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Schrödinger equation approach to Statistical Mechanics of interacting strings: Exact results

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Abstract

In this work, we consider a pair of interacting strings that may thermally fluctuate around some line-reference. We assume that the two strings interact via a q-deformed Morse potential that reproduces well the features of the real interaction. Using the Transfer Matrix Method, based on the resolution of a Schrödinger equation, we first exactly determine their solutions that were found to be bound states. Second, from the exact expression of the ground state, we compute the contact probability that is the probability to find two interacting strings at a (finite) distance apart, and obtain its exact scaling form and the associated contact exponents. The main conclusion is that, the analytical studies reveal that the q-deformed Morse potential is a good candidate for the investigation of the statistical properties of fluctuating strings.

Keywords: *Strings, Interactions, Deformed Morse potential, Statistical Mechanics.*

1. Introduction

Strings are one-dimensional objects that possess rich statistical properties due to their soft and flexible morphology. For example, DNA molecule is formed by two connected flexible polymer chains that are organized in a double helice configuration. In particular, a pair of strings may exhibit an unbinding transition [1]. We emphasize that the mechanism ruling this phenomenon is analog to that governing interfacial wetting [2] and adsorption-desorption transitions of polymers [3]. The common feature of these interfacial phenomena is that, they have a behavior similar to that of 1-dimensional lines or strings of finite tension [4], such as ledges on crystal surfaces, stretched (or directed) polymers and vortex lines in superconductors.

We note that the unbinding transition from strings, as from bilayer membranes, is often driven by steric shape-fluctuations [5] whose amplitude increases with temperature. These repulsives entropic forces are actually in competition with the van der Waals attractive ones. There exists a certain value of the Hamaker amplitude (threshold) beyond which the van der Waals attractive interactions are sufficient to bind the string together, while below this characteristic amplitude, the membrane undulations dominate the attractive forces, and then, the string separate completely.

An interesting alternative tool to quantitatively investigate the statistical properties of string-pairs is the so-called *Transfer Matrix Method* (TMM) usually encountered in Quantum Mechanics [6-8] and Critical Phenomena [9,10]. Very recently, TMM was applied to extract the statistical properties of adjacent strings using the generalized Morse potential [11].

In this paper, we apply TMM to some new potential we introduce, for the first time, which is the q-deformed Morse potential (MP). The value $q=0$ gives the standard Morse potential used in Atomic Physics to study the atoms vibrations within molecules [12]. Also, such a potential was recently used for the study of DNA denaturation problem [13,14]. While the value $q=-1$ defines a generalized Morse potential that was introduced by Deng and Fan [15], in Quantum Mechanics context.

The choice of this q-deformed MP can be motived by the fact that its shape models well the real interaction potential (repulsive at short-distances and attractive at high-distances). Another virtue of this potential is that, its associated energy spectrum is discrete, and then, all its eigenfunctions are bound states. The existence of these states makes it a good candidate for the study of the statiscal properties of adjacent strings.

This paper is organized as follows. In Section 2, we present the used string model and the analytical expression of the q-deformed MP. In Section 3, we solve the associated Schrödinger equation to get the exact form of the contact propability. Finally, some concluding remarks are drawn in the last section.

2. String model

Consider two interacting strings that move on a two-dimensional space. We assume that, on average, they fluctuate around a line-reference, say x-axis, and in addition, their associated elongations remain perpendicular to this axis. The conformation of strings can be described by the local field-separation [16], $l(x) > 0$, which is perpendicular to the line-reference. The Statistical Mechanics of strings is based on the Hamiltonian

$$H[l] = \int_0^L \left[\frac{\sigma}{2}\left(\frac{dl}{dx}\right)^2 + V_q(x)\right] dx \, . \quad (1)$$

Here, L is the string length, σ is the effective tension, and $V_q(x)$ represents the interaction potential, whose form is the following

$$V_q(l) = D\left[\left(1 - \frac{b}{e^{\alpha l} + q}\right)^2 - 1\right], \ 0 \le l < \infty \, , \quad (2)$$

with the notation

$$b = e^{\alpha l_m} + q \, , \quad (3)$$

where l_m denotes the minimum point of the potential. We assume that the parameter q is such that $q > 0$ or $-1 \le q < 0$. In fact, the parameter q acts as an important deformation parameter. There, D is the potential deepth and $\alpha > 0$ defines the potential-range. As physically required, the potential $V_q(l)$ fails to 0^-, at infinity, that is for $l \to +\infty$.

Notice that, the proposed potential is a four-parameter exponential-type one that already pointed out in Ref. [17], and it may reduce to the most well-known exponential-type molecule potentials by choosing appropriate parameters (D, b, α, q). The values $q = 0$ and $q = -1$ describe the standard and generalized MPs, respectively. Hence, potential $V_q(l)$ is more general and may be a good candidate for the study of a large class of interacting molecular systems.

The potential $V_q(l)$ possesses one root for

$$l_0 = \alpha^{-1} ln\left(\frac{b}{2} - q\right), \quad (4)$$

provided that $b > 2(q+1)$ is fulfilled. Then, the condition that $b > 0$ is ensured.

We show that the unique minimum point of the potential, l_m, is above the zero l_0, and it is given, in terms of parameters (b, q), by

$$l_m = \alpha^{-1} ln(b - q) \, . \quad (5)$$

It is easy to that the interaction potential presents no asymptote at non-vanishing positive abscissa, for $-1 < q < 0$ or $q > 0$. But, it does for $q = -1$, where it becomes infinite at the distance-origin $l = 0$.

In Fig. 1, we report the q-deformed MP, for various values of the parameter q keeping fixed the other ones (D, b, α). In particular, this figure shows that, the potential minimum is shifted towards its smaller values, as the parameter q is increased.

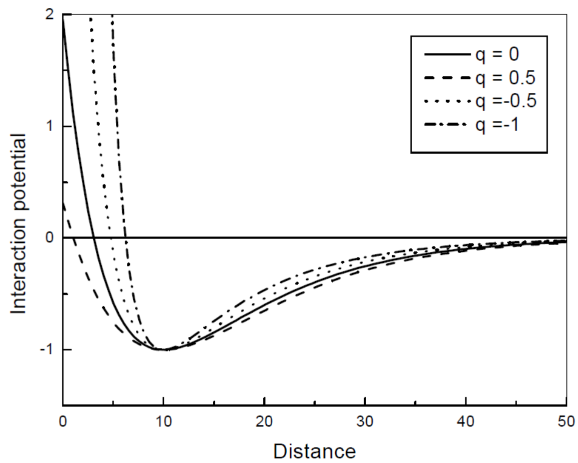

Figure 1 : Reduced Morse potential, $V_q(l)/D$, versus distance l (in nanometer unit), for various parameters $q = -1, -0.5$, 0 and 0.5. These curves are drawn with the parameters : $l_m = 10nm$ and $\alpha = 0.1nm^{-1}$.

2. Exact contact probability

In the framework of TMM, the contact probabilty to have the two strings at some distance apart is given by the knowledge of the ground state that solves a Schrödinger equation described below.

Let us start by recalling the useful *Katos's mathematical theorem* [18] :

Suppose that the potential $V(l)$ of the Schrödinger operator $H = -(d^2/dl^2) + V(l)$ is bounded from below and that

$$\lim_{l\to\infty} V(l) = 0 \, . \quad (6)$$

Notice that H has no positive eigenvalues. Indeed, if $H\varphi = E\varphi$, with $E > 0$ and $\varphi \in L^2(R)$, then, $\varphi = 0$.

Therefore, all eigenfunctions of the Schrödinger equation are bound states, of *negative* eigenvalues. The eigenvalues spectrum is then discrete. As remark [18], the point $E = 0$ can be an eigenvalue of the operator $H = -(d^2/dl^2) + V(l)$, even when $V(l) \in C^\infty(R)$.

The considered q-deformed MP effectively satisfies the above theorem conditions. First, it is bounded from below, since $V(l) \ge -D$, for all values of distance l. Second, the limit (6) is also fulfilled, due to the presence of exponential tails in the potential expression (2). In addition, according to the above remark, this potential may have a ground state, since it is infinitely differentiable. The conclusion is that, the Schrödinger equation with a q-deformed MP has only bound states as solutions and a discrete spectrum.

Now, we note that, in the thermodynamic limit, that is for $L \to \infty$, the statistical properties of model (1) can be studied using TMM that is based on the resolution of a Schrödinger-equation type [6-8],

$$\frac{(k_B T)^2}{2\sigma}\frac{d^2\varphi_n}{dl^2} + V_q(l)\varphi_n = E_n\varphi_n \,, \tag{7}$$

where T is the absolute temperature and k_B is the Boltzmann's constant. In the above differential equation, the parameters E_n's and φ_n's denote the set of eigenvalues and wave-functions, respectively. The eigenvalues E_n's are ordered in such a way that $E_0 \le E_1 \le E_2 \le \cdots$.

The ground state eigenvalue E_0 defines the free energy density, f, that is $f = E_0$, while the corresponding eigenvector, $\varphi_0(l)$, determines the probability distribution, $P(l)$. In fact, $P(l)dl$ represents the probability of finding two strings at a separation between l and $l + dl$. The probability distribution is then given by

$$P(l) = \frac{|\varphi_0(l)|^2}{\int|\varphi_0(l)|^2 dl} \,. \tag{8}$$

With the help of this distribution, we can calculate, for example, its first and second moments,

$$\langle l\rangle = \int lP(l)dl \;, \langle l^2\rangle = \int l^2 P(l)dl \,. \tag{9}$$

The string roughness is given by

$$\xi_\perp = [\langle l^2\rangle - \langle l\rangle^2]^{1/2} \,. \tag{10}$$

Before making explicit calculations, it will be convenient to recall some backgrounds concerning the general statistical properties of the string-pairs.

First, we recall the definition of the *roughness exponent*. Consider a fluctuating manifold (string or bilayer membrane) and notice that the latter makes large transverse excursions from its average position. The manifold is rough if the typical size, $\xi_\perp$, of its transverse excursions grows with its lateral size, $\xi_\parallel$. It is admitted that the two lengths obey the following scaling relation [1,19]

$$\xi_\perp \sim {\xi_\parallel}^{\zeta} \,. \tag{11}$$

This relation then defines the *roughness ex*ponent ζ. The latter crucially depends on the nature of the considered manifold. For example, for strings, $\zeta = 1/2$, and $\zeta = 1$, for almost-flat fluid membranes.

The last and interesting exponent to recall is the *contact exponent*. This characterizes the singular behavior at roughening of the contact probability of two adjacent manifolds. The latter scales as [1]

$$P \sim {\xi_\parallel}^{-\zeta_0} \sim {\xi_\perp}^{-\zeta_0/\zeta} \,. \tag{12}$$

On the other hand, we can put the probability distribution on the following scaling form

$$P(l) = {\xi_\perp}^{-1}\Omega(l/\xi_\perp) \,. \tag{13}$$

Here, the explicit factor ${\xi_\perp}^{-1}$ arises from normalization. To recover relationship (12), the scaling function $\Omega(s)$ must behave as

$$\Omega(s) \sim s^{-1+\zeta_0/\zeta} \,, \text{ for small } s \text{ (with } \zeta_0 > 0) \,. \tag{14}$$

This scaling behavior remains valid as long as the mean-separation is such that $\langle l\rangle \sim \xi_\perp$.

Now, to determine the scaling behaviour of the contact probability, we must solve the differential equation (7). We first note that it is very similar to the traditional Schrödinger equation

$$\frac{\hbar^2}{2\mu}\frac{d^2\varphi_n}{dl^2} + V_q(l)\varphi_n = E_n\varphi_n \,, \tag{15}$$

where μ is the reduced mass and $\hbar$ is the renormalized Planck's constant, making the substitution

$$\frac{(k_B T)^2}{2\sigma} \to \frac{\hbar^2}{2\mu}. \tag{16}$$

This Schrödinger equation has been exactly solved [17], and it will be convenient to recall briefly the essential steps of its resolution, in particular, for the ground state, φ_0.

To determine the ground state of interest, we first write it as follows

$$\varphi_0(l) = Nexp\left\{-\frac{\sqrt{2\sigma}}{k_B T}\int W(l)dl\right\}, \tag{17}$$

where N is a normalization constant and $W(l)$ is called a *superpotential* in supersymmetric language. The latter satisfies a non-linear Riccati differential equation,

$$W^2(l) - \frac{k_B T}{\sqrt{2\sigma}}\frac{dW}{dl} = V_q(l) - E_0 \,, \tag{18}$$

where E_0 is the ground state energy. The above equation has an exact solution that is [18]

$$W(l) = -\frac{k_B T}{\sqrt{2\sigma}}\left[Q_1 + \frac{Q_2}{e^{\alpha l} - q}\right], \tag{19}$$

with

$$Q_2 = \frac{1}{2}\left[-\alpha q + \sqrt{1 + \frac{8\sigma}{(k_B T)^2}\frac{Db^2}{\alpha^2 q^2}}\right], \tag{20a}$$

$$Q_1 = \frac{\sigma D b}{(k_B T)^2}\left(\frac{b-2q}{q}\right)\frac{1}{Q_2} - \frac{Q_2}{q}, \quad (20b)$$

$$E_0 = -\frac{(k_B T)^2}{2\sigma} Q_1^2 . \quad (21)$$

It is easy to see that $Q_1 < 0$.

Now, combining Eqs. (17) and (19) gives the *exact* form of the ground state

$$\varphi_0(l) = N_0 e^{Q_1 l}\left(\frac{e^{\alpha l}}{e^{\alpha l}+q}\right)^{Q_2/\alpha q}, \quad (22)$$

The normalization constant N_0 is exactly known. This computed ground state gives the contact probability

$$P(l) = \varphi_0^2(l) = K_0 e^{2Q_1 l}\left(\frac{e^{\alpha l}}{e^{\alpha l}+q}\right)^{2Q_2/\alpha q}, \quad (23)$$

with the known normalization constant K_0. From the above exact formula, we can compute all moments of separation between adjacent strings.

The above formula clearly shows that the contact probability has a finite (small) value at the origin

$$P(0) = K_0(1+q)^{-2Q_2/\alpha q} . \quad (23a)$$

While at infinity, it decays with the average-separation as

$$P(l) \sim K_0 e^{2Q_1 l},\ l \to +\infty \quad (23b)$$

It is easy to see that the contact probability obeys the following scaling form

$$P(l) = \frac{1}{\xi_\perp}\Omega\left(\frac{l}{\xi_\perp}\right), \quad (24)$$

with the scaling function

$$\Omega(s) = K_0 e^{-s}\left(\frac{e^{s\xi_\perp \alpha}}{e^{s\xi_\perp \alpha}+q}\right)^{2Q_2/\alpha q} . \quad (25)$$

Thus, the associated contact exponent *exactly* reads

$$\zeta_0 = \zeta . \quad (26b)$$

Then, $\zeta_0 = 1/2$, for strings.

We emphasize that the discussion of the temperature-dependence of all separation-moments will be presented in another publication.

Conclusion

The aim of this paper is an analytical study of the statistical properties of string-pairs, from a q-deformed Morse potential, using the Schrödinger equation method. It was found that its solutions where bound states.

From the exact ground state expression, we computed the contact probability that is defined as the probability to find the two interacting strings at a (finite) distance each other. This probability gives all length-scales, which are the average-separation and roughness.

The main conclusion is that, our analytical studies reveal that the q-deformed Morse potential is a good candidate for the description of the statistical properties of interacting strings.

We emphasize that the study of the unbinding transition from string-pairs with this potential will be appeared elsewhere.

This work must be considered as a natural extension of some very recently published one [11], dealt with an exact study of the statistical properties of string-pairs from standard $q = 0$ and generalized $q = -1$ Morse potentials.

Finally, the present analysis may be extended to more than two strings.

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