

H-bond simulation in DNA using a harmonic oscillator isospectral potential

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A harmonic oscillator isospectral potential obtained by supersymmetric algebra applied to quantum mechanics is suggested to simulate DNA H bonds. Thermic denaturation is studied with this potential. [S1063-651X(97)11209-0]

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I. INTRODUCTION

In recent years several new potentials obtained from the supersymmetric formalism have been applied to quantum mechanics [1,2]. These potentials were derived from shape invariant potentials, and their mathematical and formal aspects have been discussed [3]. However, they have not been applied to any real physical system.

In this work, we propose a problem where a harmonic oscillator isospectral potential obtained from superalgebra can be applied. The problem is the thermic denaturation of the DNA macromolecules, whose stability depends on the H bonds between the complementary base pairs as well as on the stacking interactions between adjacent bases along the strands. To achieve this goal, two ribbons of DNA are simulated by springs and masses linked together by anharmonic springs. Integral transfer operator formalism [4] is used to study this system.

The applicability and free parameters of the proposed potential will be discussed in the context of thermal denaturation of the poly(A-T)-poly(A-T) DNA. The melting temperature of the poly(A)-poly(T) DNA can be reproduced by a change of the stacking interactions parameter.

II. MODEL

The model used here follows one proposed by Peyrard and Bishop [4], which includes two degrees of freedom (u_n and v_n) corresponding to displacements of the bases from their equilibrium position along the H bond direction. Harmonic coupling is assumed for the stacking interactions between neighboring bases along the strands with a common value for both the coupling constant k and mass m for each base.

The classical Hamiltonian for the system is written

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

where $x_n = (u_n + v_n)/\sqrt{2}$, $y_n = (u_n - v_n)/\sqrt{2}$, $p_n = m\dot{x}_n$, $q_n = m\dot{y}_n$, and $V(y_n)$ is the H-bond potential. The index n is related to the n th base pair in the chain.

The transfer integral operator formalism and the thermodynamic limit ($N \rightarrow \infty$) show that the mean stretching $\langle y_n \rangle$ of the H bond is obtained from

$$\langle y \rangle = \langle \phi_0(y) | y | \phi_0(y) \rangle = \int \phi_0^2(y) y dy, \quad (2)$$

$\phi_0(y)$ standing for the ground-state eigenfunction of a Schrödinger-type equation

$$\left\{ -\frac{1}{2\beta^2 k} \frac{\partial^2}{\partial y^2} + V(y) \right\} \phi_i(y) = \left\{ \epsilon_i + \frac{1}{2\beta} \ln \frac{2\pi}{\beta k} \right\} \phi_i(y). \quad (3)$$

The physical information is embodied in the eigenfunctions of Eq. (3), and the forms of these solutions are fundamental in determining the average values of $\langle y \rangle$. The generalized harmonic potential does not change the ground-state eigenvalue, but the eigenfunction is sensitive to it. Therefore, thermic denaturation of DNA seems to be a convenient problem to test the applicability of the potential generated from the superalgebra formalism.

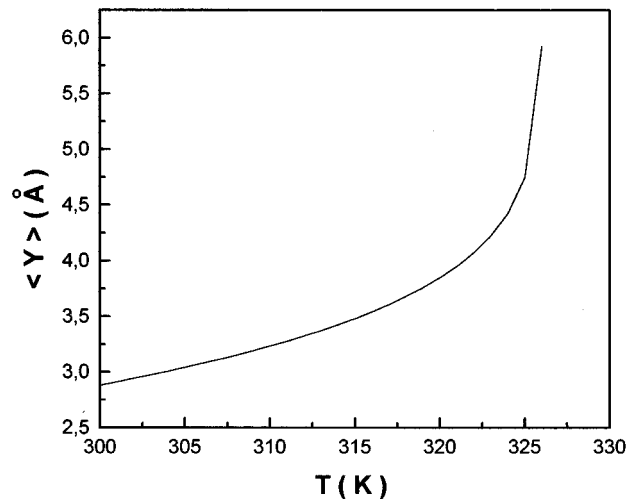


FIG. 1. Variation of $\langle y \rangle$ as a function of temperature for poly(A-T)-poly(T-A) DNA for the parameters $a = 7.45 \times 10^{-2}$ eV/Å, $k = 4.83 \times 10^{-4}$ eV/Å, and $\Gamma = -1.918$. The melting temperature is 326 K.

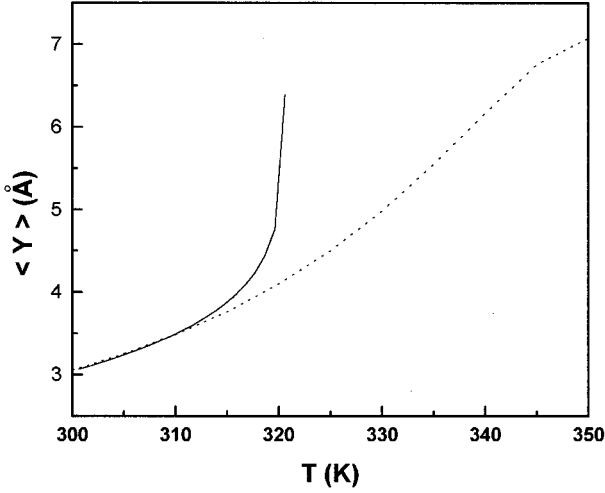


FIG. 2. Variation of $\langle y \rangle$ as function of temperature for poly(A)-poly(T) DNA. (a) The continuous line shows the results for the proposed potential where the spring constant for the stacking interaction is 96.7% from k , the other parameters are the same: $a = 7.45 \times 10^{-2}$ eV/Å and $\Gamma = -1.918$. In this case the melting temperature is 320 K. (b) The dotted line shows the results obtained for Morse potential where $D = 0.269$ eV, and $a = 1.8$ Å. The stacking interactions are supposed harmonic with $k = 3.10^{-3}$ eV/Å as suggested in Ref. [4]. To maintain a mean value $\langle y \rangle$ of about 3.0 Å, we accrete one Å in the final plot.

III. ISOSPECTRAL POTENTIAL

In supersymmetric quantum mechanics [5], the two charge operators, Q and Q^+ satisfy the anticommutation relations

$$\{Q, Q\} = \{Q^+, Q^+\} = 0 \quad \text{and} \quad \{Q, Q^+\} = H_{SS}. \quad (4)$$

The usual realization of this algebra is given by

$$Q = a^- \sigma_- = \begin{pmatrix} 0 & 0 \\ a^- & 0 \end{pmatrix} \quad \text{and} \quad Q^+ = a^+ \sigma_+ = \begin{pmatrix} 0 & a^+ \\ 0 & 0 \end{pmatrix} \quad (5)$$

where σ_- and σ_+ are written in terms of the Pauli matrix, and a^\pm are bosonic operators.

In this case, the supersymmetric Hamiltonian H_{SS} can be factorized in two partners $H_+ = a^+ a^-$ and $H_- = a^- a^+$. With exception of the ground state (only H_+ has an eigenvalue equal to zero, $E_+ = 0$) these Hamiltonians have the same spectrum.

The eigenfunctions of H_+ and H_- are related to one another by

$$\Psi_+ = a^+ \Psi_- \quad \text{and} \quad \Psi_- = a^- \Psi_+, \quad (6)$$

with bosonic operators defined by

$$a^\pm = \left\{ \mp \frac{d}{dx} + W(x) \right\}, \quad (7)$$

$W(x)$ being the superpotential.

Redefining the operators a^\pm , it is possible to obtain isospectral potentials [2]. Let A^\pm be the new operator defined by

$$A^\pm = \mp \frac{d}{dx} + F(x). \quad (8)$$

The imposition of $H_- = A^- A^+$ yields a general form from which the superpotential $F(x)$ follows. The new Hamiltonian is reformulated as

$$H_+ = A^- A^+ - 2 \frac{d}{dx} F(x). \quad (9)$$

The eigenfunctions, $\Psi_{\pm,0}$ of H_+ are related to the original Hamiltonians ($\Psi_+ = A^+ a^- \omega_+$), and the nondegenerated ground state is obtained from $A^- \Psi_{+,0} = 0$.

Different classes of potentials has been obtained with the use of this process [1]. For the harmonic oscillator system, in particular, the process has been extensively explored [2].

IV. H-BOND POTENTIAL

Some potentials have been used to simulate the H bond in DNA [6], the Morse potential being the most widely used in this context [4,7]. Using the formalism discussed, another [8] potential is suggested.

The potential is obtained by factorizing the Hamiltonian in the Schrödinger-type equation (3) and applying the superalgebra formalism to obtain the isospectral potential from the harmonic oscillator. In this case, the original potential is $V(y) = ay^2$ and the operators are $a^\pm = (1/\sqrt{k\beta}) \{ \mp (d/dy) + \sqrt{ak\beta}y \}$, i.e., $W(x) = \sqrt{ak\beta}y$. Defining A^\pm and imposing $H_- = A^- A^+$, it follows that

$$V(y) = ay^2 - \frac{1}{\beta^2 k} \frac{d}{dy} \frac{e^{-\sqrt{ak\beta}y^2}}{\Gamma + \int_0^y e^{-\sqrt{ak\beta}z^2} dz}, \quad (10)$$

where a , Γ , and k are free parameters. Inspection of this function indicates nonlinear behavior, a common feature among all other potential functions used to describe H bonds, but it is isospectral to the harmonic oscillator potential and is exactly soluble with the normalized ground-state eigenfunction ($A^- \Psi_0 = 0$) given by

$$\Psi_0(y) = \left\{ \frac{\sqrt{ak\beta}}{\pi} \left[\Gamma^2 - \frac{\pi}{4\sqrt{ak\beta}} \right]^{1/2} \times \frac{e^{-(1/2)\sqrt{ak\beta}y^2}}{\Gamma + \frac{1}{2} \left(\frac{\pi}{\sqrt{ak\beta}} \right)^{1/2} \text{erf}\{(ak)^{1/4} \beta^{1/2} y\}} \right\} \quad (11)$$

$\text{erf}(x)$ being the error function.

Before further discussing the thermic denaturation of DNA simulation with our potential, it is important to note that the mathematical aspects of the formalism used to generate the potential given in Eq. (10) is quite clear. However, the physical meaning of the transformations involved is not clear at all. Usually, in the context of superalgebra in quantum mechanics, this transformation is related to application of supercharges on the system [5], but the system under study is a classical one.

The suggested potential function embodies three parameters. The spring constant k is related to the stacking interactions, a represents the harmonic part of the H-bond potential, and Γ is related to the existing singularity of the potential. It is possible to fix these parameters considering three experimental results for a specific DNA sequence. For the poly(A)-poly(T) DNA one has so $\langle y \rangle = 2.88 \text{ \AA}$ at 300 K [9], the melting temperature is 326 K [9], and in the harmonic approach the H-bond spring constant ($k_{\text{H-bond}}$) is adjusted using the quasicontinuum model [10] as 0.81 eV/\AA^2 . This last value is obtained by expanding the potential up to second order, and comparing with the low-frequency modes of the vibration of DNA macromolecules [11].

The values for $\langle y \rangle$ follows from Eq. (2) using the ground-state eigenfunction (11). The spring constant in the harmonic approach of the H bond, on the other hand, is obtained by expanding potential (10) up to second order. The best fit provides us with the following parameters $a = 7.45 \times 10^{-2} \text{ eV/\AA}^2$, $k = 4.83 \times 10^{-4} \text{ eV/\AA}^2$, and $\Gamma = -1.918$. Figure 1 illustrates the plot of $\langle y \rangle T$ corresponding to these parameters. The abrupt behavior in the curve at 326 K indicates the melting temperature [4,8].

It is interesting to note that the new potential (10) has a qualitative advantage in establishing a connection between stacking and H-bond interactions. This property is not shared by other potentials used with the same purpose.

V. poly(A-T)-poly(A-T) DNA MELTING TEMPERATURE

As a test of the new potential applicability, the poly(A-T)-poly(A-T) DNA strand melting temperature is evaluated. As before, this strand has the same number of H bonds by base pair. However, it should be noted that the stacking interaction of this strand is around 96.7% of that in poly(A)-poly(T) DNA [9]. Considering the same relations to the k parameter, it yields $k(\text{poly(A-T)-poly(A-T)}) = 4.67 \times 10^{-4} \text{ eV/\AA}^2$.

In the present model the only difference between the two DNA macromolecules is in the k parameter (a and Γ are constants). In this case, the interpretation is that the differ-

ence between the two macromolecules is essentially the stacking interaction, other interactions being the same. This leads us to isolate the influence of stacking interactions on H bonds.

A plot of $\langle y \rangle T$ for the new value of k is shown in Fig. 2 as the continuous line, and yields a melting temperature of 320 K. For completeness, Fig. 2 shows also (dotted line) the Bishop and Peyrard [4] calculation using the Morse potential, with parameters appropriate to simulate a poly(A-T)-poly(A-T) (two H bonds by base pair). The important feature in those calculations is the rate of growing of the H-bond stretching. In this way the dotted curve was shifted by 1 \AA to permit a visual comparison with our results. It is noted that such behavior is more pronounced with the generalized potential proposed in this work than that one of Bishop and Peyrard [4], in qualitative agreement with the work of Pitici and Svirschevski [11].

VI. CONCLUSIONS

We suggest an application for potentials generated by supersymmetry. This potential has the same number of parameters (three) as the Morse potential, and has the qualitative advantage of establishing a connection between stacking and H-bond interactions. The parameters are adjusted using well-known data presented in the literature [melting temperature for poly(A)-poly(T), the mean distance at the H bond at 300 K [9], and the low-frequency modes of the vibration obtained from the quasicontinuum model [11]].

As the calculated melting temperature of the poly(A-T)-poly(A-T) DNA strand is close to the experimental one, our potential may be used successfully for DNA. However, it is important to test it in other conditions as, for example, with other sequences of bases, conformational transitions (B to Z DNA) and electrostatic interactions.

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