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Solution of a Variational inequality for charge transport DNA model with vibrational and rotational coupling motion

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Abstract- We perform a numerical computation of eigenvalues of the statistical physics of DNA using a generalized Morse potential to obtain the mean displacement of nucleotides. Likewise, applying numerical methods, we solve the Peyrard-Bishop-Holdstein model to obtain the electronic distribution in DNA. We apply semigroup theory for charge transport DNA model with vibrational and rotational coupling motion . For that we use the theory of semigroup in its equivalent vector form , that is,

$$\begin{aligned} U_t &= AU + F(U) \\ U(0) &= U_0 \end{aligned} \tag{1}$$

This system given by (2) ***stand for an initial value problem, which we show that, under suitable assumptions of the operator*** A ***and on the nonlinearity*** F ***the system supports a single global weak solution satisfying the given initial condition, for that one, we consider the Sobolev spaces which will solve the Cauchy problem. The ideas of Elena Díaz [4] have really been followed, who considers the Peyrard-Bishop-Holstein model, which introduces a description of polaronic effects for the transport of electrical charge in DNA. Consequently, a Schrödringer equation is added for electrical transport, whose indicator is the amplitude probability for an electric charge located in the nth nucleotide. Likewise, in the vibrational part, the Peyrard-Bishop model has been maintained in its continuous form, which has as its starting point the discrete form in the reference of [6] .***

Keywords: Peyrard-Bishop-Holdstein; Global weak solution; vibrational-rotational; DNA Breathing.

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I. INTRODUCTION

The Peyrard-Bishop (PB) model is a theoretical framework used to study the nonlinear dynamics of DNA, focusing on its vibrational properties and processes such as denaturation. Below are its main characteristics and applications: Fundamentals of the Peyrard-Bishop Model Mechanical Representation of DNA: The two strands of DNA are modeled as one-dimensional chains of nucleotides with a common mass m. Covalent Bonds: These are represented by harmonic potentials between adjacent nucleotides on each strand. Hydrogen Bonds: These are described using Morse potentials between complementary base pairs (A-T and G-C). Dynamic Equations: The motion of the nucleotides is governed by nonlinear differential equations that consider stacking forces (interactions between adjacent bases) and the opening of hydrogen bonds. In its helical version, harmonic couplings between bases separated in the helical ladder are included, replicating the three-dimensional structure of DNA. Applications and Benefits of the Model Study of DNA Denaturation: The model explains how heat or external forces break hydrogen bonds, separating the strands (referred to as "meltin"). It predicts the formation of local denaturation bubbles, which are relevant in processes such as transcription. Solitons and Nonlinear Waves: Analytical solutions of the model reveal the existence of solitons, localized waves that propagate energy without dispersion, suggesting an efficient mechanism for energy transfer in DNA. Methods such as Khater and Kudryashov are employed to derive exact solutions and analyze their stability using Hamiltonian systems. Viscosity Effects and Biological Environment: The inclusion of frictional forces in the model explains how the viscosity of the cellular medium affects DNA dynamics, especially during transcription from DNA to RNA. Numerical studies using methods like B-splines validate the accuracy of theoretical solutions. Extensions and Current Relevance Peyrard-Bishop-Dauxois (PBD) Model: This extension incorporates curvature effects and nonlocal couplings for a more realistic description of DNA fluctuations. Applications in Biotechnology: Understanding the nonlinear dynamics of DNA has implications for drug design, genetherapy, and nanotechnology, where the mechanical response of DNA to external stimuli is critical. In summary, the Peyrard-Bishop model provides a quantitative framework for exploring biomechanical phenomena in DNA, connecting nonlinear physics with fundamental biological processes. Its evolution into more complex versions (such as the helical or PBD models) reflects its enduring utility in molecular biophysics.

In mathematics, a weak solution or generalized solution to an ordinary or partial differential equation is a function for wich the

derivatives may not all exist but wich is nonetheless deemed to satisfy the equation in some precisely defined sense.

The theoretical study and experimental DNA has its limitations: difficulty in describing the dynamics through equations with analytical solutions, high computational costs and difficult to solve all specific problems. The mathematical tools used in the theoretical study of the problem are Finite Difference Method and Schrodinger equation with anharmonic stacking interactions for the DNA molecule. In addition we analyzed more generalizations [5] with the amplitude and the velocity of waves of DNA breathing. The results show that the amplitude increase with the generalized Morse potential. Also the connection between DNA denaturation and phase transitions can be understood through the lens of statistical mechanics and the Peyrard-Bishop model, which provides a framework for analyzing the thermodynamic behavior of DNA under varying conditions. When DNA is subjected to heat, it undergoes a denaturation transition, wherein the two strands separate due to the breaking of hydrogen bonds. This process is characterized as a first-order phase transition, meaning it involves a discontinuous change in the state of the system—specifically, a sudden increase in the fraction of unbound base pairs as temperature rises. Experimental observations support this classification, with sharp transitions noted in melting curves that indicate cooperative melting regions (CMRs) within the DNA structure1. The phase transition aspect is further elucidated by considering the interactions between bound segments and denatured loops within the DNA molecule. Theoretical models suggest that when excluded volume interactions are included, these interactions can drive the transition to be first-order, aligning with experimental findings that show critical fluctuations in properties such as loop size distributions near the transition point23. Moreover, studies employing techniques like magnetic tweezers have demonstrated how external forces can induce transitions similar to thermal denaturation, revealing a complex interplay between mechanical stress and thermal energy. This leads to a force-temperature phase diagram that captures both thermal and force-induced transitions, emphasizing that DNA's structural integrity is highly sensitive to both temperature and applied forces. In summary, the relationship between DNA denaturation and phase transitions is rooted in their shared characteristics of abrupt changes in molecular configurations under varying conditions. Theoretical models like Peyrard-Bishop provide valuable insights into these phenomena, linking molecular dynamics with broader principles of phase behavior in physical systems.

Research on DNA twisting and its implications for cancer has gained momentum, particularly focusing on how DNA structural dynamics influence genomic stability and cellular processes critical to cancer development. We have some results in this area of investigation: Transcription-Replication Conflicts: Recent studies have highlighted the role of collisions between transcription and DNA replication as significant contributors to genetic instability in cancer cells. Mutations in specific genes can lead to large tandem duplications (TDs), a type of genetic alteration associated with various cancers, including those of the upper gastrointestinal tract and breast cancer. These TDs arise when transcription machinery interferes with the DNA replication process, leading to errors that can promote tumorigenesis. Extrachromosomal DNA (ecDNA): Research has shown that ecDNA plays a pivotal role in enhancing oncogene expression and promoting genomic evolution in tumors. The presence of ecDNA is linked to increased transcription activity, which can lead to heightened transcription-replication conflicts and replication stress. This stress is characterized by slower replication fork progression and increased DNA damage, making ecDNA-containing tumors particularly vulnerable to targeted therapies that exploit these weaknesses1. Replication Stress and Genome Stability: Alterations in DNA structure can induce replication stress, a hallmark of cancer that destabilizes the genome. Understanding how specific DNA structures contribute to this stress can inform new treatment strategies across various cancer types. For instance, researchers have identified mechanisms by which structural changes in DNA impede replication, leading to genomic instability. Targeting Specific Gene Mutations: Studies have indicated that cancers characterized by large TDs are more sensitive to certain inhibitors, such as WEE1 and CHK1 inhibitors. This suggests potential therapeutic avenues for targeting tumors with specific genetic alterations linked to transcription-replication conflicts2. Role of DNA Repair Mechanisms: Investigations into mutations in genes responsible for DNA repair, such as BRCA1 and ATM, reveal their critical role in maintaining genomic integrity. Failures in these repair systems can exacerbate mutations and contribute to cancer progression, highlighting the importance of understanding how transcription and replication dynamics interact with repair pathways. In summary, ongoing research is uncovering the intricate relationships between DNA twisting, transcription-replication conflicts, and cancer development. By elucidating these connections, scientists aim to develop innovative therapeutic strategies that target the unique vulnerabilities presented by altered DNA dynamics in cancer cells.

We focus on a Global wedk solution for charge transport DNA model with vibrational and rotacional coupling using the theory of semigroups.

Recent works allow us to obtain a model coupling vibrational and rotational motion for DNA molecule [6].

Molecular-level charge transport in DNA is a physical phenomenon that serves as a theoretical complement to understanding DNA mutations. Applying the semigroup theoretical method, a new solution called the weak solution of the electrical transport system in DNA is obtained and is of multidisciplinary interest. In this context, the DNA model has become a prominent approach to understand how molecules interact and move. This model is not only relevant for the transport of biological substances, but also has implications in the development of biomedical technologies and in the manipulation of nanoscale materials. The main approaches to follow are vibrational and rotational coupling that play a fundamental role in molecular transport, since it affects the dynamics and stability of molecules during their movement. These phenomena can influence how molecules organize and move through different environments, which is crucial to optimize pro-

cesses such as drug delivery and chemical synthesis. Despite advances in molecular transport modeling, significant challenges exist. The complexity of the system, which includes multiple interactions between particles, makes analytical solutions difficult to obtain. Therefore, the development of efficient numerical solutions that can adequately capture these phenomena is required using the fourth-order Runge–Kutta numerical method based on two main equations. Firstly, the Schrodinger equation, this equation shows the probability amplitude of the localized electric charge on a nucleotide. Secondly, the Newton equation of motion that explains the displacement motion of nucleotides from the equilibrium position with its corresponding electric transport [4].

The problem for charge transport DNA model with solvent, vibrational and rotational coupling motion. The solvent interaction in the model introduces a new behaviour been analysed by [6]. from the point of view of numerical analysis.

In our case we are concerned with the global classic solution from analytical the point of view. For that, we consider an abstract initial value problem.

II. MATERIALS AND METHODS

We consider A as being an operator defined in a Hilbert space H for the scalar product $((\cdot,\cdot))$ and equipped with the norm $\|\cdot\|$, with domain $D(A)$. We say that the operator A is accretive in H if

$$\|u+\lambda Au\| \geq \|u\|,$$

for all $u \in D(A)$ and all $\lambda > 0$.

Hence, we say that an operator A in a Hilbert space H is m-accretive if the following holds

$i)$ A is accretive

$ii)$ For all $\lambda > 0$ and all $f \in H$, there exists $u \in D(A)$ such that

$$u+\lambda Au = f$$

Which is an underlying partial differential equation. It follows easily from the definition that if A is an m-accretive operator in H, the mapping $f \mapsto u$ is a contraction $H \to H$, and is one to one $H \to D(A)$, more precisely the above mapping is denoted by $J_\lambda(A)$, or $(I+\lambda A)^{-1}$. We have $J_\lambda \in \mathcal{L}(H)$, $\|J_\lambda\|_{J_\lambda} \leq 1$, and $R(J_\lambda) = D(A)$. J_λ is called the resolvent of A and A_λ is the Yosida approximation of A, defined by $A_\lambda = \lambda^{-1}(I - J_\lambda)$. It is clear that the graph $G(A)$ is closed in $H \times H$, $D(A) \hookrightarrow H$. The notation to be used is mostly standard.

The Peyrard-Bishop (PB) model has become a cornerstone in understanding DNA's nonlinear dynamics, particularly its vibrational behavior linked to thermal denaturation—the separation of double-stranded DNA into single strands under heat. This mechanical model simplifies DNA into two parallel strands of oscillators connected by a Morse potential representing hydrogen bonds, while harmonic potentials model covalent bonds along each strand. While the original PB framework focused on transverse vibrational motions of base pairs, subsequent extensions have incorporated rotational dynamics to better capture DNA's helicoidal structure and low-temperature phenomena like transcription bubbles. In the extended PB model, nucleotides exhibit both vibrational displacements (radial stretching/compression) and rotational motions (angular twists around the helical axis). The coupling between these modes arises through a nonlinear modification of the Morse potential, where the interaction energy depends on both radial displacements and angular coordinates. This dual approach allows the model to simulate how localized energy fluctuations—whether from thermal effects or protein interactions—could induce transient openings in the DNA helix, essential for processes like transcription. Remarkably, while vibrational motion dominates denaturation at high temperatures, rotational contributions become significant near physiological temperatures, influencing structural transitions. The model's biological relevance is underscored by its ability to predict realistic melting temperatures when parametrized with experimentally derived values for hydrogen bond stiffness (k 0.06 eV/$\mathring{A}^2$) and dissociation energy (D 0.03 eV). Computational studies using this framework reveal that solitonic excitations—localized waves maintaining their shape—could propagate along DNA, potentially facilitating long-range interactions between distant genomic regions. These advances demonstrate how combining vibrational and rotational dynamics in the PB paradigm bridges molecular-scale mechanics with mesoscopic biological functions, offering insights into DNA's remarkable structural adaptability.

Incorporating the Schrödinger equation into the Peyrard-Bishop (PB) DNA model enhances its ability to describe quantum charge transport mechanisms and their interplay with DNA's mechanical dynamics. Here's how this integration provides key benefits: 1. Quantum-Classical Hybrid Framework The PB model traditionally focuses on classical lattice vibrations (e.g., hydrogen bond stretching via Morse potentials). Introducing the Schödinger equation enables: Quantum treatment of charge carriers: Electrons or holes are modeled with wave functions, capturing tunneling effects and coherent transport across nucleotide bases26. Coupled dynamics: The classical equations for base-pair displacements and influence quantum parameters like effective mass and potential barriers for charges. This hybrid approach explains phenomena like polaron formation, where charges self-trap by distorting the DNA lattice. Nonlinear Schrödinger Equation (NLSE) and Solitons In extended PB models (e.g., helicoidal PB), perturbative methods reduce the system to a nonlinear Schrödinger equation for envelope solitons Solitonic solutions represent stable charge-density waves propagating without dispersion, mimicking coherent charge transport in DNA.

3. Charge-Lattice Coupling The Schrödinger equation quantifies interactions between charges and lattice v ibrations: Peyrard-Bishop-Holdstein(PBH) model: Combines charge hopping (quantum) with base-pair opening (classical), showing how displacements modulate charge mobility. Modulational instability: Small perturbations in charge density amplify under specific nonlinear conditions, leading to localized charge packets4. 4. Tunneling and Barrier Effects The Schrödinger equation models

charge tunneling through energy barriers formed by adenine (A) bases in many sequences.

Effective mass approximation: Simplifies the periodic potential of DNA into a flat profile with discontinuities, revealing distance-dependent tunneling rates. Dynamic barriers: Base-pair opening (via PB's Morse potential) alters barrier heights, affecting charge transfer efficiency. 5. Thermodynamic and Stability Insights Temperature effects: Thermal fluctuations in the PB model modify charge localization and polaron stability, critical for understanding DNA's conductivity under varying conditions. Analytical solutions: Methods like the Kudryashov technique solve coupled Schrödinger-PB systems, revealing exact soliton profiles and stability criterial.

A. Model and equations of motion

$$\begin{cases} \lambda_{tt} - c_1\lambda_{xx} + W_g(\lambda - \alpha_0\lambda^2 + \gamma_2\lambda^3) + c_3|\varphi|^2 = 0 \\ \psi_{tt} - c_2\psi_{xx} - \beta(\psi\lambda - \alpha_0\psi\lambda^2 + \gamma_2\psi\lambda^3) = 0 \\ i\varphi_t - P_1\varphi_{xx} + Q_1\varphi - Q_2\lambda\varphi = 0 \end{cases} \tag{3}$$

After making a variable change, the system (3) is equivalent to the first order system

$$\begin{aligned} U_t &= AU + F(U) \\ U(0) &= U_0 \end{aligned} \tag{4}$$

Where

$$A = \begin{pmatrix} 0 & I & 0 & 0 & 0 \\ c_1\partial_x^2 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & I & 0 \\ 0 & 0 & c_2\partial_x^2 & 0 & 0 \\ 0 & 0 & 0 & 0 & iP_1\partial_x^2 \end{pmatrix} = \begin{pmatrix} A_1 & 0 & 0 \\ 0 & A_2 & 0 \\ 0 & 0 & A_3 \end{pmatrix} \tag{5}$$

$$A_1 = \begin{pmatrix} 0 & I \\ c_1\partial_x^2 & 0 \end{pmatrix},\ A_2 = \begin{pmatrix} 0 & I \\ c_2\partial_x^2 & 0 \end{pmatrix},\ A_3 = iP_1\partial_x^2$$

According to [10], We recall that the operator A_1 is the infinitesimal generator of a C_0 group of operators on $H^1(\mathbb{R}) \times L^2(\mathbb{R})$, more precisely $\{T(t)\}_{t\in\mathbb{R}}$ and the same thing happens with the operator A_2, while for operator A_3 it is verified that it is an infinitesimal generator of a C_0 group of unitary operators on $L^2(\mathbb{R})$, that is $\{S(t)\}_{t\in\mathbb{R}}$.

$$U = \begin{pmatrix} u_1 \\ u_2 \\ u_3 \\ u_4 \\ u_5 \end{pmatrix} \tag{6}$$

Note that u_5 is a complex valued function.

$$F(U) = \begin{pmatrix} 0 \\ -W_g(u_1 - \alpha_0 u_1^2 + \gamma_2 u_1^3) - c_3|u_5|^2 \\ 0 \\ \beta(u_1u_3 - \alpha_0 u_1^2 u_3 + \gamma_2 u_1^3 u_3) \\ -i(Q_1u_5 - Q_2u_1u_5) \end{pmatrix} \tag{7}$$

In addition,

$$W_g = \frac{4a^2D}{n},\ \alpha_0 = \frac{3a\sqrt{2}}{2},\ c_1 = \frac{k}{m},\ c_2 = \frac{\xi}{I},\ \gamma_2 = \frac{7a^2}{3}$$
$$\beta = \frac{mW_g\sqrt{2}}{2I},\ Q_1 = \frac{V}{h},\ Q_2 = \frac{\chi}{h},\ P_1 = \frac{2V}{h},\ c_3 = \frac{\chi}{m}$$

In order to use the theory of semigroups, we define a suitable Hilbert space $X = (H^1(\mathbb{R} \times L^2(\mathbb{R}))^2 \times L^2(\mathbb{R})$

Given a vector $U = [u_1, u_2, u_3, u_4, u_5] \in (C_0^\infty(\mathbb{R}))^5$, we define the norm

$$\|U\|_X = \left(\int_{\mathbb{R}} |u_1|^2 + |\partial_x u_1|^2 + |u_2|^2 + |u_3|^2 + |\partial_x u_3|^2 + |u_4|^2 + |u_5|^2 + |\partial_x u_5|^2 dx \right)^{1/2} \tag{8}$$

It follows easily that the completion of $(C_0^\infty(\mathbb{R}))^5$ with respect to the norm $\|\cdot\|_X$ is the Hilbert space X.

Definition 2. We define the operator A associated with the differential operator given in the relation (5) as follows,

$$A : D(A) \subset X \to X$$

Where $D(A) = \left(H^2(\mathbb{R}) \times H^1(\mathbb{R})\right)^2 \times H^2(\mathbb{R})$ and for every $U = [u_1, u_2, u_3, u_4, u_5] \in D(A)$ let

$$AU = [u_2, c_1\partial_x^2 u_1, u_4, c_2\partial_x^2 u_3, iP_1\partial_x^2 u_5] \in B \tag{9}$$

Where $B = \left(H^1(\mathbb{R}) \times L^2(\mathbb{R})\right)^2 \times H^2(\mathbb{R})$. With the same arguments given in [10], we get that for every $f \in X$ and real λ conveniently chosen, we have that the equation

$$U - \lambda AU = f$$

Has a unique solution $U \in D(A)$, such that $\|U\|_X \leq C\|F\|_X$, for some constant $C > 0$. In addition the operator A defined in the relation (9) is the infinitesimal generator of a C_0 group on $D(A)$, more precisely $\left\{\widetilde{T}(t)\right\}_{t\in\mathbb{R}}$, satisfying

$$\|\widehat{T}(t)\|_X \leq C\|f\|_X$$

On the other hand, for the nonlinearity, one shows that $F : X \to X$ is Lipschitz, in fact for every $U = [u_1, u_2, u_3, u_4, u_5],\ V = [v_1, v_2, v_3, v_4, v_5] \in X$

$$F(U)-F(V)=\begin{pmatrix} 0 \\ -W_g(u_1-v_1-\alpha_0(u_1^2-v_1^2)+\gamma_2(u_1^3-v_1^3)-c_3(|u_5|^2-|v_5|^2)) \\ 0 \\ \beta(u_1u_3-\alpha_0u_1^2u_3+\gamma_2u_1^3u_3)-\beta(v_1v_3-\alpha_0v_1^2v_3+\gamma_2v_1^3v_3) \\ -i(Q_1u_5-Q_2u_1u_5)+i(Q_1v_5-Q_2v_1v_5) \end{pmatrix}$$

Hence, applying the norm given in the relation (8), we have

$$\begin{aligned}\|F(U)-F(V)\|_X^2 &= \|-W_g(u_1-v_1-\alpha_0(u_1^2-v_1^2)+\gamma_2(u_1^3-v_1^3)-c_3(|u_5|^2-|v_5|^2))\|_{L^2}^2 \\ &+\|\beta(u_1u_3-\alpha_0u_1^2u_3+\gamma_2u_1^3u_3)-\beta(v_1v_3-\alpha_0v_1^2v_3+\gamma_2v_1^3v_3)\|_{L^2}^2 \\ &+\|\left(Q_1(u_5-Q_2u_1u_5\right)+\left(Q_1(v_5-Q_2v_1v_5\right)\|_{L^2}^2 \\ &+\|\partial_x[(Q_1(u_5-Q_2u_1u_5)+(Q_1(v_5-Q_2v_1v_5)]\|_{L^2}^2\end{aligned}$$

DIAGRAMA DE FLUJO DEL SOFTWARE

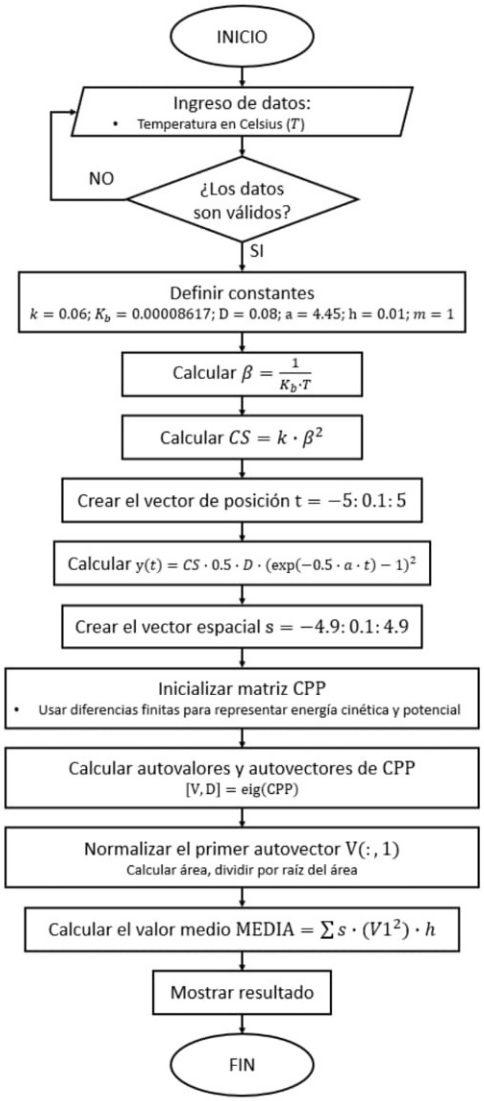

Figura 1: Flowchart for calculating the mean displacement of DNA nucleotides

We can see the solutions in the figure 2 using the generalized Morse according to [9] and the numerical computation of eigenvalues of statistical physics of DNA according to [5] and schematized in Figure 1. On the horizontal axis the parameter q and on the vertical axis the variable mean displacement pf DNA nucleotides.

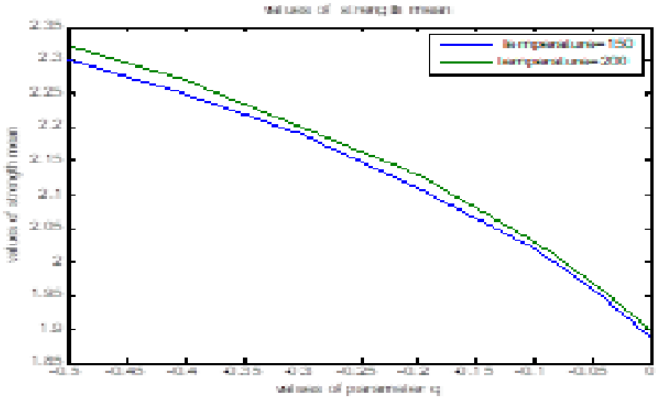

Figura 2: Average displacement of nucleotides according to the generalized Morse potential of parameter q and temperature

We can see the solution of the electronic distribution with the the model of Peyrard-Bishop-Holdstein in the figure 3. For the simulation, the following parameters have been considered as part of the software codes used in Python for the model Peyrard-Bishop-Holdstein of DNA.

Parámetros del modelo N = 23 —— Número de pares de bases m = 300.0 —— masa efectiva (arbitraria) D = 0.04 —— –profundidad del pozo de Morse (eV) a = 4.2 —— ancho del

potencial de Morse (1/Å) k = 0.025 ——- constante de acoplamiento entre bases J = 0.01 —— hopping (eV) chi = 0.05 —— acoplamiento Holstein (eV/Å)

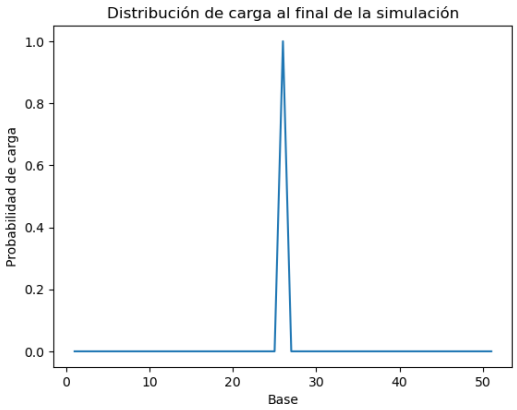

Figura 3: Electronic distribution considering 51 base pairs

After adding and subtracting terms and applying some estimates such a Sobolev embedding theorems , Cauchy- Schwartz inequalities and thus some other elementary inequalities of Sobolev spaces. It yields that there exists a constant $C > 0$, such that

$$\begin{aligned}\|F(U)-F(V)\|_X \leq C\big[&\|u_1-v_1\|_{L^2}^2+\|\partial_x(u_1-v_1)\|_{L^2}^2\\&+\|u_2-v_2\|_{L^2}^2+\|u_3-v_3\|_{L^2}^2\\&+\|\partial_x(u_3-v_3)\|_{L^2}^2+\|u_4-v_4\|_{L^2}^2\\&+\|u_5-v_5\|_{L^2}^2+\|\partial(u_5-v_5)\|_{L^2}^2\big]\end{aligned}$$

Hence, we have

$$\|F(U)-F(V)\|_X \leq C\|U-V\|_X$$

For all $U=[u_1,u_2,u_3,u_4,u_5], V=[v_1,v_2,v_3,v_4,v_5] \in X$. With the same arguments demonstrated above we deduce that

$$\begin{aligned}\|F(U)-F(V)\|_{D(A)} &= \|F(U)-F(V)\|_X\\&\quad+\|A(F(U)-F(V))\|_X\\&\leq C\|U-V\|_X+\|A(U)-A(V)\|_X\end{aligned}$$

For some positive constant C and for all $U, V \in D(A)$.

III. MAIN RESULT

Theorem 1. Given any $U_0 \in D(A)$, and the nonlinear mapping $F : D(A) \to D(A)$ verifies to be globally Lipschitz continuous for the graph norm, then there exists a unique global classical solution U for the system (4) in the sense that $U \in C^1([0,+\infty), X) \cap C^0([0,+\infty), D(A))$. Morever, if $U_0 \in D(A^2)$ then U' and AU are Lipschitz continuous on bounded sets of $[0,+\infty)$ to X. Furthermore, if X is reflexive and $U_0 \in D(A^2)$, then

$$U \in C^1([0,+\infty), D(A)) \cap C^0([0,+\infty), D(A^2))$$

Demostración. Consider the operator $\widetilde{A}$ defined by

$$\begin{cases} D(\widetilde{A}) = \{U \in D(A);\ AU \in D(A)\} \\ \widetilde{A}U = AU\ , \quad \text{For all } U \in D(\widetilde{A}) \end{cases}$$

Recall that $\widetilde{A}$ is a densely defined m-accretive operator in $D(A)$ and that the semigroup generated by $\widetilde{A}$ coincides with the restriction of $\{\widetilde{T}(t)\}_{t>0}$ to $D(A)$.

For the existence is proved by using the contraction mapping principle in the space

$$B=\left\{U \in C^0([0,+\infty), D(A));\ \sup_{t\geq 0} e^{-kt}\|U(t)\|_{D(A)} < \infty\right\}$$

Where $k > 0$ is to be chosen. B equipped with the norm

$$\|U(t)\|_B = \sup_{t\geq 0} e^{-kt}\|U(t)\|_{D(A)}$$

Is a Banach space, and so we consider the mapping

$$\Phi(U)(t) = \widetilde{T}(t)U_0 + \int_0^t \widetilde{T}(t-\sigma)F(U(\sigma))d\sigma$$

It follows easily that

$$\|\Phi(U)-\Phi(V)\|_B \leq \frac{C}{k}\|U-V\|_B$$

Choosing any $k > C$, we conclude that Φ has a fixed point $U \in B$, which is a solution of the equation (3).

On the other hand, for continuous dependency, we assume that U and V are two solutions of the system (4) associated to the initial values U_0 and V_0, respectively. Then

$$\begin{aligned}\|U(t)-V(t)\|_{D(A)} &\leq \|U_0-V_0\|_{D(A)}\\&\quad+c\int_0^t \|U(\sigma)-V(\sigma)\|_{D(A)}d\sigma\end{aligned}$$

It follows from Gronwall's inequality

$$\|U(t)-V(t)\|_{D(A)} \leq e^{ct}\|U_0-V_0\|_{D(A)}$$

In a similar way, about the Lipschitz continuity when $U_0 \in D(A)$. Let $h > 0$, we have that $U(t+h)$ is the weak solution of the system (4) with the initial value $U(h)$, from the continuous dependence, we obtain

$$\|U(t+h)-U(t)\|_{D(A)} \leq e^{ct}\|U(h)-U(0)\|_{D(A)}\ ,\ \text{for all } t \geq 0$$

In addition, we have

$$U(h) = \widetilde{T}(h)U_0 + \int_0^t \widetilde{T}(h-\sigma)F(U(\sigma))d\sigma$$

And so

$$\begin{aligned}\|U(h)-U_0\|_{D(A)} &\leq \|\widehat{T}(h)U_0-U_0\|_{D(A)}\\&\quad+h\sup_{0<\sigma<h}\|F(U(\sigma))\|_{D(A)}\\&\leq h\|AU_0\|_X+h\sup_{0<\sigma<h}\|F(U(\sigma))\|_{D(A)}\end{aligned}$$

By using

$$\left\| \frac{\widehat{T}(t)U - U}{t} \right\|_X \leq \|AU\|_X \ , \text{ for all } t \geq 0$$

$$\begin{aligned} \|U(t)\|_X &\leq \|U_0\|_X + \int_0^t \|F(U(\sigma))\|_X d\sigma \\ &\leq \|U_0\|_X + t\|F(0)\|_X + C\int_0^t \|U(\sigma)\|_X d\sigma \end{aligned}$$

By Gronwall's inequality, this implies that

$$\|U(t)\|_X \leq e^{ct}[\|U_0\|_X + \|F(0)\|_X]$$

And so,

$$\sup_{0<\sigma<h} \|F(U(\sigma))\|_X \leq \|F(0)\|_X + Ce^{ch}[\|U_0\|_X + h\|F(0)\|_X]$$

Hence, it follows the result. ■

IV. CONCLUSION

We have achieved a result of existence and uniqueness about the global classical solution of the Peyrad-Bishop-Holdstein model of DNA using the theory of semigroups. From our analysis we have a good amount of electro-dynamic software for prediction of the mean amplitudes of the mean stretch and the corresponding electronic distribution in the anorexic Gauss bell-like DNA,

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