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Nonlinear Lattice Within Supersymmetric Quantum Mechanics Formalism

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Abstract. In the last decades, the study of nonlinear one dimensional lattices has attracted much attention of the scientific community. One of these lattices is related to a simplified model for the DNA molecule, allowing to recover experimental results, such as the denaturation of DNA double helix. Inspired by this model we construct a Hamiltonian for a reflectionless potential through the Supersymmetric Quantum Mechanics formalism, SQM. Thermodynamical properties of such one dimensional lattice are evaluated aming possible biological applications.

1. Introduction

Nonlinear one dimensional lattices have been the subject of many studies for some time, such as the Fermi-Pasta-Ulam problem, [1], [2] for a review. More recently, a simple lattice model for the denaturation of the DNA was proposed, the Peyrard-Bishop model, PB, [3]. In this model, the biomolecule is described by two chains of particles coupled by nonlinear springs, simulating the hydrogen bonds that connect the two basis in a pair. The potential for the hydrogen bonds is approximated by a Morse potential. The Hamiltonian system generates a partition function which allows the evaluation of thermodynamical quantities such as the mean strength of the basis pairs. As a byproduct the dynamics of the Hamiltonian system is shown to be a NLSE (Nonlinear Schrödinger Equation) admiting soliton solutions, [4].

On the other hand, a reflectionless potential with one bound state, construted using Supersymmetric Quantum Mechanics, SQM, can be shown to be identical to a initial soliton solution of the KdV equation. Thus, motivated by the Hamiltonian problem generated in the PB model, here we propose the use a reflectionless potential constructed using the formalism of SQM, [5], [6], to study a nonlinear one dimensional lattice in order to evaluate thermodynamical quantities.

In what follows, we briefly review the main principles of SQM, introduce the reflectionless potential a give a sketch of the PB model. We then introduce a reflectionless potential in place of the Morse potential to evaluate the mean stretching of the model as a preliminar test and give our conclusions.

2. Supersymmetric Quantum Mechanics and the Reflectionless Potential

Consider a system described by a given one-dimensional potential $V_1(x)$. The associated Hamiltonian H_1 can be factorized in terms of bosonic operators, in $\hbar = c = 1$ units, [5]

$$H_1 = -\frac{1}{2}\frac{d^2}{dx^2} + V_1(x) = A_1^+ A_1^- + E_0^{(1)} \tag{1}$$

where $E_0^{(1)}$ is the lowest eigenvalue. The bosonic operators are defined in terms of the so called superpotential $W_1(r)$,

$$A_1^{\pm} = \frac{1}{\sqrt{2}}\left(\mp\frac{d}{dx} + W_1(x)\right). \tag{2}$$

As a consequence of the factorization of the Hamiltonian H_1, the Riccati equation must be satisfied,

$$W_1^2 - W_1' = 2\left(V_1(x) - E_0^{(1)}\right). \tag{3}$$

Through the superalgebra, the eigenfunction for the lowest state is related to the superpotential W_1 by

$$\Psi_0^{(1)}(x) = Nexp(-\int_0^x W_1(\bar{x})d\bar{x}). \tag{4}$$

Now it is possible to construct the supersymmetric partner Hamiltonian

$$H_2 = A_1^- A_1^+ + E_0^{(1)} = -\frac{1}{2}\frac{d^2}{dx^2} + \frac{1}{2}(W_1^2 + W_1') + E_0^{(1)}. \tag{5}$$

If one factorizes H_2 in terms of a new pair of bosonic operators, $A_2^{\pm}$ one gets,

$$H_2 = A_2^+ A_2^- + E_0^{(2)} = -\frac{1}{2}\frac{d^2}{dx^2} + \frac{1}{2}(W_2^2 - W_2') + E_0^{(2)} \tag{6}$$

where $E_0^{(2)}$ is the lowest eigenvalue of H_2 and W_2 satisfy the Riccati equation,

$$W_2^2 - W_2' = 2V_2(x) - 2E_0^{(2)}. \tag{7}$$

The potential $V_2(x)$ can be written as

$$V_2(x) = V_1(x) - \frac{d^2}{dx^2} ln\Psi_0^{(1)}(x). \tag{8}$$

Thus, setting $V_1(x) = 0$ in (1), the Hamiltonian H_1 has a positive energy spectrum and for negative energies $E = -\gamma^2/2$, the equation $H\Psi = E\Psi$ has solutions given by, [6]

$$\Psi_0^{(1)}(x, E) = cosh\gamma x + \alpha sinh\gamma x\ . \tag{9}$$

Thus the partner potential $V_2(x)$, with $|\alpha| < 1$ is given by

$$V_2(x) = V_1(x) - \frac{d^2}{dx^2} ln\Psi_0^{(1)}(x, E) = -\frac{\gamma^2(1-\alpha^2)}{(cosh\gamma x + \alpha sinh\gamma x)^2} \tag{10}$$

has a single bound state at energy

$$\bar{E} = -\gamma^2/2 \tag{11}$$

and energy eigenfunction given by

$$\bar{\Psi} = \frac{1}{cosh\gamma x + \alpha sinh\gamma x}. \tag{12}$$

Therefore, through the algebra of SQM, the free particle potential $V_1(x) = 0$ has supersymmetric partner V_2 whose ground state energy is $E = -\gamma^2/2$ and groundstate wavefunction given by equation (12). The potential V_2, rewritten as

$$V_2(x) = -\gamma^2 sech^2(\gamma x + tanh^{-1}\alpha) \tag{13}$$

has the same reflectionless property of V_1, which is inherently reflectionless, [6], [7]. V_2 is the potential that we shall address later.

3. The Peyrard-Bishop model

In the Peyrard-Bishop model (PB), [3], the molecule is represented by two linear chains of N particles describing the nucleotides harmonically coupled; the interstrand interactions are restricted to facing nucleotides. For each base pair the model includes two degrees of freedom u_n and v_n, Figure 1. Denoting by p_u and p_v the conjugated momentum to the spatial positions u and v, the Hamiltonian model can be written as,

$$\begin{aligned} H &= \sum_n \left(\frac{p_{u,n}^2}{2m} + \frac{K}{2}(u_n - u_{n-1})^2 + \right. \\ &\left. \frac{p_{v,n}^2}{2m} + \frac{K}{2}(v_n - v_{n-1})^2 + V(\frac{u_n - v_n}{\sqrt{2}}) \right) \end{aligned} \tag{14}$$

where $p_{u,n}$ and $p_{v,n}$ are the momenta corresponding to the respective coordinates u_n and v_n.

The transformation of variables

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

decouples the two degrees of freedom such that the Hamiltonian can be rewritten as

$$H = H_x + H_y$$

where

$$H_x = \sum_n \left(\frac{p_{x,n}^2}{2m} + \frac{K}{2}(x_n - x_{n-1})^2 \right)$$

and

$$H_y = \sum_n \left(\frac{p_{y,n}^2}{2m} + \frac{K}{2}(y_n - y_{n-1})^2 + V(y_n) \right) \tag{15}$$

The Hamiltonian H_x is purelly harmonic. In the PB model, the potential $V(y_n)$ was taken to be the Morse potential, simulating the hydrogen bonds between the basis of the macromolecule. The Morse potential is known to describe very well diatomic molecules, [9].

At this point it is important to remark that, as a result of the transfer integral method, the statistical mechanics of this one-dimensional Hamiltonian is equivalent to solving the following Schrödinger equation, [8]

$$-\frac{1}{2\beta^2 K}\frac{d^2\Psi}{dy^2} + V(y)\Psi = E\Psi \tag{16}$$

where $\beta = \frac{1}{k_B T}$, k_B is the Boltzmann constant, T is the temperature and K is the string constant, determined experimentally. Notice that the y index has been omitted.

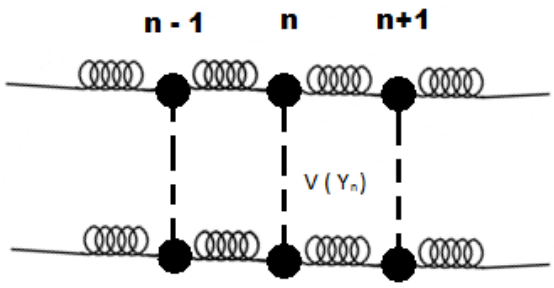

Figure 1. The lattice model.

4. The reflectionless potential in the lattice model

The starting point is equation (16) with the potential given by (10). The potential V_2 can be rewritten as

$$V_2(x) = -\gamma^2 sech^2(\gamma x + tanh^{-1}\alpha). \tag{17}$$

and is, by construction, a reflectionless potential. Notice that α must be different from zero in order to be reflectionless.

The groundstate wavefunction is equivalently given by

$$\bar{\Psi} = N(cosh\gamma y + \alpha sinh\gamma y)^{-B} \tag{18}$$

where $B = -\frac{1}{2} + \frac{1}{2}\sqrt{1 + 8\beta^2 K}$. The equivalent groundstate energy is

$$E = -\frac{\gamma^2 B^2}{2\beta^2 K} \ . \tag{19}$$

Next step is the evaluation of the mean stretching of this model, $< y >$, given by,

$$< y >= \frac{\int_{-\infty}^{+\infty} y|\bar{\Psi}(y)|^2 dy}{\int_{-\infty}^{+\infty} |\bar{\Psi}(y)|^2 dy} \ . \tag{20}$$

Thus, the parameters were fixed in such a way that γ maintains the depth of the potential close to the depth of the Morse potential, $\gamma^2 = 0.01eV$ and $K = 1.10^{-4} eV/\mathring{A}^2$, [10]. The α parameter is set to $\frac{1}{2}$ and the constant $\frac{8K}{k_B^2}$, appearing in B is of order of $1.10^5 K^2$. The evaluation of the mean stretching shows that the denaturation begins at temperature around $500K$, as shown in Figure 2 below. It should be noted that the denaturation temperature obtained in the PB model is $460K$, [3].

Concerning the connection of the reflectionless potential with the soliton propagation in the lattice, (17) can be considered a one-soliton solution of the Korteweg-de-Vries equation, KdV, $V_2(x) = v(x, 0)$ in the form

$$(\partial_{xxx} - 12v\partial_x + \partial_t)\, v(x,t) = 0 \ . \tag{21}$$

The general solution for all t is

$$v(x,t) = -\gamma^2 sech^2(\gamma x - 4\gamma^3 t + tanh^{-1}\alpha). \tag{22}$$

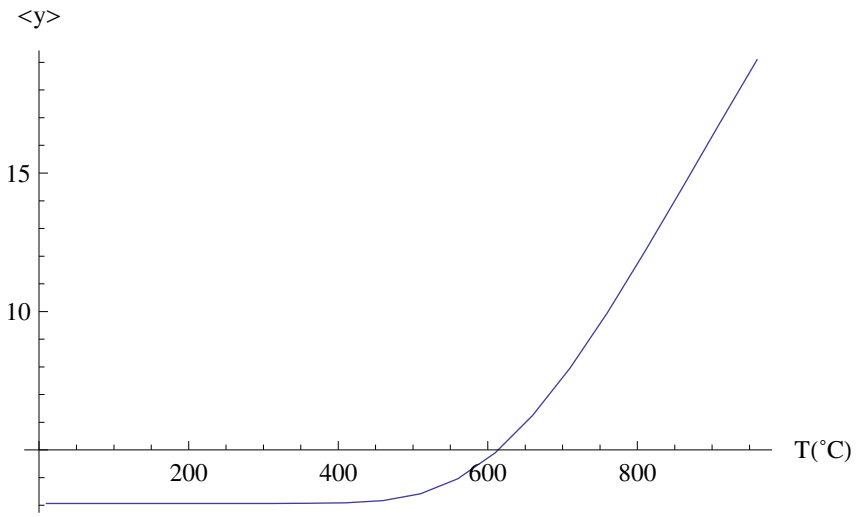

Figure 2. Plot of $< y >$ (in angstrons) as function of temperature.

5. Results and conclusions

The reflectionless potential obtained through SQM was employed in the study of the thermodynamic behaviour of a nonlinear one dimensional lattice. In particular the thermodynamic denaturation was shown to be in qualitative agreement with the result achieved with the Morse potential in the PB model, indicating that this approach is promising to future investigations.

The fact that the potential is reflectionless is particularly interesting in the sense that information can be transmitted through the nonlinear excitations of the lattice, which is compatible with soliton propagation on the lattice.

In conclusion, we remark that the association of the reflectionless potential may be a promising approach to analyse the dynamics of a nonlinear lattice with possible biological applications, subject of further analysis. Moreover we stress that SQM is used here as a quantum mechanical tool to solve a classical problem of a nonlinear one dimensional lattice, a peculiar quality or new attribute of SQM.

Acknowledgments

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