Using a one-dimensional lattice applied to the thermodynamic study of DNA

2010 J. Phys.: Conf. Ser. 246 012037

(http://iopscience.iop.org/1742-6596/246/1/012037)

Using a one-dimensional lattice applied to the thermodynamic study of DNA.

N. F. Ribeiro, E. Drigo Filho

São Paulo State University – UNESP, Instituto de Biociências, Letras e Ciências
Exatas, Rua Cristóvão Colombo, 2265, CEP 15054-000, São José do Rio Preto, SP,
Brazil

E-mail: nataliafavaro@hotmail.com, elso@ibilce.unesp.br

Abstract. In this work it is analyzed a one-dimensional lattice which is composed by mass-spring systems with one additional Rosen-Morse potential on site. This kind of lattice is used to study thermodynamic properties of DNA, especially its thermal denaturation. On the context of this work, the Rosen-Morse potential simulates hydrogen bonds between double strands of the molecule. From the graphic of the average stretching of base pairs versus temperature it is possible to observe the thermal denaturation of the system. This result shows that it is possible to obtain phase transition with an asymmetric potential without an infinite barrier.

The Peyrard-Bishop (PB) model proposed in 1989 [1] has been used a lot to describe the thermal denaturation of DNA [2]. In the original model the double strand of DNA is described by two chains of particles, in which the harmonic potential simulates the stacking interactions. On the other hand, the Morse potential describes the hydrogen bonds that are one of the main interactions responsible for maintaining stable the double strand of the molecule. From this model, several dynamic and thermodynamic aspects of the DNA have been explored, for example, formation of domain wall [3, 4], energy location [5], formation and stability of breathers [6-8].

Several modifications have been proposed in the PB model in order to obtain a better description of the phase transition for a DNA molecule. One way to alter the model consists on the modification of stacking interaction. Originally, this interaction was taken as purely harmonic [1], but in more recent works [9-11], an exponential term was introduced with this harmonic term. Another way to alter the original model is to substitute the Morse potential for others potentials with different characteristics. This can be made by the addition of a new term to the Morse potential as it is done, for instance, in ref. [12]. In this reference, the additional term was interpreted as interactions of the macromolecule with the solvent.

Concerning the general behavior of non-linear lattices of the type here studied, Angelani et all [13] show that phase transitions are related to topological changes occurred in the system. One important result indicated in reference [13] is that the system does not presents phase transition when the potential on site has a symmetrical well. This happens because these potential have symmetric waves functions, obtained in the Schrödinger-type equation that emerges from the formalism, and centered in the origin. Therefore, the average value of the stretching of base pairs is always zero, what results on the impossibility of existing phase transition. This result contrasts with the one obtained for potentials with infinite barrier in one extremity of the potential well, like the Morse potential, in which the transition happens. This property is emphasized in reference [3], in which the transition is discussed both by using the dynamical method of domain wall as by using statistic mechanic. Thus, when the potential that simulates hydrogen bonds has an asymmetric well with an infinite barrier in one extremity and a finite barrier in the other one, the phase transition always occurs. This can be observed by following the evolution of one order parameter, in this case, the average stretching of base pairs, which divers for a critical temperature.

The main result here presented is that the use of Rosen-Morse potential on site in the studied lattice allows characterizing a phase transition similar to those obtained in the literature models [1-3]. As it is doing with the Morse potential [1], the use of Rosen-Morse potential permits an analytical treatment, what a priori makes easier the obtaining and interpretation of the results, besides in applications to obtain the probe design [14]. Another remarkable result is that the use of a finite and asymmetrical potential on site in a lattice used in PB model presents phase transition. The kind of potential, not yet treated in literature, can be considered as having intermediate characteristics between the symmetrical potentials [13] and the asymmetrical potential with infinite barrier in one extremity [3].

The Rosen-Morse potential is explored a lot in literature, both in the formal aspect [15-17] as in physical applications. It has been used, for example in studies of vibration on polyatomic molecules [18] and on polarons models [19]. This potential is defined as:

$$V(y_i) = B_0 \tanh(\alpha y_i) - \frac{U_0}{\cosh^2(\alpha y_i)}, \tag{1}$$

where B_0 and U_0 are parameters related, respectively, with asymmetrical and depth of the potential, and α is a parameter related with the width of the well. By adopting B_0 equals zero, the potential acquires a symmetrical shape. The variables y_i represent, in the PB model, the stretching between the i-th base pair, as shown in figure 1.

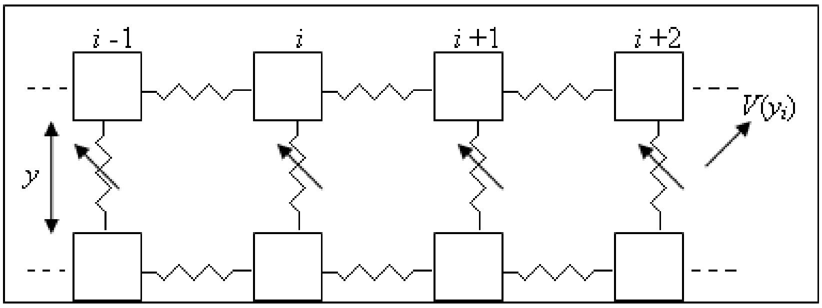

Figure 1: Representation of DNA model proposed by Peyrard and Bishop

The values of the parameters (α, B_0, U_0) here used were chosen in order to obtain a good adjustment with the Morse potential, $V_M(y) = D(1-e^{-ay})^2 - D$, with $D = 0.03 eV$ and $a = 2.81 \text{Å}^{-1}$, used to describe the hydrogen bonds on DNA [20]. The figure 2 shows a comparison between the originally Morse potential and the proposed Rosen-Morse one. The adjusted result, used in figure 2, points to $B_0 = -0.02 eV$, $U_0 = 0.047 eV$ and $\alpha = 4.3 \text{Å}^{-1}$.

Following the usual PB model [1, 2] and replacing the Morse potential by the Rosen Morse potential in order to simulate the hydrogen bonds, the thermodynamic properties of the system are described by the partition function Z. The partition function of physical prominence, written in terms of the variable that represents the average stretching of hydrogen bonds, can be calculated by using the transfer integral operator method [21]. 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:

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

where $\beta = \dfrac{1}{k_B T}$, $k_B = 8.617 \times 10^{-5} eV/K$ is the Boltzmann constant, T is the temperature, $k = 0.06 eV.\text{Å}^{-2}$ is the elastic constant related to the interaction alongside the chain (a purely harmonic potential is adopted to simulate the stacking interactions [2, 20]) and $V(y_i)$, in this case, is the Rosen-Morse potential which is given by the equation (1). The variables y_i represent, as usual, the stretching between the two springs [1-14], i.e., the distance between two bases that form the i-th base pair.

The partition function of the system is given by the sum $Z = \sum_n e^{-N\beta\varepsilon_n}$, where N is the particles number of the system. However, in the thermodynamically limit ($N \to \infty$) the result is dominated by the ground state and the others terms of the sum can be despised. Therefore, for ours purposes, we limit to calculate the eigenfunction and the energy eigenvalue for the ground state of equation (2).

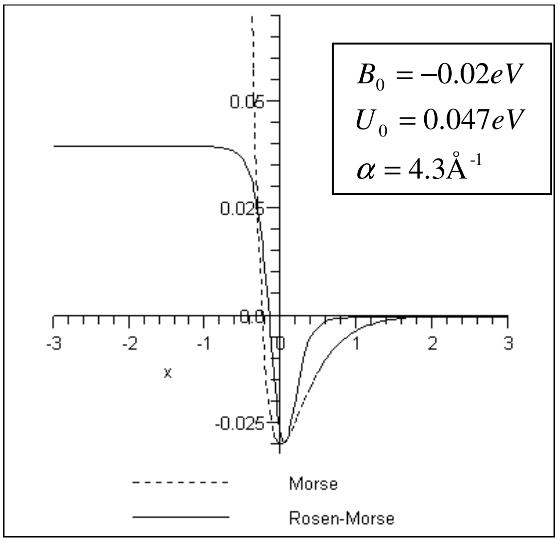

Figure 2: Graphic of the Morse potential (dotted curve) and the Rosen-Morse potential (solid curve). In the text box on the right of the graphic, there are the values obtained for the parameters of Rosen-Morse potential.

There are several methods that can be used to find the equation solutions (2), one of them is the Frobenius method [22]. Another approach is related to the factorization and supersymmetric method, as indicated in reference [23]. Anyway, for the ground state, the eigenfunction found is:

$$\psi = \frac{Ae^{az}}{\cosh^b z}, \tag{3}$$

where the new variable is $z = \alpha y$, A is the normalization constant, $a = -\dfrac{k\beta^2}{\alpha^2}\dfrac{B_0}{b}$ and $b = -\dfrac{1}{2} + \dfrac{1}{2}\left(1 + \dfrac{8\beta^2 k}{\alpha^2} U_0\right)^{\frac{1}{2}}$. The energy eigenvalue corresponded to the eigenfunction (3) is:

$$\varepsilon_0 = -\frac{\alpha^2}{2k\beta^2}\left(a^2 + b^2\right) - \frac{1}{2\beta}\ln\left(\frac{2\pi}{\beta k}\right). \tag{4}$$

From the eigenfunction (3) it is possible to find the average stretching between the base pairs ($< y >$) through the equation:

$$< y >= \frac{\int_{-\infty}^{\infty} y\psi^2 dy}{\int_{-\infty}^{\infty} \psi^2 dy}. \tag{5}$$

The integrals indicated in equation (5) can be solved numerically. When the indicated parameters are used, the integration result depends only on the temperature, then, it is possible to follow the values of $< y >$ in terms of the temperature. The obtained result is showed in figure 3, where is presented a graphic of the average stretching of base pairs ($< y >$) versus temperature. For comparison effects, it is also presented in figure 3 the curve of the average stretching of base pairs versus temperature for the Morse potential on site. This curve was made by using the eigenfunction of the ground state for Morse potential, given in reference [1]. In this figure can be clearly observed that in the temperature interval between 300 and 350K there was an increase in the average stretching of base pairs. This indicates that in this temperature interval a thermal denaturation of the molecule occurred. It can be observed that in the obtained curve for Rosen-Morse potential the transition was similar to that obtained for Morse potential.

The fact that an exact/analytical solution exists for the studied system allows an alternative way to determine the temperature in which occurs the break of the double strand. This can be done through direct inspection of the wave function given by equation (3). For this function leads to on bound states, it is necessary that it be normalized in all space. By a direct inspection of the wave function (3) one observes that for ψ not divers it is necessary that a and b parameters of the wave function follow the condition $0 < \frac{a}{b} < 1$. From this condition can be established that $a < b$ to have bound estates. Thus, the critical temperature must occurs when $a = b$, what means,

$$\frac{\beta_C}{\alpha}\left(k|B_0|\right)^{\frac{1}{2}} = -\frac{1}{2} + \frac{1}{2}\left(1 + \frac{8\beta_C k U_0}{\alpha^2}\right)^{\frac{1}{2}}, \tag{6}$$

where $\beta_C = \frac{1}{k_B T_C}$, T_C in this case represents the critical temperature.

From expression (6) it is possible to obtain a critical temperature as a function of the potential parameters. The result is:

$$T_c = -\frac{k}{\alpha k_B}\frac{\left(|B_0| - 2U_0\right)}{\left(k|B_0|\right)^{\frac{1}{2}}}. \tag{7}$$

By substituting all the parameters in equation (7), the value of the critical temperature is approximately $T_C = 346K$.

This procedure also can be done to determine the critical temperature for Morse Potential. The expression for the critical temperature, was obtained in reference [2] as $T_C = \frac{2\sqrt{kD}}{ak_B}$, where a and D are the parameters of the Morse potential, k_B is the Boltzmann constant and k is the elastic constant. By substituting this parameters and constants in equation (8), the value of the critical temperature for Morse potential is approximately 350K which is close to the result obtained from (7).

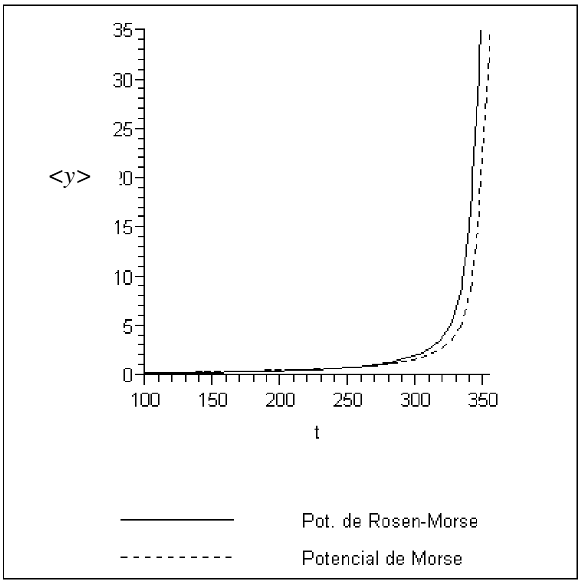

Figure 3: Graphic of the average stretching of base pairs, <*y*>, versus temperature, t, obtained from Morse and Rosen-Morse potential for temperature interval between 100K and 350K.

According to the reference [24] the denaturation temperature of DNA molecule varies between 318K and 372K, depending on the nucleotides involved in chain. Therefore, the obtained temperature for both potentials, Rosen-Morse and Morse, are in agreement with the values that exist in literature. In the studied scope, this result indicates that the potential used and the adopted parameters can describe both qualitative as quantitative the thermal denaturation of DNA and the similarity between the graphics of <*y*> for Morse and Rosen-Morse potentials indicates that it is possible to obtain a phase transition like that in ref. [1] with a asymmetrical potential that not presents an infinite barrier.

To conclude, the obtained results in this work show that is possible to characterize the thermal denaturation of DNA molecule with the use of Rosen-Morse potential to simulate the hydrogen bonds of the molecule. This result shows that it is possible to obtain a phase transition in PB-type models [1] without the potential on site having an infinite barrier. This result complements the discuss made in literature about the non-existence of phase transitions for symmetrical potential [13] and the well known fact [3] that the use of an asymmetrical potential, with wells that have an infinite barrier in one extremity and a finite barrier in another, allows the appearing of this transition. Thus, in way to be transition in one-dimensional lattices that emerges from a PB approach is necessary that the potential shows as asymmetrical well, and it is not necessary that exists an infinite barrier.

Finally, the fact of the obtained transition temperature in this system matches the values existed in literature [24] makes the adopted parameters reliable.

Acknowledgments

The authors are grateful to CAPES and FAPESP for the financial support.

References

[1] Peyrard M and Bishop A R 1989 *Phys. Rev. Lett.* **62** 2755.
[2] Peyrard M 2004 *Nonlinearity* **17** R1.
[3] Qasmi H, Barré J and Dauxois T 2004 *arXiv:cond-mat/0407662v1.*
[4] Theodorakopoulos N 2006 *Phys. D* **216** 185.
[5] Deluca J, Drigo Filho E, Ponno A and Ruggiero J R 2004 *Phys. Rev. E* **70** 026213.
[6] Cuevas J, Archilla J F R, Gaididei Yu B And Romero F R 2002 *Physica D* **163** 106.
[7] Cuevas J, Starikov E B, Archilla J F R and Hennig D 2004 *Modern Phys. Lett. B* **18** 1319.

[8] Alvarez A, Romero F R, Archilla J F R, Cuevas J and Larsen P V 2006 *European Phys. J. B* **51** 119.
[9] Dauxois T, Peyrard M and Bishop A R 1993 *Phys. Rev. E* **47** R44.
[10] Dauxois T and Peyrard M 1995 *Phys Rev. E* **51** 4027.
[11] Joyeux M and Buyukdagli S 2005 *Phys Rev. E* **72** 051902.
[12] Weber G 2006 *Europhys. Lett.* **73** 806.
[13] Angelani L, Ruocco G and Zamponi F 2005 *Phys. Rev. E* **72** 016122.
[14] Weber G, Haslam N, Essex J W and Neylon C 2009 *J. Phys.: Condens. Matter* **21** 034106.
[15] Lévai G 2008 *Phys. Lett. A* **372** 6484.
[16] Jia C S, Yi L Z and Sum Y 2008 *J. Math. Chem.* **43** 435
[17] Tezcan C and Sever R 2007 *J. Math. Chem.* **42** 387.
[18] Rosen N and Morse P M 1932 *Phys. Rev.* **42** 210.
[19] Smondyrev M A, Gerlach B and Dzero M O 2000 *Phys. Rev. B* **62** 692.
[20] Silva R A S, Drigo Filho E and Ruggiero J R 2008 *J. Biol. Phys.* **34** 511.
[21] Scalapino D J, Sears M and Ferrel R A 1972 *Phys. Rev. B* **6** 3409.
[22] Nieto M M 1978 *Phys. Rev. A* **17** 1273.
[23] Drigo Filho E 1990 *Rev. Bras. Fís.* **20** 258.
[24] Saenger W 1984 *Principles of Nucleic Acid Structure* (New York: Springer-Verlag Press).