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Thermodynamics of DNA with "hump" Morse potential

Hernán C. Gutiérrez[1], Elso Drigo Filho[2], José R. Ruggiero[2], Milton C. Gutierrez[3], Liv C. F. Rivera[4]

Resumo: A desnaturação térmica do DNA, ou seja, a separação das duas cadeias, é um fenômeno causado pela amplitude das vibrações das bases, portanto, é necessário saber como essa separação é gerada para implementar o modelo alternativo do comportamento de fusão como uma função da sequência de nucleotídeos e terapias para combater o câncer. Propomos usar o modelo de Peyrard-Bishop (PB) de DNA não linear estendido para incluir um potencial enarmônico que represente a interação de empilhamento aromático entre n- e (n-1)-enésimos pares de bases consecutivos para tratar o problema. Nós usamos métodos de diferença finita para determinar o valor médio do deslocamento para o potencial "corcunda de Morse" do modelo Peyrard-Bishop do DNA. Mostramos como o "pseudo-Schrödinger" estendido combinado com método de diferença finita pode ser usado para obter os deslocamentos do valor médio para a desnaturação térmica do DNA com o potencial Morse "da corcunda".

Palavras-chave: Método das diferenças finitas, equação pseudo-Schrödinger, "corcunda" do potencial de Morse

Abstract: The thermal denaturation of DNA, i.e. the separation of the two strands is a phenomenon caused by the amplitude of the vibrations of the bases, therefore it is necessary to know how such separation is generated in order to implement alternative model of the melting behavior as a function of nucleotide sequence and therapies to combat the cancer. We propose to use the extended nonlinear Peyrard-Bishop(PB) model of DNA to include an anharmonic potential representing the aromatic stacking interaction between n- and (n-1)-th consecutive base pairs to treat the problem. We use Finite-difference methods for determine the mean value of the displacement for the "hump Morse" potential of the Peyrard-Bishop model of DNA. We show how the extended "pseudo-Schrödinger" combined with finite difference method can be used to obtain the mean value displacements for the thermal denaturation of DNA with "hump" Morse potential.

Keywords: Finite-difference methods, "pseudo-Schrödinger" equation, "hump" Morse potential

[1] *UNAC, Universidad Nacional Del Callao, Facultad de Ciências de la Salud, Callao, Perú*
[2] *UNESP, Universidade Estadual Paulista, Departamento de Física, São José Rio Preto, Brasil*
[3] *Universidad de Trujillo, Departamento de Matematica, Trujillo, Perú*
[4] *Universidad San Juan Bautista, Facultad de Medicina, Lima, Perú*
Correspondent author: hcortez@unac.pe

INTRODUCTION

We explore the thermodynamic properties solving the pseudo-Schrödinger equation of the transfer integral[1-7] for the "hump Morse". The mathematical tools used in the theoretical study of the problem are Finite Difference Method (FDM) and pseudo-Schrödinger equation with anharmonic stacking interactions for the DNA molecule.

THE MODELS

The Hamiltonian for the BP model is given by

$$H = \sum_{n=1}^{N} \frac{m}{2}(\dot{x}_n^2 + \dot{y}_n^2) + \sum_{n=1}^{N} \frac{\mu}{2}\left(x_n - x_{n-1}\right)^2 + \sum_{n=1}^{N} \frac{\mu}{2}\left(y_n - y_{n-1}\right)^2 + \sum_{n=1}^{N} V\left(y_n - x_n\right) \quad (1)$$

or in the general form:

$$H = \sum_{n=1}^{N} \frac{m}{2}(\dot{x}_n^2 + \dot{y}_n^2) + \sum_{n=1}^{N} W\left(x_n - x_{n-1}\right)^2 + \sum_{n=1}^{N} W\left(y_n - y_{n-1}\right)^2 + \sum_{n=1}^{N} V\left(y_n - x_n\right) \quad (1.1)$$

where W is given by:

$$W = \frac{\mu(1+\rho e^{-\delta(y_n + y_{n-1})})}{2} \quad (1.2)$$

where x_n and y_n denote the relative displacements of the n^{th} nucleotide bases at each strand and N denotes the number of nucleotides. This expression can be viewed as a non-harmonic interaction with the parameter $\rho \neq 0$. The potential $V(y_n - x_n)$ in the original (PB) model is taken as a Morse potential.

Using a suitable change of coordinates ("stretching" and "center of mass") in equation (1), defined by

$$u_n = \frac{x_n - y_n}{\sqrt{2}} \text{ and } v_n = \frac{x_n + y_n}{\sqrt{2}} \quad , \quad (2)$$

the Hamiltonian (1) is divided in two parts, the acoustic (H_{ac}) and optical (H_{op}) parts. They are given by

$$H_{ac} = \sum_{n=1}^{N} \frac{m}{2} \dot{v}_n^2 + \sum_{n=1}^{N} \frac{\mu}{2}\left(v_n - v_{n-1}\right)^2 \quad (3)$$

and

$$H_{op} = \sum_{n=1}^{N} \frac{m}{2} \dot{u}_n^2 + \sum_{n=1}^{N} \frac{\mu}{2}\left(u_n - u_{n-1}\right)^2 + \sum_{n=1}^{N} V(\sqrt{2}u_n), \quad (4)$$

respectively.

The general form is:

$$H_{op} = \sum_{n=1}^{N} \frac{m}{2} \dot{u}_n^2 + \sum_{n=1}^{N} W\left(u_n - u_{n-1}\right)^2 + \sum_{n=1}^{N} V(\sqrt{2}u_n) \quad (4.1)$$

The main interest here is in the optical Hamiltonian (4), because it contains the non-linearity of the problem. The equations of motion for equation (4) are a system of discrete nonlinear Klein-Gordon (KG) equations (n=1, 2... N):

$$\ddot{u}_n + V'(u_n) + \mu(2u_n - u_{n-1} - u_{n+1}) = 0, \qquad (5)$$

with $V'(u_n)$ being the derivative of the potential with respect the coordinate u_n .

The evaluation of the partition of equation (4.1) using the transfer integral operator method in the thermodynamic limit reduces to solving the "pseudo-Schrödinger" equation:

$$\{-1/(2.\beta^2.\mu.h(u_n))d^2 \ / d\ u_n^{\ 2} + U_{eff}(u_n, \beta)\}\psi(u_n) = \varepsilon^*\ \psi\ (u_n) \qquad (5.1)$$

$$U_{eff}(u_n, \beta) = V(\sqrt{2}u_n) + (1/2\beta)\ln(\beta\mu/2\pi) + (1/2\beta)\ln h(u_n) \qquad (5.2)$$

where

$$h(u_n) = 1 + \rho e^{-2\delta u_n} \qquad (5.3)$$

We use the hump Morse potential[28] in equation (4). The Morse Potential (PB model),

$$V(u) = \frac{D}{2}\left[\exp(-au) - 1\right]^2, \qquad (6)$$

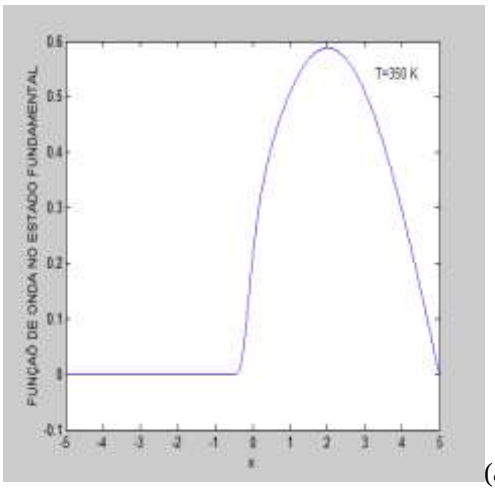
was solved in[32]. The case for the symmetric Morse potential (SPB model) given by

$$V(u) = \frac{D}{2}\left[\exp(-a|u|) - 1\right]^2. \qquad (7)$$

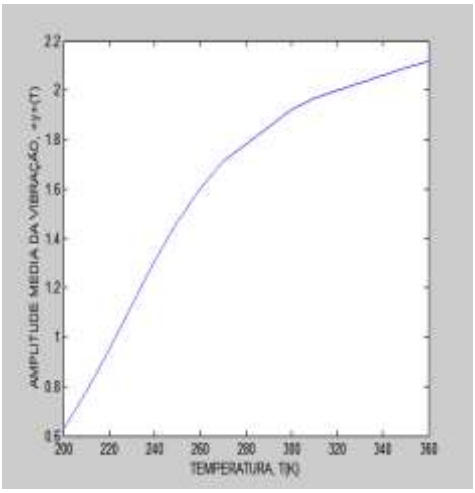
was solved in[29].

THERMODYNAMICS: THE MEAN VALUE OF THE DISPLACEMENTS

We can use the Finite difference methods for obtain the ground state wave function and the mean value of the displacement using the formulas of the literature[7]. We use the model (1) with the Morse Potential and the parameters μ =0.06, a= 4.45 and D=0.04. The Figure 1(b) shows that the mean of the amplitude is approximately 2.0 Å.



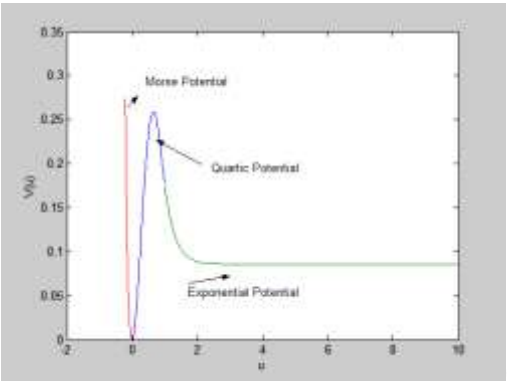
(a)

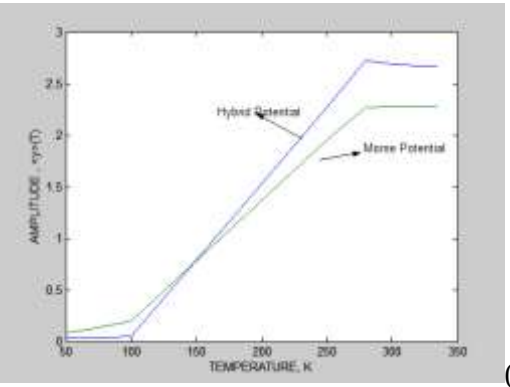


(b)

Figure 1. The ground state wave function ψ_0 for the Schrödinger equation (5.3) (a) and the mean of the displacements (b) using the formula: $< u >= \int_{-\infty}^{+\infty} \psi^2{}_0 u du$ [7]. We solve the equation 5.3 using the Finite-difference methods with the parameter ρ=0.

We can use the Finite difference methods for obtain the ground state wave function and the mean value of the displacement for the Hybrid potential ("hump Morse")[28] when the temperature is low and high. The results of this method is showed in Fig. 2(b).



(a)


(b)

Figure 2. The "hump Morse"[28](a) and the mean of the displacements (b) using the formula: $< u >= \int_{-\infty}^{+\infty} \psi^2{}_0 u du$ [7]. We solve the equation 5.3 using the Finite-difference methods with the parameter ρ=3, μ=0.01 and δ=0.8.

Also a model coupling vibrational and rotational motion for the DNA molecule[30] extend the original PB model and the denaturation with anharmonic staking interaction (equation (1.2)) in DNA has the features of a first order phase transition. It is a consequence of the evaluation of the final average stretching using the partition function and the entropic barrier (the third term in equation (5.2)).

CONCLUSIONS

For the PB model we solve the "pseudo-Schrödinger" equation using the finite difference to determine eigenfunctions, the mean value of the displacements with a threshold value of 2.0 Å for the denaturation temperature of 350 K. The "Hump Morse" allow the model to describe the tunneling currents and the sharp thermal denaturation of DNA. Finally, it is important to emphasize the importance of the partition function in the numerical evaluation of the average stretching of the original PB model[3] with rotational motions for nucleotides[30] and anharmonic stacking for the existence of a first order phase transition.

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