Journal of Posthumanism
2025
Volume: 5, No: 1, pp. 1440–1449
ISSN: 2634-3576 (Print) | ISSN 2634-3584 (Online)
posthumanism.co.uk

DOI: https://doi.org/10.63332/joph.v5i1.688

New Solution for Charge Transport in Dna Model with Generalized Morse Potential

Milton Milciades Cortez Gutierrez[1], Hernan Oscar Cortez Gutiérrez[2], Lenin Rolando Cabracancha Montesinos[3], Pascual Fermín Onofre Mayta[4], Liv Jois Cortez Fuentes Rivera[5], Jesús Yuncar Alvaron[6]

Abstract

This paper is concerned with the global weak solution for charge transport DNA model with vibrational and rotational coupling motion. For that we use the theory of semigroup according to rewrite in vector form the system obtained from the dynamics of the Peyrard-Bishop model for vibrational motion of DNA dynamics. We consider an abstract initial value problem, which we show that, under suitable assumptions 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. We present our result developed in Matlab for the calculation of the average stretching amplitude for a Morse potential dependent on a parameter q (generalized Morse potential). The emphasis is on the inverse relationship between of the average distance of a DNA breathing and the "q" values of the generalized Morse potential.

Keywords: *Charge Transport, Peyrard-Bishop, Global Weak Solution, DNA Breathing, Generalized Morse Potential.*

Introduction

The equations of motion for DNA are a system of discrete nonlinear Klein-Gordon (KG) equations (n=1, 2... N)

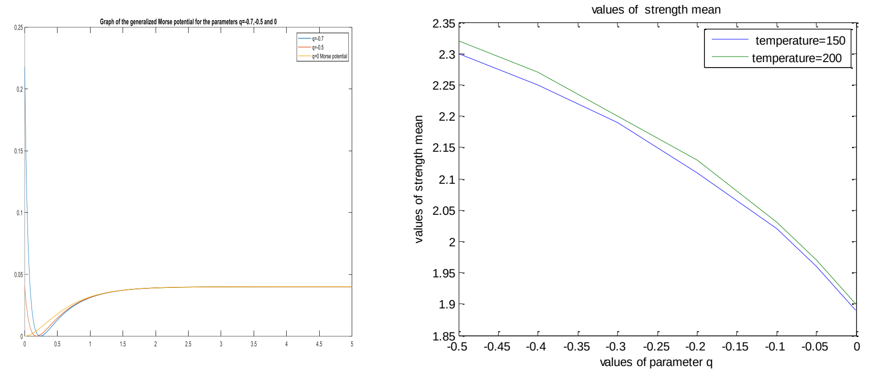
$$\ddot{u}_n + V'(u_n) + \mu(2u_n - u_{n-1} - u_{n+1}) = 0, \qquad (1)$$

with $V'(u_n)$ being the derivative of the potential with respect the coordinate u_n wich represents the stretching of DNA.

As a motivation we present our result developed in Matlab for the calculation of the average stretching amplitude of DNA for a Morse potential dependent on a parameter q:

$$V_q(W_n - v_n) = D\left(\left(1 - \frac{b}{e^{a(w_n - v_n)/\sqrt{2}} + q}\right)^2 - 1\right).(1.0)$$

[1] Universidad Nacional de trujillo.
[2] Universidad nacional del Callao, Email: hocortezg@unacvirtual.edu.pe, (Corresponding Author)
[3] Universidad nacional del Callao.
[4] Universidad nacional del Callao.
[5] Universidad nacional del Callao. Email: ljcortezf@unacvirtual.edu.pe.
[6] Universidad nacional del Callao.



(a) (b)

Figure 1. Solution for the strength mean of the vibration of DNA (b) and the generalized Morse depending of parameter q (a).

The problem for charge transport in DNA model with solvent interaction has been analysed from the point of view of numerical analysis. In our case we are concerned with the global weak solution from analytical the point of view. For that, we consider an abstract initial value problem.

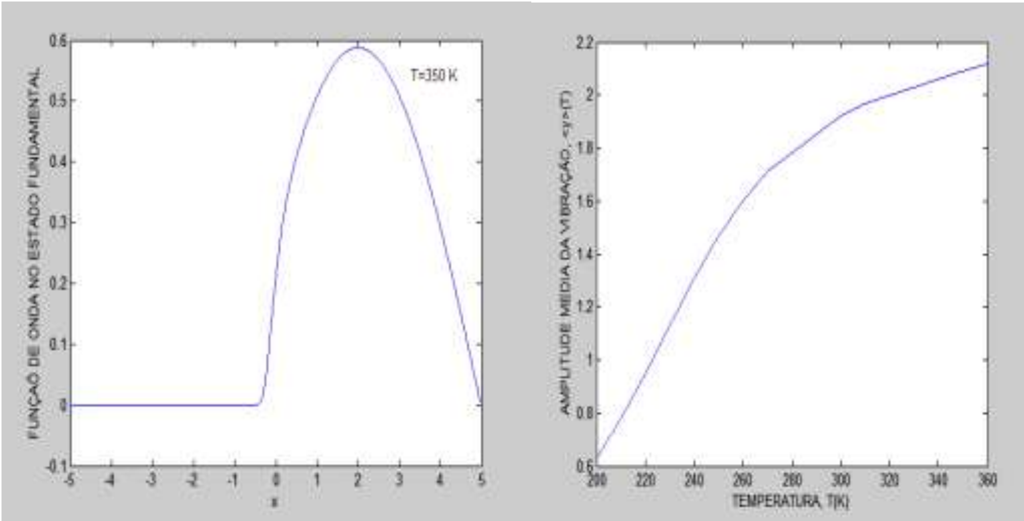
$$U_t = AU + F(U) \qquad (1.1)$$

$$U(0) = U_0$$

Where A will be a densely defined linear m-accretive operator in a Hilbert space X, with the norm $\|\quad\|$, $F: X \to X$ is a nonlinear mapping that will satisfy the condition of being globally Lipschitz continuous. Hence, we use the semigroup theory according (2), to obtain a family of operators $\{\tilde{T}(t)\}_{t\in\mathbb{R}}$. That will play an important role in proving the existence.

Méthod

Numerical methods with software MATLAB: The DNA vibrations of DNA are numerically resolved based on statistical physics, which allows us to estimate the average stretching amplitude of DNA.(1)



(a) (b)

Figure 2. Energy localizations with the ground state wave function ψ_0 for the Schrodinger equation (a) and the mean of the displacements (b) using the formula: $<u>=\int_{-\infty}^{+\infty}\psi^2{}_0 u du$ (1.2)

Abstracts methods with semigroup theory: We consider A as being an operator defined in a Hilbert space H for the scalar product ((,)) and equipped with the norm $\| \quad \|$, 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 $H \rightarrow H$, and is one to one $H \rightarrow D(A)$ 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 $H \times H$, $D(A) \hookrightarrow H$. (9).

The notation to be used is mostly standard.

Charge Transport In A DNA Model With Solvent Interaction

$$\boldsymbol{\lambda_{tt}} + c_0\partial_x^2\lambda + A\lambda + B\lambda^2 + \mathrm{Wg}\lambda^3 + c_2|\varphi|^2 = 0 \qquad (2.1)$$

$$\psi_{tt} + c_1\partial_x^2\psi + Q_3\lambda\psi + Q_4\lambda^2\psi - \gamma\beta\psi\lambda^3 + Q_5\psi = 0 \quad (2.2)$$

$$i\,\varphi_t = P_1\partial_x^2\varphi + Q_1\varphi + Q_2\lambda\phi \qquad (2.3)$$

With initial conditions

$$\varphi(x,0) = \varphi^0(x)\,,\ \lambda(x,0) = \lambda^0(x)\,,\ \lambda_t(x,0) = \lambda^1(x)\,,$$

$$\psi(x,0) = \psi^0(x),\ \ \psi_t(x,0) = \psi^1(x) \qquad (2.4)$$

After making a variable change, the system $(2.1) - (2.4)$ is equivalent to the first order system

$$U_t = \mathcal{A}U + F(U) \qquad (2.2)$$

$$U(0) = U_0$$

Where

$$\mathcal{A} = \begin{pmatrix} 0 & I & 0 & 0 & 0 \\ -c_0\partial_x^2 - A & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & I & 0 \\ 0 & 0 & -c_1\partial_x^2 - Q_5 & 0 & 0 \\ 0 & 0 & 0 & 0 & -iP_1\partial_x^2 - iQ_1 \end{pmatrix} = \begin{pmatrix} A_1 & 0 & 0 \\ 0 & A_2 & 0 \\ 0 & 0 & A_3 \end{pmatrix}$$

(2.3)

$$A_1 = \begin{pmatrix} 0 & I \\ -c_0\partial_x^2 - A & 0 \end{pmatrix}, A_2 = \begin{pmatrix} 0 & I \\ -c_1\partial_x^2 - Q_5 & 0 \end{pmatrix}, A_3 = -iP_1\partial_x^2 - iQ_1$$

According (3), 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 , we apply Stone's theorem which it is verified that it is an infinitesimal generator of a C_0 group of unitary operators on $L^2(\mathbb{R})$, that is $\{S(t)\}_{t\in\mathbb{R}}$. (8)

$$U = \begin{pmatrix} u_1 \\ u_2 \\ u_3 \\ u_4 \\ u_5 \end{pmatrix} \qquad (2.4)$$

Note that u_5 is a complex valued function.

$$F(U) = \begin{pmatrix} 0 \\ -Bu_1^2 - W_g u_1^3 - c_2|u_5|^2 \\ 0 \\ -Q_3u_1u_3 - Q_4u_1^2u_3 - \gamma\beta u_1^3 \\ -iQ_2u_1u_5 \end{pmatrix} \qquad (2.5)$$

In addition,

$$W_g = \frac{4a^2D}{m} \ , \alpha_0 = \frac{3a\sqrt{2}}{2} \ , c_0 = -\frac{k}{m} \, , c_1 = \frac{-\xi}{I} \ , \gamma = \frac{7a^2}{3}$$

$$\beta = \frac{mW_g\sqrt{2}}{2I} \ , Q_1 = -\frac{V}{h} \, , Q_2 = \frac{\chi}{h} \ , P_1 = -\frac{2V}{h} \, , c_3 = \frac{\chi}{m}, A = \frac{8rD_jf_s}{l_s^3} + W_g$$

$$B = \alpha_0 W_g + \frac{2\sqrt{2}D_jf_s}{l_s^3} \, , Q_4 = \frac{-4rD_jf_s}{l_s^3} + \beta\alpha_0 \, , Q_5 = \frac{2rD_jf_s}{ml_s}\left(1 - \frac{4r^2}{l_s^2}\right)$$

$$Q_3 = \frac{8\sqrt{2}r^2D_jf_s}{l_s^3} - \beta$$

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

$\|U\|_X = \left(\int_{\mathbb{R}} |u_1|^2 + |\partial_x u_1|^2 + |u_2|^2 + |u_3|^2 + |\partial_x u_3|^2 + |u_4|^2 + |u_5|^2 + |\partial_x u_5|^2 dx\right)^{1/2}$ (2.6)

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

Definition 1.- We define the operator $\mathcal{A}$ associated with the differential operator given in the relation (2.3) as follows,

$$\mathcal{A}: D(\mathcal{A}) \subset X \to X$$

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

$\mathcal{A}U = [u_2, -c_0\partial_x^2 u_1 - A, u_4, -c_1\partial_x^2 u_3 - Q_5, -iP_1\partial_x^2 u_5 - iQ_1 u_5] \in \left(H^1(\mathbb{R}) \times L^2(\mathbb{R})\right)^2 \times H^2(\mathbb{R})$).

With the same arguments given in (4) , we get that for every $f \in X$ and real λ conveniently chosen, we have that the equation

$$U - \lambda\mathcal{A}U = f$$

Has a unique solution $\in D(\mathcal{A})$, such that $\|U\|_X \leq C\|F\|_X$, for some constant $C > 0$. In addition the operator A defined in the relation (2.7) is the infinitesimal generator of a C_0 group on $(\mathcal{A})$, more precisely $\{\tilde{T}(t)\}_{t\in\mathbb{R}}$, satisfying (10).

$$\left\|\tilde{T}(t)\right\|_X \leq C\|F\|_X$$

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

$$F(U) - F(V) = \begin{pmatrix} 0 \\ -Bu_1^2 - W_g u_1^3 - c_2|u_5|^2 - (-Bv_1^2 - W_g v_1^3 - c_2|v_5|^2) \\ 0 \\ -Q_3 u_1 u_3 - Q_4 u_1^2 u_3 - \gamma\beta u_1^3 - (-Q_3 v_1 v_3 - Q_4 v_1^2 v_3 - \gamma\beta v_1^3) \\ -iQ_2 u_1 u_5 - (-iQ_2 v_1 v_5) \end{pmatrix}$$

Hence, applying the norm given in the relation (2.6), we have

$$\|F(U) - F(V)\|_X^2 = \left\| -W_g(u_1 - v_1 - \alpha_0(u_1^2 - v_1^2) + \gamma_2(u_1^3 - v_1^3) - c_3(|u_5|^2 - |v_5|^2 \right\|_{L^2}^2 +$$
$$+ \left\| \beta(u_1 u_3 - \alpha_0 u_1^2 u_3 + \gamma_2 u_1^3 u_3) - \beta(v_1 v_3 - \alpha_0 v_1^2 v_3 + \gamma_2 v_1^3 v_3) \right\|_{L^2}^2 +$$
$$+ \|(Q_1(u_5 - Q_2 u_1 u_5) + (Q_1(v_5 - Q_2 v_1 v_5)\|_{L^2}^2 +$$
$$+ \|\partial_x[(Q_1(u_5 - Q_2 u_1 u_5) + (Q_1(v_5 - Q_2 v_1 v_5)]\|_{L^2}^2$$

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 (5).

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

Hence, we have

$\|F(U) - F(V)\|_X \le C\|U - V\|_X$, for all $U = [u_1, u_2, u_3, u_4, u_5], V = [v_1, v_2, v_3, v_4, v_5] \in X.$

Results and Discussions

Theorem 1. Given any $U_0 \in X$, there exists a unique global weak solution U for the system (2.2) in the sense that $U \in C^0([0, +\infty), X)$ and

$$U(t) = \tilde{T}(t)U_0 + \int_0^t \tilde{T}(t - \sigma)\, F(U(\sigma))d\sigma \ , \quad \forall t \ge 0 \qquad (3.1)$$

In addition, there is continuous dependence of U with respect to U_0

$\|U(t) - V(t)\|_X \le e^{ct}\|U_0 - V_0\|_X$ for all $t \ge 0$, where $V(t)$ is the solution of the system (2.2) with the initial value V_0.

Morever, if $U_0 \in D(\mathcal{A})$ then U is Lipschitz continuous on bounded sets of $[0, +\infty)$;that is, for every $T < \infty$ there exists a constant $M_T > 0$ such that

$\|U(t_1) - U(t_2)\|_X \le M_T|t_1 - t_2|$ for all $0 \le t_1, t_2 \le T$

Proof

For the uniqueness, we consider U and V two solutions of the system (2.2). Then we have

$$\|U(t)-V(t)\|_X \le C\int_0^t \|U(\sigma)-V(\sigma)\|_X d\sigma$$

Thus by Gronwall's inequality,

$$\|U(t)-V(t)\|_X \le e^{cT}\|U_0-V_0\|_X = 0$$

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

$$B=\left\{U\in C^0([0,+\infty),X);\ \operatorname*{Sup}_{t\ge 0} e^{-kt}\|U(t)\|_X<\infty\right\}$$

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

$$\|U(t)\|_B = \operatorname*{Sup}_{t\ge 0}\ e^{-kt}\|U(t)\|_X$$

Is a Banach space, and so we consider the mapping

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

It follows easily that

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

Choosing any $>C$, we conclude that Φ has a fixed point $U\in B$, which is a solution of the equation (3.1).

On the other hand, for continuous dependency, we assume that U and V are two solutions of the system (2.2) associated to the initial values U_0 and V_0 , respectively. Then (6).

$$\|U(t)-V(t)\|_X \le \|U_0-V_0\|_X + C\int_0^t \|U(\sigma)-V(\sigma)\|_X\, d\sigma$$

It follows from Gronwall's inequality

$$\|U(t)-V(t)\|_X \le e^{ct}\|U_0-V_0\|_X$$

In a similar way, about the Lipschitz continuity when $U_0\in D(\mathcal{A})$. Let $h>0$, we have that

$U(t+h)$ is the weak solution of the system (2.2) with the initial value $U(h)$, from the continuous dependence, we obtain

$\|U(t+h)-U(t)\|_X \le e^{ct}\|U(h)-U(0)\|_X$, for all $t\ge 0$

Furtheremore, we have

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

And so

$$\|U(h)-U_0\|_X \leq \left\|\tilde{T}(h)U_0 - U_0\right\|_X + h \underset{0<\sigma<h}{\text{Sup}} \|F(U(\sigma))\|_X \leq$$

$$\leq h\|\mathcal{A}U_0\|_X + h \underset{0<\sigma<h}{\text{Sup}} \|F(U(\sigma))\|_X \leq$$

By using

$$\left\|\frac{\tilde{T}(t)U-U}{t}\right\|_X \leq \|\mathcal{A}U\|_X \quad , \text{ for all } t \geq 0$$

$$\|U(t)\|_X \leq \|U_0\|_X + \int_0^t \left\|F\big(U(\sigma)\big)\right\|_X d\sigma \ \leq \ \|U_0\|_X + t\|F(0)\|_X + C\int_0^t \|U(\sigma)\|_X \, d\sigma$$

By Gronwall's inequality, this implies that

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

And so,

$$\underset{0<\sigma<h}{\textbf{Sup}} \|\boldsymbol{F}(\boldsymbol{U}(\boldsymbol{\sigma}))\|_X \leq \|\boldsymbol{F}(\boldsymbol{0})\|_X + \boldsymbol{C}e^{\boldsymbol{ch}}[\|\boldsymbol{U_0}\|_X + \boldsymbol{h}\|\boldsymbol{F}(\boldsymbol{0})\|_X]$$

Hence, it follows the result.

The case that $F: X \to X$ is globally Lipschitz continuous allows to use Banach´s fixed point contraction theorem, precisely defining a mapping to obtain the mild solution. On the other hand, both the uniqueness and the continuous dependence of the data make strong use of the Gonwall inequality, including the result.

Conclusions

We have achieved a result of existence and uniqueness in the weak sense such as one shows in the theorem 1. Which the theory of semigroups was strongly applied.

The dynamic software developed in Matlab allow us to simulate vibrations for each temperature input and generalized Morse potential dependent on the poarameter q. We can also find a inverse correspondence law. That is, to emphasize that there is an inverse relationship between of the average distance of a DNA breathing and the "q" values of the generalized Morse potential. Dynamic software in Matlab helps solve bioinformatics problems and represents and educational strategy in today's world.

References

Gutierrez HO, Gutierrez MM, Rivera GI, Rivera LJ, Vallejo. Dark Breather using symmetric Morse, solvent and external potentials for DNA breathing . Ecletica Quimica Journal. 2018 Dec; 43(4):44-49.

Peyrard M, Bishop AR. Statistical mechanics of a nonlinear model for DNA denaturation. Physical review letters. 1989 Jun 5;62(23):2755.

Fialko NS, Lakhno VD. Nonlinear dynamics of excitations in DNA. Physics Letters A. 2000 Dec 18;278(1-2):108-12.

Silva RA, Filho ED, Ruggiero JR. A model coupling vibrational and rotational motion for the DNA molecule. Journal of Biological Physics. 2008 Oct;34:511-9.

Tabi CB, Mohamadou A, Kofané TC. Modulational instability of charge transport in the Peyrard–Bishop–Holstein model. Journal of Physics: Condensed Matter. 2009 Jul 8;21(33):335101.

Dauxois T, Peyrard M, Willis CR. Localized breather-like solution in a discrete Klein-Gordon model and application to DNA. Physica D: Nonlinear Phenomena. 1992 Aug 15;57(3-4):267-82.

Ngoubi H, Ben-Bolie GH, Kofané TC. Charge transport in DNA model with vibrational and rotational coupling motions. Journal of Biological Physics. 2017 Sep;43:341-53.

Pazy A, Pazy A. Applications to Partial Differential Equations—Nonlinear Equations. Semigroups of Linear Operators and Applications to Partial Differential Equations. 1983:230-51.

Renardy M, Rogers RC. An introduction to partial differential equations. Springer Science & Business Media; 2006 Apr 18.

Gutiérrez MM, Gutiérrez HO, Rivera GI, Rivera LJ, Vallejo DE. Local existence of solutions for the modified Korteweg-de Vries (mKdV) equation in weighted Sobolev spaces. South Florida Journal of Development. 2021 May 5;2(1):458-66.