbas, Soliton Solution of the Peyrard-Bishop-Dauxois Model of DNA Dynamics with M-Truncated and β-Fractional Derivatives Using Kudryashov's R Function Method, *Fractal Fract.*, **6** (2022), 616. https://doi.org/10.3390/fractalfract6100616

25. J. B. Okaly, T. Nkoa Nkomom, Nonlinear Dynamics of DNA Chain with Long-Range Interactions, In: *Nonlinear Dynamics of Nanobiophysics*, Singapore: Springer, 2022. https://doi.org/10.1007/978-981-19-5323-1_4

26. A. Bugay, Soliton excitations in a Twist-Opening Nonlinear DNA Model, In: *Nonlinear Dynamics of Nanobiophysics*, Singapore: Springer, 2022. https://doi.org/10.1007/978-981-19-5323-1_7

27. I. Hubac, F. Blaschke, O. N. Karpisek, Quantum information in biomolecules: Transcription and replication of DNA using a soliton model, *Opava, Proceedings of RAGtime 22: Workshops on Black Holes and Neutron Stars*, 2020, 55–71.

28. N. Ayyappan, C. M. Joy, L. Kavitha, Stability analysis of DNA with the effect of twist and Morse potential, *Mater. Today: Proc.*, **51** (2022), 1793–1796.

29. M. A. Abdou, L. Ouahid, J. S. Al Shahrani, M. M. Alanazi, S. Kumar, New analytical solutions and efficient methodologies for DNA (Double-Chain Model) in mathematical biology, *Modern Phys. Lett. B*, **36** (2022), 2250124. https://doi.org/10.1142/S021798492250124X

30. R. Saleh, S. M. Mabrouk, A. M. Wazwaz, Lie symmetry analysis of a stochastic gene evolution in double-chain deoxyribonucleic acid system, *Waves Random Complex Media*, **32** (2022), 2903–2917. https://doi.org/10.1080/17455030.2020.1871109

31. D. Shi, H. U. Rehman, I. Iqbal, M. Vivas-Cortez, M. S. Saleem, X. Zhang, Analytical study of the dynamics in the double-chain model of DNA, *Results Phys.*, **52** (2023), 106787. https://doi.org/10.1016/j.rinp.2023.106787

32. M. Vivas-Cortez, S. Arshed, M. Sadaf, Z. Perveen, G. Akram, Numerical simulations of the soliton dynamics for a nonlinear biological model: Modulation instability analysis, *PLoS One*, **18** (2023), e0281318. https://doi.org/10.1371/journal.pone.0281318

33. T. Han, K. Zhang, Y. Jiang, H. Rezazadeh, Chaotic Pattern and Solitary Solutions for the (21)-Dimensional Beta-Fractional Double-Chain DNA System, *Fractal Fract.*, **8** (2024), 415. https://doi.org/10.3390/fractalfract8070415

34. N. O. Nfor, Higher order periodic base pairs opening in a finite stacking enthalpy DNA model, *J. Modern Phys.*, **12** (2021), 1843–1865.

35. S. W. Yao, S. M. Mabrouk, M. Inc, A. S. Rashed, Analysis of double-chain deoxyribonucleic acid dynamical system in pandemic confrontation, *Results Phys.*, **42** (2022), 105966. https://doi.org/10.1016/j.rinp.2022.105966