Solution of the Schrödinger equation for a particular form of Morse potential using the Laplace transform

M. Zarezadeh[1] M. K. Tavassoly[1,2;1)]

[1] Atomic and Molecular Group, Faculty of Physics, Yazd University, Yazd, Iran
[2] Photonics Research Group, Engineering Research Center, Yazd University, Yazd, Iran

Abstract: In this paper, we have solved the Schrödinger equation for a particular kind of Morse potential and find its normalized eigenfunctions and eigenvalues, exactly. Our work is based on the Laplace transform technique which reduces the second-order differential equation to a first-order.

Key words: Schrödinger equation, Laplace transform, Morse potential, bound state

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1 Introduction

The exact solution of the Schrödinger equation for various potentials is an important task in non-relativistic quantum mechanics, because considerable information is found in the wave functions of any quantum system. Therefore, researchers have focused on this issue and have studied known potentials, for example the Morse potential [1] which is in our present consideration. This quantum system is one of a class of potentials [2] in which the Schrödinger equations have been exactly solved. Indeed, this potential is the most appropriate candidate for the description of the interaction between the two atoms in diatomic molecules. It is known that the two atoms in a diatomic molecule have a balance distance and oscillate around their equilibrium point. If the distance between the two atoms is greater than this value, the chemical bond between them is broken; this phenomenon is well illustrated by the Morse potential. In addition, this potential is also used in spectroscopy, diatomic molecular vibration, scattering and in the description of vibrations of polyatomic molecules [3–6]. [7] investigated the controllability of a quantum system for a Morse potential which possesses a finite dimensional energy spectrum.

From another view, the Morse potential is one class of potentials which is introduced in the finite-dimensional Hilbert space, as we have also shown in this paper. In fact, the intention of our presentation is to construct the coherent states of such a system which particularly deals with a finite-dimensional Hilbert space. Our motivation arises from the fact that the coherent states play an important role in various fields of physics [8–10] (for a recent set of papers in this field refer to [11]). These states were firstly introduced in the infinite-dimensional Hilbert space of a harmonic oscillator. But in recent decades, the concept of coherent states has been generalized in very many ways. One of these generalizations that has attracted a lot of attention is the extension of coherent states to the finite-dimensional space, for instance, the physical systems in which their energy spectrum contains a finite number of states [12]. In this typical work the energy spectrum and eigenfunctions of the potential are the first necessary tools for constructing coherent states and then one can investigate the nonclassical properties for the obtained states.

Moreover, in recent years, several methods have been proposed to solve the Schrödinger equation for the Morse potential. Dayi and Duru introduced the q-Schrödinger equation for the potential $V(u)=u^2+1/u^2;\ u\geqslant 0$ [13]. Then, they studied a relationship between the Morse potential with the above potential by a q-canonical transformation, through which the q-Schrödinger equation for the Morse potential may be defined and solved. Aktas and Ramazan have calculated the bound-state energies of the q-deformed Morse potential by using the Hamiltonian Hierarchy method within the framework of the SUSYQM [14]. This is indeed the same method that was introduced by Schrödinger, i.e., the factorization method [15], in which the solvable models can be transformed in terms of appropriate creation and annihilation operators. Another method is the Laplace (or integral) transform which has been used for solving differential and integral equations. Chen has used this technique for solving the Schrödinger equation of the Morse potential [16].

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1) E-mail: mktavassoly@yazd.ac.ir

Recently, the Nikiforov-Uvarov (NU) method [17] is introduced which is based on the solution of a second-order differential equation with special orthogonal functions [18]. By means of this method , the Schrödinger equation is reduced to a generalized equation of hypergeometric type functions. Berkdemir and Han have used the NU method for rotational correction on the Morse potential [19]. Other techniques for solving the Schrödinger equation for the Morse potential are: the asymptotic iteration method (AIM) [20, 21], the path integral method [22], etc. In this paper, we focus on solving the Schrödinger equation and finding the energy spectrum together with the corresponding eigenfunctions of a special type of Morse potential (which we call the l-parameter Morse potential) by using the Laplace transform.

2 Exact solution of the Schrödinger equation for the Morse potential

In this paper we want to consider the (shifted) Morse potential

$$V^l(x)=(l+1)^2-(2l+3)\mathrm{e}^{-x}+\mathrm{e}^{-2x}, \tag{1}$$

where l is a constant. It is obvious that this particular form of Morse potential considered in Ref. [23] is rather different from the one considered in Ref. [16], $V(x)=D_\mathrm{e}\mathrm{e}^{-2ax}-2D_\mathrm{e}\mathrm{e}^{-ax}$; i.e. they cannot be obtained again from each other by a change of variable and so on (this will be more clear from our final obtained results). Substituting Eq. (1) into the time independent Schrödinger equation yields

$$\left(-\frac{\mathrm{d}^2}{\mathrm{d}x^2}+\mathrm{e}^{-2x}-(2l+3)\mathrm{e}^{-x}+(l+1)^2-E_n^l\right)\psi_n^l(x)=0, \tag{2}$$

where we have set $\hbar^2/2m=1$. Now we define k and β^2 as

$$k = 2l+3, \tag{3}$$
$$\beta^2 = (l+1)^2-E_n^l. \tag{4}$$

Thus, Eq. (2) simplifies to

$$\left(\frac{\mathrm{d}^2}{\mathrm{d}x^2}-\mathrm{e}^{-2x}+k\mathrm{e}^{-x}-\beta^2\right)\psi_n^l(x)=0. \tag{5}$$

After a change of variable as $y=\mathrm{e}^{-x}$, Eq. (5) can be rewritten as

$$\left(y^2\frac{\mathrm{d}^2}{\mathrm{d}y^2}+y\frac{\mathrm{d}}{\mathrm{d}y}-y^2+ky-\beta^2\right)\psi_n^l(y)=0. \tag{6}$$

If we introduce $\psi(y)$ as follows

$$\psi(y)=y^A f(y), \tag{7}$$

where A is a constant, then by inserting (7) into (6), one obtains

$$\left[y^2\frac{\mathrm{d}^2}{\mathrm{d}y^2}+(2A+1)y\frac{\mathrm{d}}{\mathrm{d}y}-y^2+ky+(A^2-\beta^2)\right]f(y)=0. \tag{8}$$

Let us take $A=-\beta$ (the case $A=\beta$ is clearly not valid), thus we have the second-order differential equation

$$\left[y\frac{\mathrm{d}^2}{\mathrm{d}y^2}-(2\beta-1)y\frac{\mathrm{d}}{\mathrm{d}y}-y+k\right]f(y)=0. \tag{9}$$

The next step is to reduce the above second-order differential equation to the first-order differential equation by using the Laplace transform technique. The necessary Laplace transforms are as follows [24]

$$\pounds\left(y\frac{\mathrm{d}^2f(y)}{\mathrm{d}y^2}\right) = -2pF(p)-p^2\frac{\mathrm{d}F}{\mathrm{d}p}, \tag{10}$$

$$\pounds(yf(y))=-\frac{\mathrm{d}F(p)}{\mathrm{d}p}, \tag{11}$$

$$\pounds\left(\frac{\mathrm{d}f(y)}{\mathrm{d}y}\right)=pF(p), \tag{12}$$

$$\pounds(f(y))=F(p). \tag{13}$$

Using (10)–(13), in Eq. (9), it reduces to the following first-order differential equation:

$$(1-p^2)\frac{\mathrm{d}F(p)}{\mathrm{d}p}+[k-(1+2\beta)p]F(p)=0. \tag{14}$$

Therefore, we find $F(p)$ with a simple integration procedure results in:

$$F(p)=N(p-1)^{\frac{k-2\beta-1}{2}}(p+1)^{\frac{-k-2\beta-1}{2}}, \tag{15}$$

where N is an integration constant. Our further goal is to obtain $f(y)$, which is possible by taking the inverse Laplace transform of Eq. (15) giving us:

$$f(y)=N\mathrm{e}^{-y}y^{2\beta}\frac{{}_1F_1\left(\frac{2\beta-k+1}{2};2\beta+1;2y\right)}{\Gamma(2\beta+1)}, \tag{16}$$

where ${}_1F_1(a;b;y)$ is the Kummer confluent hypergeometric function. In obtaining (16) we have used the following integral relationship [24]

$$\int_0^y f_1(t)f_2(y-t)\mathrm{d}t=F_1(s)F_2(s), \tag{17}$$

where $f_1(t)$ and $f_2(t)$ are the inverse Laplace transforms of $F_1(s)$ and $F_2(s)$, respectively. The relationship between Kummer confluent hypergeometric function and associated Laguerre polynomials reads as

$${}_1F_1(-n;u+1;y)=\frac{n!\Gamma(u+1)}{\Gamma(u+n+1)}L_n^u(y), \tag{18}$$

where $L_n^u(y)$ is the associated Laguerre polynomials. Substituting Eq. (18) into (16) gives us the following result

$$f(y)=N\frac{n!}{\Gamma(k-n)}\mathrm{e}^{-y}y^{k-2n-1}L_n^{k-2n-1}(2y), \tag{19}$$

where we have assumed that

$$u=2\beta,\ \ 2\beta-k+1=-2n, \tag{20}$$

and N may be determined from the normalization condition. Inserting (19) into Eq. (7) yields the final form of the eigenfunctions as:

$$\psi_n^l(y)=N_n\mathrm{e}^{-y}y^{l-n+1}L_n^{2(l-n+1)}(2y),\quad N_n=N\frac{n!}{\Gamma(k-n)}, \tag{21}$$

where N_n can be obtained from the normalization condition as follows:

$$N_n=\left(\frac{n!2^{2l-2n+3}}{(2l-n+2)!}\right)^{1/2}. \tag{22}$$

Equation (21) may be expressed in terms of the main variable x as:

$$\psi_n^l(x)=N_n\exp(-\mathrm{e}^{-x})\mathrm{e}^{-(l-n+1)x}L_n^{2(l-n+1)}(2\mathrm{e}^{-x}). \tag{23}$$

Lastly, considering (3), (4) and (20) gives the spectrum of the Morse potential with l-parameters introduced in (1) as

$$\begin{aligned}E_n^l &= (l+1)^2-(l+1-n)^2\\ &= -n^2+2(l+1)n.\end{aligned} \tag{24}$$

Noticing that in Eq. (23) the associated Laguerre polynomial, $L_n^{2(l-n+1)}(2x)$, is valid for $2l-2n+2>-1$, thus the values of n are limited to $n=0,\ 1,\ 2,\ \cdots,l$, i.e., the associated spectrum is in a bound state. We end our discussion by emphasizing the fact that our considered Morse potential and the case considered in Ref. [16] are two different sets of the family of Morse potentials.

3 Conclusion

We have used a certain type of Morse potential and solved its Schrödinger equation by using a Laplace transform. We reduced the second-order differential equation to a first-order differential equation and we found the energy spectrum and corresponding eigenfunctions. Our main results are summarized in Eqs. (23) and (24)[1)].

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1) Notice that in Ref. [6], the solution of first-order differential equation in (10) of the paper should be corrected as

$$F(p)=N\left(1-\frac{1}{p+\frac{1}{2}}\right)^{\frac{k-2\beta-1}{2}}\left(p+\frac{1}{2}\right)^{-(2\beta+1)}.$$