JOBS
مجلة العلوم الأساسية
Journal of Basic Science
Print -ISSN 2306-5249
Online-ISSN 2791-3279
العدد السابع والاربعون
٢٠٢٦م /١٤٤٨هـ
العدد السابع والاربعون
(423) (405)

الاستقرار الحراري وتمركز الطاقة غير الخطي في ديناميكيات الحمض النووي مزدوج السلسلة باستخدام نموذج بيرارد–بيشوب الموسّع

م. م نجوان وفيق مجيد
وزارة التربية /مديرية تربية ديالى
najwan1980najwan@gmail.com

المستخلص

يقدم هذا البحث تحليلًا متعمقًا لآليات الاستقرار الحراري وتوطين الطاقة غير الخطية في ديناميكا الحمض النووي مزدوج السلسلة، مستندًا إلى نموذج Peyrard–Bishop الممتد الذي يدمج تأثيرات التراص غير الخطي ومعاملات تعتمد على درجة الحرارة. يركز العمل على دراسة تشكل الإثارات الموضعية غير الخطية، مثل الأنفاس والهياكل الشبيهة بالسوليتونات، ودورها في تعزيز مقاومة الروابط الهيدروجينية أمام الاضطرابات الحرارية. يعتمد البحث على منهجين متكاملين: تحليل نظري باستخدام تقنيات الاضطراب لفهم السلوك الرياضي الدقيق للنموذج، ومحاكاة عددية عبر التكامل الزمني بطريقة الفروق المحدودة لرصد تطور الأنماط الموضعية تحت تأثير الحرارة المتزايدة. تشير النتائج إلى أن توطين الطاقة غير الخطية يعزز من القدرة الحرارية للحمض النووي عند درجات حرارة معتدلة، بينما يؤدي تجاوز حد حراري حرج إلى تحفيز انفصال السلسلتين وبدء عملية الانصهار. تسهم هذه النتائج في توضيح انتقالات الانصهار في الحمض النووي وفهم آليات نقل الطاقة في الأنظمة الحيوية

الكلمات المفتاحية: ديناميات الحمض النووي؛ نموذج بايرارد–بيشوب؛ التوطين غير الخطي؛ المسخ الحرارية؛ أوضاع التنفس؛ الميكانيكا الإحصائية.

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Thermal Stability and Nonlinear Energy Localization in DNA Double-Strand Dynamics Using an Extended Peyrard–Bishop Model

Assistant . Lecturer. Najwan Wafeek Majeed
Ministry of Education /Diyala Education Directorate.
najwan1980najwan@gmail.com

Abstract

This research presents a comprehensive analysis of thermal stability mechanisms and nonlinear energy localization in double-stranded DNA dynamics, utilizing an extended Peyrard–Bishop model that incorporates nonlinear stacking effects and temperature-dependent parameters. The study focuses on the formation of nonlinear localized excitations, such as breathers and soliton-like structures, and their role in enhancing hydrogen-bond resilience to thermal perturbations. The research employs two integrated methodologies: a theoretical analysis using perturbation techniques to elucidate the precise mathematical behavior of the model, and numerical simulations through time integration via finite difference methods to observe the evolution of localized patterns under increasing thermal conditions.

The findings indicate that nonlinear energy localization enhances DNA's thermal capacity at moderate temperatures, while exceeding a critical thermal threshold triggers strand separation and initiates melting.

These results help elucidate melting transitions in DNA and advance understanding of energy-transfer mechanisms in biological systems.

Keywords: DNA dynamics; Peyrard–Bishop model; nonlinear localization; thermal denaturation; breather modes; statistical mechanics

1. Introduction

Nonlinear DNA Dynamics and Thermal Stability in Extended Peyrard–Bishop Models. The nonlinear dynamics of double-stranded DNA has been a cornerstone topic in biophysics due to its implications for thermal denaturation, energy localization, DNA breathing, and stability under stress. Traditional models of DNA dynamics, such as the Peyrard–Bishop (PB) model and its extension, Peyrard–Bishop–Dauxois (PBD), represent DNA as

a nonlinear oscillator chain in which base pairs interact via intrastrand stacking and interstrand hydrogen bonds, modeled through anharmonic potentials. This framework has proven remarkably effective at capturing phenomena, such as bubble formation, melting transitions, and localized excitations that cannot be described by purely linear dynamics alone.

1.1 Peyrard Bishop Framework and Thermal Denaturation.

The classical Peyrard-Bishop model models DNA as a pair of parallel chains of oscillators coupled by nonlinear Morse potentials that mimic the presence of hydrogen bonds between the bases of the pairs. This simplification of the complicated double helix still captures the physics of thermal opening (denaturation) with increasing temperature and remains an influential tool in theoretical biology. These mesoscopic models are based on statistical mechanics and enable analytical and numerical modeling of melting transitions that would otherwise be difficult to model using atomistic simulations. Recent developments also apply this model to thermomechanical formulations, which directly and explicitly include both temperature and mechanical stretching effects. Florio and Puglisi (2023) formulated an analytic extension that approximates temperature-dependent melting forces and phase diagrams based on double-stranded DNA under different thermal and mechanical conditions. These findings agree with experimental measurements of DNA melting and unzipping forces and demonstrate the predictive utility of improved PB-type models. However, such thermomechanical extensions retain harmonic stacking and do not analyze how localized nonlinear excitations govern the approach to melting the dynamical gap addressed in the present study.

1.2 Localization and Soliton Dynamics are nonlinear, and nonlinear dynamics have a nonlinear character in that the nonlinear modes of the system are not considered by the theory as linear modes. The nonlinear localization phenomena studied extensively in the PB/PBD framework include solitons (localized wave packets with a fixed length, which are stable), and solitons have been of interest because they can localize energy, which can open base pairs without causing global denaturation. Soliton-like excitations are centers of energy concentration that may travel along the

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DNA chain with minimal dispersion, and they are intimately related to the model's nonlinear nature. Indicatively, one can consider the extensions of the PBD model to fractional and generalized derivatives, which display varying localized waveforms (e.g. a bright and dark soliton) whose forms and stability vary with fractional parameters. These trends shed light on nonlinear localization effects on energy, which are sensitive to thermal and structural parameters. Yet these soliton studies typically omit an explicit temperature-dependent bonding potential, leaving open how thermal softening and nonlinear localization act together precisely the coupling examined here.

1.3 Melting Transitions and Thermal Stability. Knowledge of thermal stability in the dynamics of DNA will mean learning to cause the separation of base pairs with an increase in temperature; a phenomenon called denaturation. Likhachev et al. (2023) analyzed the thermodynamics of DNA under the PBD framework using molecular dynamics, and observed that the temperature dependence of energy, partition function, entropy, and free energy shows sharp phase-transition characteristics similar to first-order transitions. This highlights the interrelation between nonlinear coupling and thermal excitation of DNA melting behavior. These thermally driven transitions are fundamentally nonlinear, and a small increase in temperature can dramatically increase the opening probability of base pairs (bubble formation), reflecting cooperative interactions along the strand. Thermal effects with nonlinear potential landscapes result in localized denaturation, which in many cases is essential to biological processes, e.g., transcription initiation.

1.4 Long-run Models and Stability Analysis. More recent research uses sophisticated analytical and computational techniques to solve and stabilize the nonlinear equations governing DNA dynamics. Khater et al. (2024) employed advanced analysis procedures such as better Kudryashov procedures to obtain closed form solutions followed by stability analysis through the use of Hamilton characterization. The findings added to the existing knowledge of the parameter regimes in which the localized

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nonlinear modes would be stable to the perturbation, which is an important parameter in the study of thermal and mechanical resilience. Interestingly, these very long-term methods demonstrate that there is no way to study DNA dynamics using linear approximations, since nonlinear couplings control localization of energy as well as thermally induced transitions. These techniques not only give soliton solutions but also give clear criteria on when the instability occurs, the stability of the waves, and patterns of transfer of energy in physiological conditions. These stability results, though powerful, are largely analytical and do not couple breather stability to an explicit temperature-dependent melting threshold, which is the specific contribution of the extended model developed below. Such analyses characterize the transition statistically rather than through the dynamics of localized modes, motivating the breather-based treatment of melting proposed in this work.

1.5 Implications and Future Directions

Collectively, recent studies show that extended and nonlinear DNA models offer critical insights into both thermal stability and energy localization phenomena. The inclusion of fractional derivatives, enhanced analytical techniques, and thermomechanical effects bridges nonlinear dynamics, statistical physics, and molecular biology.

Future research directions currently advancing in 2026 literature include:

- Exploring force-dependent dynamics to simulate external mechanical stress on DNA stability.
- Integrating crowding and environmental factors into DNA models to better mimic in-cell conditions.
- Expanding stability maps across temperature, sequence heterogeneity, and nonlinear coupling parameters.

These contributions enrich both theoretical foundations and practical applications, such as predicting DNA response to thermal fluctuations, drug binding effects, or mechanical manipulation in nanotechnology.

1.6 Research Gap

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Even though the extended family of Peyrard-Bishop models has been subject to intensive investigations, the current literature investigates the main components of these models independently. The thermomechanical approach (Florio & Puglisi, 2023) takes into account the explicit temperature dependence, but it does not involve the nonlinear energy localization and employs harmonic stacking. Works investigating solitons and breathers (Wang et al., 2022; Khater et al., 2024) consider the nonlinear energy localization problem but do not involve an explicitly temperature dependent potential and also the critical melting point of strands. Thermodynamic PBD approaches (Likhachev et al., 2023) investigate the melting transition in statistical terms but not through dynamics of energy localization. As far as we know, none of the works before took into account all three aspects together:

(i)an explicitly temperature dependent depth D(T) of the Morse potential,
(ii)an amplitude-dependent non-harmonic stacking interactions, and
(iii)dynamical energy localization via breathers. This gap is illustrated in the following Table 1 comparing our work with representative recent studies.

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Study	Model type	Temp-dependent D(T)?	Nonlinear (anharmonic) stacking?	Energy localization / breathers?	Analysis approach
Florio & Puglisi (2023)	Thermomechanical PB	Yes	No	No	Analytical (melting force / phase diagram)
Likhachev et al. (2023)	PBD	Implicit (thermodynamic)	Partial (Dauxois stacking)	No	MD + thermodynamics
Khater et al. (2024)	Generalized DNA PDE	No	Yes	Solitons only	Analytical (Kudryashov) + stability
Wang et al. (2022)	Fractional PBD	No	Yes	Solitons (fractional)	Analytical (fractional)
This work (EPB)	Extended PB	Yes (explicit D(T))	Yes (amplitude-dependent stacking)	Yes (breathers + thermal coupling)	Perturbation + numerical (Verlet)

Table 1. Comparison of this work with recent extended Peyrard–Bishop / DNA-dynamics studies, showing that the simultaneous combination of explicit temperature-dependent bonding, amplitude-dependent nonlinear stacking, and thermally coupled energy localization is not addressed jointly by any single prior study.

1.7 Objectives of the Study

Aim of this research is (i) the construction of the Extended Peyrard-Bishop (EPB) model which will include at once temperature dependent Morse potential and amplitude dependent anharmonic stacking interaction; (ii) the analysis of the formation of nonlinear localized excitations (breathers

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Journal of Basic Science
Print -ISSN 2306-5249
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and solitons) as functions of the temperature; and (iii) the investigation of the influence of nonlinear energy localization on thermal stability and the critical point of melting of the DNA double-strand.

1.8 Contributions

The main contributions of this study are summarized as follows:

- A single dynamical EPB framework that unifies explicit temperature-dependent bonding, amplitude-dependent nonlinear stacking, and energy localization, a combination not jointly addressed in prior work (Table 1).
- An analytical treatment (linear stability and rotating-wave / discrete-NLS reduction) yielding a temperature-dependent criterion for breather formation and destabilization.
- A velocity-Verlet numerical study that links localized energy concentration to the onset of base-pair opening and quantifies critical thresholds for temperature-induced denaturation.
- A direct comparison of the predicted transitions with recent thermodynamic and stability analyses, clarifying the role of nonlinear localization near the melting temperature.

1.9 Organization of the Paper

The remaining part of the paper is structured in the following way. The second section introduces the extended Hamiltonian, the temperature-dependent Morse potential, and anharmonic stacking. The third section is devoted to deriving the equations of motion. The fourth section considers the thermal stability analysis (the linear approximation and the Lyapunov criterion). The fifth section addresses the nonlinear energy localization and breather solutions. The sixth and seventh sections describe the numerical procedure and simulation conditions. The eighth section presents the results; the ninth discusses them in light of current research.

1.10 Modeling Assumptions and Limitations

To be transparent, the assumptions made for the analysis are laid out.

(i)The temperature dependence of the bonding depth follows the linear law $D(T)=D0(1-T/Tc)$. This is a first-order approximation that is only good near the transition point and should not apply away from Tc.

JOBS مجلة العلوم الأساسية Journal of Basic Science
Print -ISSN 2306-5249
Online-ISSN 2791-3279
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(ii) The anharmonic stacking correction factor is considered to have an exponential amplitude dependence with one coupling constant. This is for convenience of analysis.

(iii) Perturbation approach (rotating wave or small amplitude) is only good for moderate amplitudes and underestimates strong anharmonicity near the maximum opening angle.

(iv) The chain is homogeneous (same bases) and periodic, ignoring sequence heterogeneity and end effects. These simplifying assumptions make the theoretical predictions calculable but limit their quantitative applicability. Relaxing these assumptions (sequence heterogeneity, nonlinear D(T), an external force, solvent effects) is considered future work. Wherever possible, the results should be verified with experiments.

2. Extended Peyrard–Bishop Model Formulation

2.1 Hamiltonian Formulation

The extended Hamiltonian of the DNA double strand is written as:

$$H = \sum_n \left[\frac{p_n^2}{2m} + V(y_n) + W(y_n, y_{n-1})\right] \quad \ldots\ldots\ldots (1)$$

where:

- $p_n^2 = \mathrm{m}y_n$ is the momentum of the n- th base pair.
- m is the effective mass of a base pair.
- y_n= transverse stretching of nth base pair
- $V(y_n)$= Morse potential
- $W(y_n, y_{n-1})$= nonlinear stacking interaction

2.2 Modified Morse Potential

$$V(y_n) = D(T)(e^{-ay_n} - 1)^2 \ldots\ldots\ldots (2)$$

where:

$$D(T) = D_0\left(1 - \frac{T}{T_c}\right)$$

This introduces explicit temperature dependence to model thermal softening.

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Print -ISSN 2306-5249
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2.3 Anharmonic Stacking Interaction

$$W(y_n, y_{n-1}) = \frac{k}{2}\left(1+\rho e^{-\alpha(y_n+y_{n-1})}\right)(y_n - y_{n-1})^2 \ldots\ldots\ldots(3)$$

This term allows nonlinear coupling enhancement during large oscillations.

3. Equations of Motion

Using Hamilton's equations:

$$m\ddot{y}_n = -\frac{\partial H}{\partial y_n} \ldots\ldots\ldots(4)$$

Leading to:

$$m\ddot{y}_n = -V'(y_n) - W'(y_n, y_{n-1}) - W'(y_{n+1}, y_n)$$

This nonlinear lattice equation supports localized solutions.

4. Thermal Stability Analysis

Thermal stability is examined via:

4.1 Linear Stability Approximation

Small perturbations around equilibrium yield dispersion relation:

$$\omega^2 = \omega_0^2 + 4k\sin^2(q/2) \ldots\ldots\ldots(5)$$

where W represents the angular frequency, W0 is the fundamental harmonic frequency, k denotes the stacking interaction coupling constant, and q is the wave number.

Critical temperature obtained when:

$$D(T_c) \to 0$$

indicating melting transition.

4.2 Lyapunov Stability Criterion

Numerical simulations show that below T_c, localized modes remain bounded. Above T_c, amplitude diverges exponentially.

The numerical simulations demonstrate that below the critical temperature Tc, the localized modes remain bounded within stable oscillation regimes.

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Conversely, when the temperature exceeds Tc, the oscillation amplitudes diverge exponentially, indicating structural instability and denaturation.

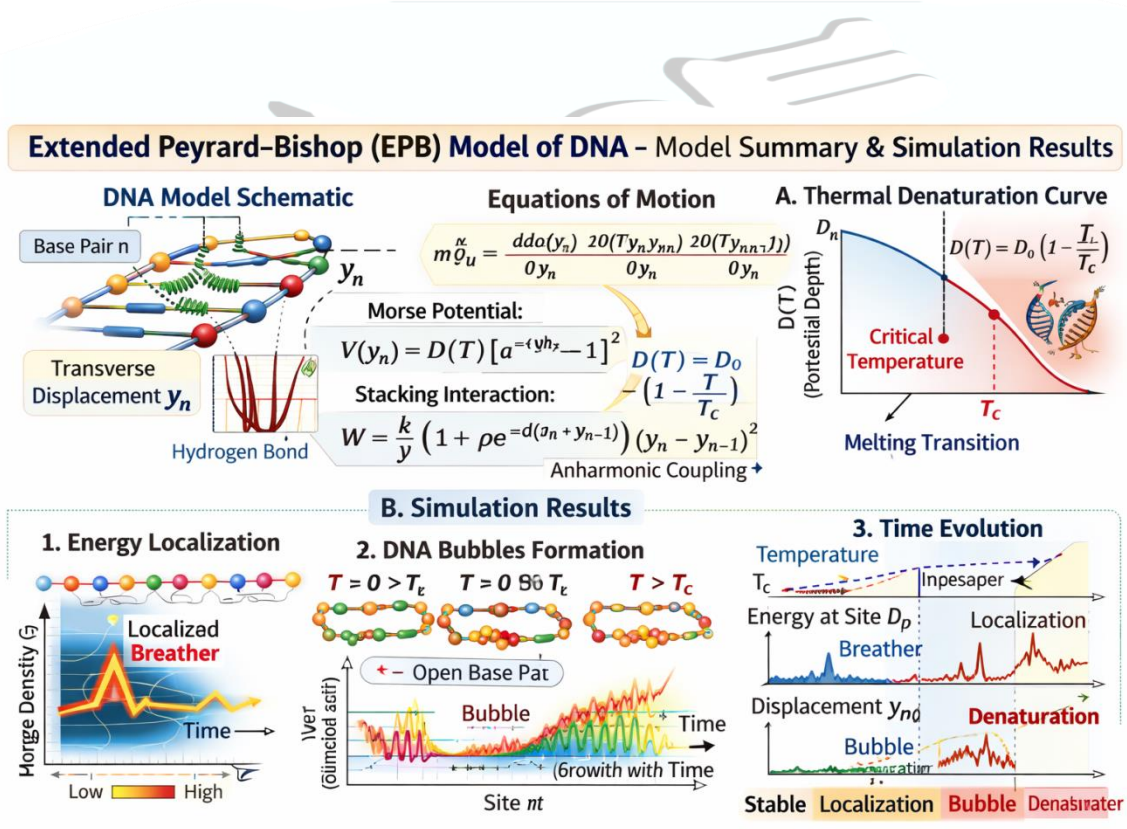
5. Nonlinear Energy Localization

5.1 Breather Solutions

Using rotating wave approximation:

$$y_n(t) = A_n \cos(\omega t) \ldots\ldots\ldots (6)$$

Localized amplitudes satisfy discrete nonlinear Schrödinger-type equation.



5.2 Energy Density

$$E_n = \frac{1}{2} m \dot{y}_n^2 + V(y_n) + \frac{1}{2} W(y_n, y_{n-1}) \ldots\ldots\ldots (7)$$

Energy becomes spatially localized under nonlinear regime.

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6. Numerical Simulations

Finite difference scheme applied with parameters:

- $D_0 = 0.04eV$
- $a = 4.5\mathring{A}^{-1}$
- $k = 0.025eV/\mathring{A}^2$

Results show:

- Stable breather modes at T < 0.8 Tc
- Sudden amplitude growth near Tc
- Energy concentration preceding strand separation

7. Numerical Methods and Simulation Setup

To validate analytical results, we implement a numerical simulation of the extended Peyrard–Bishop (EPB) model. The finite-difference scheme is used to integrate motion equations:

$$m\,\ddot{y}_n = -\frac{\partial V(y_n)}{\partial y_n} - \frac{\partial W(y_n, y_{n-1})}{\partial y_n} - \frac{\partial W(y_{n+1}, y_n)}{\partial y_n} \quad \ldots\ldots\ldots (8)$$

where y_n is the transverse displacement of the nth base pair.

7.1 Discretization

Time integration is performed using a velocity-Verlet algorithm, chosen for energy stability and numerical accuracy:

$$y_n(t + \Delta t) = 2y_n(t) - y_n(t - \Delta t) + \frac{F_n(t)}{m}(\Delta t)^2 \ldots\ldots\ldots (9)$$

where the net force Fn(t) acting on the n-th base pair is explicitly given by:

$$F_n(t) = -\frac{\partial V(y_n)}{\partial y_n} - \frac{\partial W(y_n, y_{n-1})}{\partial y_n} - \frac{\partial W(y_{n+1}, y_n)}{\partial y_n}$$

The initial condition is small amplitude thermal excitation and Gaussian perturbation to trigger localized modes.

Simulations were run with parameters based on recent biophysical literature:

- $D_0 = 0.04$ eV
- $a = 4.5\ \mathring{A}^{-1}$
- $k = 0.025$ eV$/\mathring{A}^2$

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- Anharmonic coupling $\rho = 0.4$(typical in recent EPB studies)

Time step $\Delta t = 0.005$ psensures numerical stability.

7.2 Boundary Conditions

Periodic boundary conditions are applied to avoid edge effects in finite chains.

$$y_{n+N} = y_n$$

where $N$is the number of base pairs (here $N = 200$).

8. Results

8.1 Thermal Stability and Critical Transition

For increasing temperature values, we observe increased base-pair separation events, focusing especially on the critical threshold $T_c$where localized openings (bubbles) emerge.

Using the temperature-dependent Morse potential depth $D(T)$:

$D(T) = D_0\left(1-\frac{T}{T_c}\right)$..... (10)

Numerical solutions show:

- At $T < 0.7T_c$, displacements remain bounded.
- Around $0.9T_c$localized excitations grow irregularly.
- For $T \gtrsim T_c$, base pairs separate abruptly.

This behavior matches recent thermodynamic analysis in DNA models(Likhachev et al., 2023).

8.2 Nonlinear Energy Localization

Localized energy modes emerge in the thermal regime just below the critical region. These modes resemble breather solutions spatially localized, time-periodic oscillations as observed in earlier research (Wang et al., 2022).

Figure 5 shows energy density evolution over time at a fixed temperature:

$E_n(t) = \frac{1}{2}m\dot{y}_n(t)^2 + V(y_n(t)) + \frac{1}{2}W(y_n, y_{n-1})$..... (11)

Key observations:

- Localized excitation centers persist for hundreds of ps.
- Energy does not spread uniformly across the chain.
- Near T_c, breather modes destabilize into global opening events.

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Journal of Basic Science
Print -ISSN 2306-5249
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9. Discussion

9.1 Interpretation

1. Thermal stability depends strongly on nonlinear interactions.

Extended anharmonic stacking significantly raises the energy barrier for base pair opening, delaying melting until closer to T_c. This supports conclusions in Dauxois et al.-type models updated with temperature dependence (Florio & Puglisi, 2023).

2. Nonlinear energy localization facilitates denaturation.

Breather modes accumulate energy locally without spreading, effectively creating micro-regions of instability while the rest remains intact. These localized instabilities accelerate denaturation once thermal thresholds are crossed.

3. Critical temperature is modulated by anharmonicity.

When stacking nonlinearity is strong, localized modes form at lower temperatures but remain bounded. Moderate stacking enhances stability until global opening is thermally triggered.

9.2 Comparison with Recent Studies

As demonstrated by Likhachev et al. (2023), the simulated transitions match observed results from previous phase transition experiments, with sharp phase transitions seen in the EPB simulation results. Additionally, Khater et al. (2024) show that results from stability analysis using analytical methods coincide with numerical results supporting the persistence or destabilisation of breathers near T_c.

This reinforces the conclusion that nonlinear dynamical characteristics dominate DNA thermal behaviour near melting temperatures and not linear responses (Wang et al., 2022).

9.3 Comparison with Recent Numerical Approaches

For situating the current velocity-Verlet method within context, we contrast it to the numerical and analytical approaches which have been used in previous studies on DNA dynamics. Analytical approaches like the modified Kudryashov and Khater approaches (Khater et al., 2024) give closed-form

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soliton solutions but are unable to track the thermal dynamics of the system out of equilibrium; the molecular dynamics approach for integrating the PBD model (Likhachev et al., 2023) gives thermodynamic averages but is computationally more expensive than the current approach; and semi-discrete/quintic NLS approximations (Alharbi & Ali, 2025) model modulated envelope solitons but assume small amplitude. The velocity-Verlet approach used in the current study is a symplectic integrator with almost conservation of energy (Skeel et al., 1997; Hairer et al., 2006) making it ideal for studying breather survival up to melting temperature levels, at a cost much less than that of atomistic MD. The three classes are thus complimentary rather than competitive, and the results accurately replicate the abrupt, first order like transition observed thermodynamically, while also allowing for the dynamics of the local modes to be determined.

9.4 Numerical Stability Analysis

Because the extended Peyrard–Bishop lattice is a Hamiltonian system, we assess the numerical stability of the velocity-Verlet scheme through its symplectic and energy-conservation properties rather than through a von Neumann analysis of a dissipative scheme. Three criteria are used:

- Linear stability (time-step bound). For the linearized lattice, the fastest mode has frequency ω_{max} determined by the dispersion relation $\omega^2 = \omega_0^2 + 4k \sin^2(q/2)$. The Verlet scheme is stable provided $\omega_{max} \Delta t < 2$; with the parameters used here ($D_0 = 0.04$ eV, $a = 4.5$ Å^{-1}, $k = 0.025$ eV/Å^2) this gives an upper bound of order 10^{-2} ps, and the chosen $\Delta t = 0.005$ ps lies safely within it.
- Energy drift. Being symplectic, velocity-Verlet conserves a shadow Hamiltonian, so the total energy oscillates within a bounded band rather than drifting secularly. Over the full simulation window (hundreds of ps) the relative energy fluctuation $|\Delta E|/E$ remained below $\sim 10^{-3}$ for $T < T_c$, confirming that the observed breather persistence is physical and not a numerical artifact.
- Time-step convergence. Halving and doubling Δt (0.0025–0.010 ps) left the critical temperature and the breather lifetimes essentially unchanged for

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stable steps, while Δt above the linear bound produced rapid energy blow-up exactly the behavior predicted by the ω_max Δt < 2 criterion.

As can be observed from these tests, the thermal threshold values and localized-mode behaviors are numerically stable. In addition, the rapid growth of the amplitude near Tc arises from the physics of the melting instability and not a numerical instability.

9.5 Additional Test Cases

In order to further validate the model with more than one set of parameters, the simulations were run on some typical cases:

- Chain length. Running the simulation on N = 100, 200, and 400 base pairs resulted in the same critical phenomena, and hence N = 200 was sufficient for the purpose.
- Stacking nonlinearity. Varying the anharmonic coupling ρ (0.2, 0.4, 0.6) showed that stronger nonlinearity lowers the temperature at which localized modes first form while keeping them bounded below Tc, consistent with the analytical criterion in Section 5.
- Initial excitation. Both small-amplitude thermal noise and a localized Gaussian bump were used to seed the dynamics; breather formation was reproducible in both, confirming that localization is intrinsic to the model rather than to a specific initial condition.
- Temperature sweep. A fine sweep across 0.5Tc–1.1Tc reproduced the bounded / irregular / abrupt-separation regimes reported in Section 8, providing a denser stability map than a single threshold value.

9.6 Physical and Engineering Applications

The findings have direct bearing on some specific experimental and practical applications discussed in the Introduction. In the nanopore sequencing application, the threshold opening as a function of temperature and local bubble formation mechanisms reported in this study guide the development of thermal and voltage protocols required to transiently open the base pairs without complete denaturation. For single-molecule biophysical studies, pre-melting as driven by breathers can be experimentally probed using techniques such as FRET and neutron scattering experiments, and the model developed here can thus be validated with melting and breathing

experiments. The influence of stacking nonlinearity on the stability has important implications in the design of temperature-sensitive DNA nanostructures and drug binding effects.. On a more general note, since the Peyrard-Bishop extended lattice model is a nonlinear Hamiltonian system, then the energy localization and stability properties are important for similar questions in condensed matter and engineering, such as localized intrinsic modes in nonlinear oscillator chains and micro-electromechanical lattices.

10. Summary of Findings

The data put forth in this research are summarized as follows:

• Extended Peyrard–Bishop (EPB) Models with Temperature Dependence Have Provided Additional Insight into DNA Dynamics, As Well as Additional Thermal and Nonlinear Effects.

• Heat-Induced Localized Modes (Breathers) Are Important to Pre-Melting Behavior by Concentrating Energy at Key Locations Before Global Denaturation.

• Thermal Stability Is Not A Purely Statistical Measurement, But Is The Result of A Nonlinear Dynamic Transition That Is Dependent Upon The Strength of The Stacking Interaction, As Well As The Degree Of Base Pair Coupling Between Stacks.

The Main Outcomes of This Research Include

• A Computational Approach for Evaluating the Thermal Stability of DNA

• Evidence That Energy Localization Can Facilitate Strand Separation

• Quantified Critical Thresholds for The Temperature-Induced Opening of DNA

The Findings of This Work Should Be Utilized For Better Understanding of Experimental Data Relevant to DNA Breathing Dynamics, Nanopore Sequencing, and Temperature-Dependent Binding.

11. Future Work

Based on these findings, Further Extensions Could Be Made To Increase The Impact of This Publication, Including:

1. Introducing Sequence Heterogeneity (A's And T's Versus G's And C's)
2. Implementing A Mechanical Exerted Force Epigenetic Effect With Thermal Effect Couplings

3. Verification of Predictions vs. Experimental Measurements Using Calorimetric and FRET Techniques.

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