



Brazilian Journal of Physics

ISSN: 0103-9733

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Sociedade Brasileira de Física
Brasil

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Brazilian Journal of Physics, vol. 41, núm. 2-3, septiembre, 2011, pp. 195-200

Sociedade Brasileira de Física

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Thermodynamics of a Peyrard–Bishop One-Dimensional Lattice with On-site “Hump” Potential

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Received: 11 January 2011 / Published online: 30 April 2011
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Abstract This paper presents a thermodynamic study of DNA through a Peyrard–Bishop one-dimensional lattice with an on-site “hump” potential. The transfer integral operator method was used to obtain the thermodynamic properties of the system and the solution of the Schrödinger-type equation that emerges from this formalism was determined by the variational method. With the parameters of the potential, commonly used in literature, the value obtained for the denaturation temperature was extremely high. This work suggests different parameters to describe the thermodynamics of DNA macromolecule.

Keywords Lattice theory · Thermodynamics · DNA · Statistical mechanics

1 Introduction

The DNA is a molecule of extreme importance to life since it carries all the genetic information of the living beings. Its double-helix structure was proposed in 1953 by James Watson and Francis Crick [1], and this has impelled scientists from various areas to develop studies and models as an attempt to explain how this complex molecule transmits genetic information.

Peyrard and Bishop proposed a physical model of DNA in 1989 [2] in order to describe the thermal denaturation of the molecule [3]. In this model, the

double helix of DNA is described by two chains of particles. The stacking interactions that bind the adjacent bases of each strand are simulated by the harmonic potential. On the other hand, the hydrogen bonds—which are some of the main interactions responsible for maintaining the stability of the double helix of the molecule—are described by the Morse potential. This model was used to explore several dynamic and thermodynamic aspects of DNA such as the formation of domain wall [4, 5], energy location [6], formation, and stability of breathers [7–9].

With the original model of PB, it is possible to describe the thermal denaturation of DNA. However, the phase transition obtained is not as abrupt as indicated by the experimental results. Considering this, several modifications of this model were proposed in order to improve the phase transition for the DNA molecule. One of the suggested alterations consists in modifying the stacking interaction. Some more recent works [10–12] introduce an exponential term to the harmonic potential used in the original model [2]. Another way to alter the original model was to add a new term to the Morse potential, interpreting the additional term as interactions of the macromolecule with the solvent [13, 14]. There are other adaptations of this kind of model that aim at making it more realistic [15, 16].

In a recent work [17], Peyrard et al. have shown that, from the thermodynamic point of view, the alteration of the stacking interaction done in references [10, 11] enables the DNA to describe the experimental data of the molecule very well. However, from the dynamic point of view, the lifetimes of open states of base pairs do not agree with the experimental results, indicating that the model does not adjust qualitatively to the description of the dynamic properties of the DNA.

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To obtain a better description for the dynamic of the molecule, it was suggested [17] that the hydrogen bonds, initially simulated by the Morse potential, could be described by a more complex potential, denominated “hump” potential. It was also numerically shown that a phase transition of the DNA molecule occurs when using the lattice model with the on-site “hump” potential and the nonharmonic potential in the stacking interactions. This transition occurs in a temperature very close to the one obtained for the on-site Morse potential, because the parameters of the “hump” potential were chosen for that. However, the authors also analyzed a nonlinear model inspired by DNA in which a harmonic potential was used to simulate the stacking interaction.

The aim of this study is to calculate the thermodynamic properties of a lattice composed by the on-site “hump” potential and the harmonic potential describing the stacking interactions [17]. Particularly, we intended to investigate if the denaturation temperature obtained to this lattice agrees with the expected results to the denaturation of DNA. In order to do this, the transfer integral operator method [18] was used. The solutions of the eigenfunctions and the energy eigenvalues that emerge from this formalism were obtained by a semi-analytical method that is the variational method [19].

2 The Nonlinear Lattice Model

In the nonlinear lattice model used, the stacking interactions of DNA are described by the harmonic potential and the hydrogen bonds are simulated by the “hump” potential ($V(y_n)$). The thermodynamic properties of the lattice are given in function of the variable y_n that represents the stretching between the n th base pair. An outline of this model is presented in Fig. 1.

The “hump” potential is defined by the following expressions [17]:

$$V(y) = \begin{cases} A[e^{-\alpha y} - 1]^2 & \text{if } y < 0 \\ ay^2 + by^3 + cy^4 & \text{if } 0 \leq y \leq 1 \\ D + Fe^{-\beta y} \left(y + \frac{1}{\beta}\right) & \text{if } y > 1 \end{cases} \quad (1)$$

This potential is determined by the choice of the parameters D , F , α , and β . The other parameters are determined by the conditions of continuity of the potential and of its first and second derivatives. The values of the parameters used are given in reference [17],

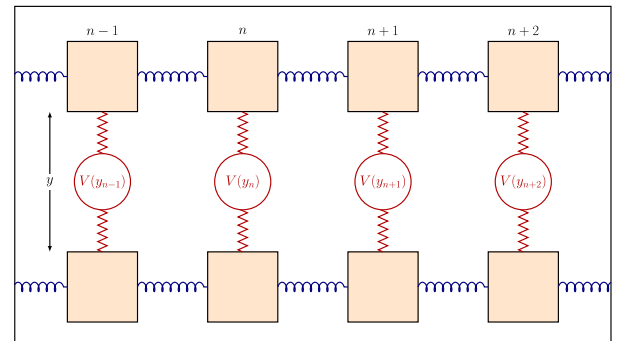


Fig. 1 (Color online) Outline of the studied DNA model

i.e., $D = 0.0857\text{eV}$, $\alpha = \beta = 4\text{\AA}^{-1}$, and $F = 4\text{eV}\cdot\text{\AA}^{-1}$. The graphic of this potential to the parameters used is shown in Fig. 2.

The Hamiltonian of interest, which emerges from the model, is given by the sum of the kinetic energy of the bases with the harmonic and “hump” potentials, in other words,

$$H = \sum_n \frac{p_n^2}{2m} + \frac{1}{2}k(y_n - y_{n-1})^2 + V(y_n), \quad (2)$$

where the first term is that of the kinetic energy of the base pairs, $m = 300\text{ amu}$ is the average mass of the nucleotide, $p_n = m \frac{dy_n}{dt}$ is the linear momentum, and the second term is the harmonic potential which simulates the stacking interactions and $V(y_n)$ is the “hump” potential.

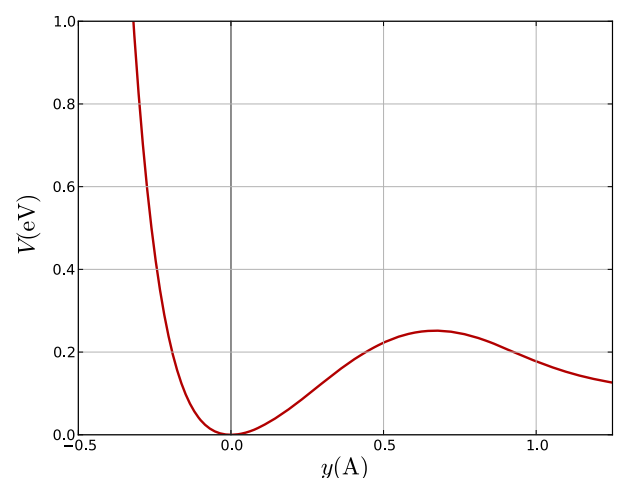


Fig. 2 (Color online) Plot of the “hump” potential (1), with $D = 0.0857\text{eV}$, $\alpha = \beta = 4\text{\AA}^{-1}$, and $F = 4\text{eV}\cdot\text{\AA}^{-1}$

3 Calculation of the Thermodynamic Properties of the Model

The thermodynamic properties of the model are described by the partition function Z . To calculate the partition function—written in terms of the variable that represents the stretching of the base pairs of the chain—the transfer integral operator method [18] was used. This technique relates the partition function with eigenfunctions ψ_n and energy eigenvalues ε_n obtained through a Schrödinger-type equation. Thus, the problem can be synthesized in finding the eigenfunctions and eigenvalues, expressed by the equation:

$$\left[-\frac{1}{2\beta^2 k} \frac{d^2}{dy_i^2} + V(y_i) \right] \psi_n(y_i) = \left[\varepsilon_n + \frac{1}{2\beta} \ln \left(\frac{2\pi}{\beta k} \right) \right] \psi_n(y_i), \quad (3)$$

where $\beta = \frac{1}{k_B T}$, $k_B = 8.617 \times 10^{-5} \text{ eV/K}$ is the Boltzmann constant, T is the temperature, $k = 0.01 \text{ eV} \cdot \text{\AA}^{-2}$ is the elastic constant of the interaction alongside the chain and $V(y_i)$, in this case, is the “hump” potential given by Eq. 1. The variables y_i represent, as usual, the stretching between the two springs, i.e., the distance between two bases that form the i th base pair.

With the eigenvalues given by Eq. 3, the partition function of the system can be obtained by the sum $Z = \sum_n e^{-N\beta\varepsilon_n}$, where N is the total number of particles from the system. However, in the thermodynamic limit, where the particles number is very big ($N \rightarrow \infty$), the result of the partition function is dominated by the ground state and the other terms of the sum can be neglected. This approximation has been used since the introduction of the Peyrard–Bishop model, as in references [2, 3, 10, 11]. Therefore, for our purposes, we have limited ourselves to calculating the eigenfunction and the energy eigenvalue of Eq. 3 only for the ground state.

The Schrödinger-type Eq. 3 has an analytical solution only for some potentials, such as Morse and Rosen-Morse [20]. In the case of the “hump” potential, the solutions can be found by using numerical methods. However, in this study, the solution of Eq. 3 will be found with the use of a semi-analytical method known as variational method [19].

In order to study the phase transition of the DNA, the average stretching of the base pairs, $\langle y \rangle$, will be used as an order parameter. As the square of the wave function—which emerges from the formalism of the

transfer integral operator method—gives the probability distribution, $\langle y \rangle$ can be calculated by the equation:

$$\langle y \rangle = \frac{\int_{-\infty}^{\infty} y \psi^2 dy}{\int_{-\infty}^{\infty} \psi^2 dy}. \quad (4)$$

4 Variational Method

The variational method [19] is an approximation method used to solve the Schrödinger equation, which consists of the choice of an arbitrary eigenfunction (ψ_μ) that is used to calculate the energy eigenvalue. The variational principle guarantees that the energy obtained is always an upper limit of the real energy of the system (E_0). To refine the result, the chosen eigenfunction is written in terms of a set of parameters, called variational parameters $\{\mu\}$. The variational parameters chosen will be the ones that minimize the energy.

Thus, in agreement with the variational principle, we have:

$$E_0 \leq \bar{H} = \frac{\int_V \psi_\mu^* H \psi_\mu dV}{\int_V \psi_\mu^* \psi_\mu dV}, \quad (5)$$

where V is the total volume of the system. Using only one variational parameter (μ), the energy eigenvalue can be found by the minimization of the right side of Eq. 5 regarding this parameter.

The trial eigenfunction chosen to solve Eq. 3 with the potential (1) is the wave function, which is the solution for the Morse potential [2, 3] with the parameters adjusted, so that the depth and width of the Morse potential well is the closest possible to the “hump” potential. This choice was made because the aim of this work is to study the phase transition of the molecule. This phenomena is strongly dependent on the potential well shape and it is believed that the wave function inside the potential well will have similar characteristics to the real eigenfunction of the “hump” potential because in this region the “hump” potential has the same shape of the Morse potential. This choice may not be good in a region after the potential well, but this part of the potential is not the focus of this work. Following this reasoning, the chosen trial function with only one variational parameter was:

$$\psi_{0\mu} = \exp(-de^{-\mu \cdot y}) \exp \left[- \left(d - \frac{1}{2} \right) \mu \cdot y \right], \quad (6)$$

where $d \equiv \left(\frac{\beta}{a} \right) (k D_M)^{1/2} > \frac{1}{2}$, $\beta = \frac{1}{k_B T}$, k_B is the Boltzmann constant, T is the temperature, $k = 0.01 \text{ eV} \cdot \text{\AA}^{-2}$ is the

elastic constant of the interaction alongside the chain [17], y is the variable that represents the stretching of the base pairs, μ is the variational parameter, D_M , and a are the Morse potential parameters ($V(y) = D_M(e^{-ay} - 1)^2$) that are related, respectively, to the depth and width of the potential well. The values used for DM and a , which were obtained through the adjustment between the Morse and “hump” potentials, are $D_M = 0.33028\text{eV}$ and $a = 0.77848\text{Å}^{-1}$.

The solutions of Eq. 3 are dependent on the temperature T of the system. So, knowing the trial wave function (Eq. 6) and the parameters D_M and a , we can calculate the energy of the system as a function of the variational parameter for several temperatures by Eq. 5 and, after that, we can minimize it in relation to the variational parameter to obtain the value of μ .

Having the value of the variational parameter, the shape of the trial wave function can be obtained. This process was performed for several temperatures; therefore, it is possible to know the behavior of the average stretching of the base pairs given by Eq. 4, with the variation of temperature.

5 Results

To find the approximate solutions of Eq. 3 by the variational method, it was necessary to solve the integral given in Eq. 5 with the trial eigenfunction (Eq. 6). This integration was done numerically. In order to obtain the variational parameter value, a plot of the energy eigenvalue in function of the variational parameter was done. The value of μ that provides the best solution is the one that minimizes the energy and, therefore, is the

value found in the global minimum of the plot of \bar{H} versus μ . This procedure was accomplished for several values of temperature.

After the value of the variational parameter is obtained, all the parameters of the trial eigenfunction (Eq. 6) are known and, thus, we can obtain the average stretching of the base pairs given by Eq. 4. The values of $\langle y \rangle$ in function of the temperature are found in Fig. 3.

Figure 3 indicates that the average stretching of the base pairs remains always very small in relation to the physically acceptable temperatures to study the thermodynamic of DNA. According to reference [21], the denaturation temperature of the DNA is around 318 and 372 K depending on the nucleotides present in the chain. Figure 3 shows that, with the parameters indicated in reference [17], nothing happens in this range of temperature with the average stretching of the base pairs. The high denaturation temperature found was expected because it depends on the depth of the potential well. Reference [17] presents a comparative figure between the Morse potential, used primarily in the DNA model, and the “hump” potential. This figure indicates a potential well much more pronounced in the “hump” potential. Therefore, it suggests that the critical temperature for the “hump” potential would be much larger than the 350 K obtained for the Morse potential.

As the critical temperature obtained with the “hump” potential with the parameters used in [17] is not physically acceptable to study the DNA, it is necessary to seek better parameters for the potential in order to find a better description for the thermodynamics of this macromolecule when the harmonic potential is used to simulate the stacking interactions.

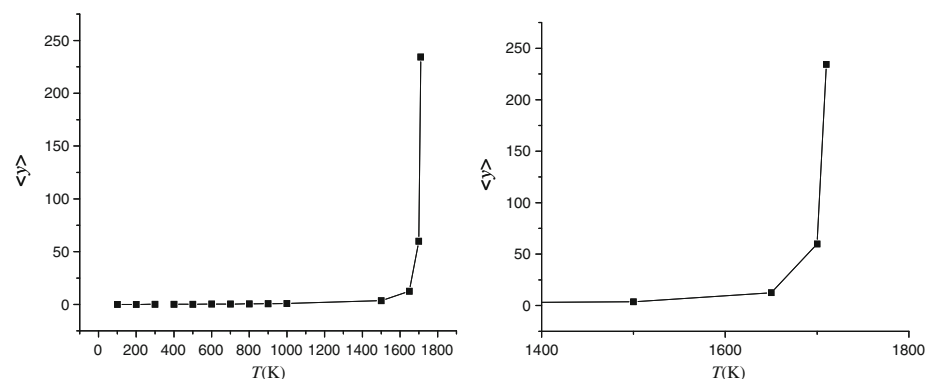


Fig. 3 Graphic of the average stretching of the base pairs ($\langle y \rangle$) as a function of the temperature. The parameters of the “hump” potential are $D = 0.0857\text{eV}$, $\alpha = \beta = 4\text{Å}^{-1}$ and $F = 4\text{eV.Å}^{-1}$; the parameters of the trial eigenfunction are $D_M = 0.33028\text{eV}$ and $a = 0.77848\text{Å}^{-1}$ and the spring constant is $k = 0.01\text{eV.Å}^{-2}$. The

variational parameters were adjusted in order to minimize the energy as indicated in the text. In the right side of the figure the interval of the curve was restricted in order to emphasize the growth of the average stretching of the base pairs

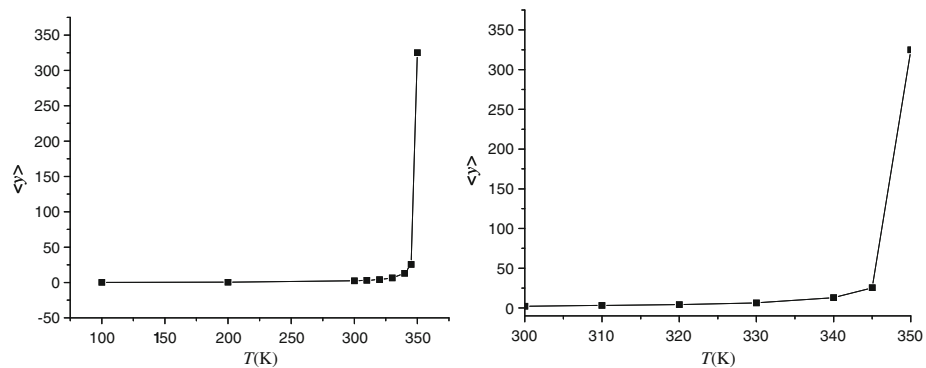


Fig. 4 Graphic of the average stretching of the base pairs ($\langle y \rangle$) as a function of the temperature. The parameters of the “hump” potential are $D = 0.03\text{eV}$, $\alpha = 1.2\text{\AA}^{-1}$, $\beta = 4\text{\AA}^{-1}$ and $F = 0.1\text{eV}\cdot\text{\AA}^{-1}$; the parameters of the trial eigenfunction are

$D_M = 0.03\text{eV}$ and $a = 2.81\text{\AA}^{-1}$ and the spring constant is $k = 0.06\text{eV}\cdot\text{\AA}^{-2}$. In the right side of the figure, the interval of the curve was restricted in order to emphasize the growth of the average stretching of the base pairs

Due to the dependence of the denaturation temperature with the depth and width of the potential well, it is expected that an acceptable critical temperature of the “hump” potential would be obtained if these characteristics of the potential well were similar to the Morse potential. Therefore, an adjustment was made between these two potentials to find the parameters of the “hump” potential used in the thermodynamics calculations. In this case, the parameters used to the Morse potential were taken from reference [16], as well as the elastic constant k ; they are $D_M = 0.03\text{eV}$, $a = 2.81\text{\AA}^{-1}$ and $k = 0.06\text{eV}\cdot\text{\AA}^{-2}$. The parameters obtained from the adjustment to the “hump” potential were $D = 0.03\text{eV}$, $\alpha = 1.2\text{\AA}^{-1}$, $\beta = 4\text{\AA}^{-1}$ and $F = 0.1\text{eV}\cdot\text{\AA}^{-1}$.

In order to calculate the thermodynamic properties of the lattice with the new parameters, the same procedures already presented were used. The behavior of the average stretching of the base pairs $\langle y \rangle$ in function of the temperature variation is shown in Fig. 4.

Figure 4 indicates that, with the new parameters used in the “hump” potential, the critical temperature in which the denaturation of the DNA molecule occurs declines to approximately 350 K. This result agrees with the experimental results found in literature [21] for the DNA.

6 Discussion and Conclusions

This study used the variational method to estimate the critical temperature in which the thermal denaturation of the DNA molecule occurs, using the lattice model proposed by Peyrard et al. in [17]. Despite the fact that, in this reference, there are results of the thermodynamic of the lattice with the on-site “hump” potential

and the nonharmonic potential describing the stacking interactions; it is also studied a nonlinear model inspired by DNA macromolecule in which it is used the harmonic potential in the stacking interactions. This paper demonstrated that the change of the nonharmonic potential by the harmonic potential makes the thermodynamic results of the model completely different from the ones expected for a lattice that aims to simulate the thermodynamic properties of the DNA molecule.

The results show that, with the change of the stacking potential, the denaturation temperature of the lattice grows unreasonably. This result indicates that the parameters used in reference [17] for the “hump” potential are not good to simultaneously study the dynamic and thermodynamic properties of the DNA when the stacking interaction is simulated by the harmonic potential, since these parameters do not allow the phase transition of the molecule to occur in a physically acceptable temperature.

A suggestion of new parameters for the “hump” potential is also presented in this study. These new parameters enable a better description of the thermodynamic properties of DNA to the lattice with the harmonic potential in the stacking interaction. With the new parameters it was possible to obtain a denaturation temperature for the DNA molecule, which agrees with the experimental values presented in literature.

Keeping fixed the constants of the “hump” potential, it is also possible to bring the denaturation temperature to realistic values by modifying the spring constant used in the stacking interaction. The use of $k = 4.2 \times 10^{-4}\text{eV}\cdot\text{\AA}^{-2}$ takes the denaturation temperature to approximately 350 K. Concerning the dynamics, the relation between the lifetimes of open and closed base pairs more specifically, a new computational study is

needed to verify whether the times involved remain in agreement with what is experimentally expected. However, this study must constitute a new work which emphasizes the dynamic of the model.

Acknowledgments The authors are grateful to J.R. Ruggiero and G.G. Slade for the inspiring discussions. This study was partially supported by the Coordination for the Improvement of Higher Education Personnel (CAPES).

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