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Analytical Bound-State solution of the Schrodinger equation for the morse potential within the Nikiforov-Uvarov method

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Abstract: The Morse potential has important and significance rule to describe the diatomic molecule energy and structure. However, there is no any analytical solution for Schrodinger equation with this potential without approximation, therefore other ways such as numerical, perturbation, variation and so on are taken to deal with this potential. In this work the the Nikiforov-Uvarov method is taken to obtain its energy eigenvalues and eigenfunctions. In the ground state the Schrodinger equation with this potential have exact solution but with arbitrary l-state the Morse potential with centrifugal term have no exact solution therefore it is solved analytically with use the Pekeris approximation. Here in this work we solved the Schrodinger in the space of D dimension and use the Nikiforove-Uvarov method which is based on solving the hyper geometric type second-order differential equations by means of the special orthogonal functions.

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1 Introduction

Solving of the Schrodinger equation in quantum mechanics for various potential has great interest. Time independent Schrodinger equation can give us the eigenvalues of energies and also the wave functions, which include all the necessary information about the quantum system under consideration. Due to this fact, analytic solutions have generated great interest in all physical branches. It is well known that, there are a few potentials which for them the Schrodinger equation has analytic solution. The Nikiforov-Uvarov (NU) method is an alternative procedure which sometimes is used to solve the Schrodinger equation [4,16]. The NU procedure gives an exact solution of the time independent Schrodinger equation for some kinds of potentials. Solving of

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the second order and linear differential equations forms the basis of this procedure [20]. In this method with use an appropriate transformation of coordinate, the time-independent Schrodinger equation is changed to an equation of the hyper geometric type. This procedure is also used to solve the Schrodinger equation with potentials which they have an exponential terms and also with central and non-central potentials [21,22]. This approach is a general method which is used beyond the Schrodinger equation and used to solve some other equation, such as Dirac [5] relativistic finite-difference equation [15] Klein–Fock–Gordon equation [1] and Klein-Gordon equations. In order to explain physical states of the systems, usually taking potentials depend on the case of study. Parabolic potentials such as the Eckart [23], Rosen-Morse, Scarf and Ginocchio barrier potential are some of those potentials [9,19]. The Morse potential, named after physicist Philip M. Morse, is a convenient interatomic interaction model for the potential energy of a diatomic molecule [11,14]. It is a better approximation for the vibrational structure of the molecule than the quantum harmonic oscillator because it explicitly includes the effects of bond breaking, such as the existence of unbound states. It also accounts for the anharmonicity of real bonds and the non-zero transition probability for overtone and combination bands. The Morse potential can also be used to model other interactions such as the interaction between an atom and a surface. Due to its simplicity (only three fitting parameters), it is not used in modern spectroscopy. However, its mathematical form inspired the MLR (Morse/Long-range) potential, which is the most popular potential energy function used for fitting spectroscopic data.

It's not possible to solve the Schrodinger equation exact and analytically for each potential. So, the approximated procedure widely used to calculate this equation analytically. Almost researchers approximate the centrifugal term as Pekeris do [6,18] or Greene and Aldrich approximation [10]. Exponential potential is a wide class of potentials which have an important role in various physics problems. The Hulthen [2,17], Manning Rosen plus Hulthen [3], Poschl & Teller [13], WS [7,21], Rosen & Morse type [24], the Manning & Rosen (MR) [8,19] potential are some of these potentials.

In next section we describe the Schrodinger equation for radial Morse potential in D dimension. In section 3 the Nikiforov-Uvarov method is explained. After that in section 4 the eigenvalue and wave functions are obtained via Nikiforov-Uvarov method.

2 The D-dimensional Schrodinger equation

In the n-dimensional n ≥ 2 space, the Schrodinger equation with spherically symmetric potential V (r) is of the form [2]

$$\left[-\frac{\hbar^2}{2m}\nabla_D^2 + V(r) - E_{nl}\right]\psi_{nlm}(r,\Omega_D) = 0 \tag{1}$$

Where D is dimension of space, m is the reduced mass, r is hyperradius, $\Omega_D = (\theta_1, \theta_2, \cdots, \theta_{D-2}, \phi)$ is hyperangle, $\hbar$ is the Planck's constant, $\Delta_D = \nabla_D^2$ is the Laplacian operator and

$$\psi_{nlm}(r,\Omega_D) = R_{nl}(r)Y_{lm}(\Omega_D) \tag{2}$$

The Laplacian operator divides into a hyper-radial part $r^{1-n}\frac{\partial}{\partial r}\left(r^{n-1}\frac{\partial}{\partial r}\right)$ and an angular part $\frac{\hat{L}_D^2}{\hbar^2 r^2}$ i.e.

$$\nabla_D^2 = r^{1-D}\frac{\partial}{\partial r}\left(r^{D-1}\frac{\partial}{\partial r}\right) - \frac{\hat{L}_D^2}{\hbar^2 r^2} \tag{3}$$

where $\hat{L}_D$ is the grand orbital angular momentum operator. The eigenfunctions of $\hat{L}_D^2$ are the hyper-spherical harmonics:

$$\hat{L}_D^2 Y_{lm}(\Omega_D) = \hbar^2(l + D - 2)Y_{lm}(\Omega_D) \tag{4}$$

where l is the angular momentum quantum number. After substituting Eqs. (2), (3) and (4) into (1), and using $\psi_{nlm}(r,\Omega_D)$ as the eigenfunction of $\hat{L}_D^2$ with eigenvalue $\hbar^2 l(l+D-2)$, we obtain an equation known as the hyper-radial Schrodinger equation with the Morse potential:

$$\frac{d^2R_{nl}}{dr^2} + \frac{D-1}{r}\frac{dR_{nl}}{dr^2} + \frac{2m}{\hbar^2}\left[E_{nl} - V(r) - \frac{\hbar^2 l(l+D-2)}{2mr^2}\right]R_{nl} = 0 \tag{5}$$

With introducing a new function $\psi_{nl}(r) = r^{\frac{D-1}{2}}R_{nl}(r)$ and a new parameter $\tilde{l} = l + (D-3)/2$ Eq. (5) reduces to

$$\frac{d^2\psi_{nl}}{dr^2} + \frac{2m}{\hbar^2}\left[E_{nl} - V(r) - \frac{\hbar^2\tilde{l}(\tilde{l}+1)}{2mr^2}\right]\psi_{nl} = 0 \tag{6}$$

This equation has the same form as the equation for a radial part of a particle in a radial potential in three dimensions.

3 The Nikiforov-Uvarov method

The Nikiforov-Uvarov method (NU method), which is introduced by Nikiforov-Uvarov, is a method for solving a second order differential equation. Each second order differential equation cannot be solved by this method, but only those equations have special coefficient function can be solved by this method. This method gives us an exact analytic solution of the equation.

By using of this method, the exact energy eigenvalues and the wave functions of the Schrodinger equation are obtained analytically by a systematically scheme, which this method introduced. In order to solve a second order differential equation with this method, some constraint should be satisfied. Due to those constraints the

Schrodinger equation with only some special potential is solved analytically. The mean equation and those constraints are given as follow;

$$\psi''(s)+\left(\frac{\tilde{\tau}(s)}{\sigma(s)}\right)\psi'(s)+\left(\frac{\tilde{\sigma}(s)}{\sigma^2(s)}\right)\psi(s)=0 \tag{7}$$

Here the constraints on the $\sigma(s)$ and $\tilde{\sigma}(s)$ are so that they are polynomials at most second-degree, $\tilde{\tau}(s)$ is a first degree polynomial or is a constant.

To obtain a special solution of Eq. (7) by factorization, the following replacement is used:

$$\psi(s)=\phi(s)y(s) \tag{8}$$

This replacement changes the Schrodinger equation, to an equation of the hyper geometric type as follow,

$$\sigma(s)y''(s)+\tau(s)y'(s)+\lambda y(s)=0 \tag{9}$$

Where λ is a constant ($\lambda=k+\pi'$, k is constant), $\phi(s)$ satisfies

$$\frac{\phi'(s)}{\phi(s)}=\frac{\pi(s)}{\sigma(s)} \tag{10}$$

And

$$\tau(s)=\tilde{\tau}(s)+2\pi(s) \tag{11}$$

Where, $\pi(s)$ is a constant or a first order polynomial which depends on the variable s, and determined as fallow

$$\pi(s)=\frac{\sigma'(s)-\tilde{\tau}(s)}{2}\pm\sqrt{\left(\frac{\sigma'(s)-\tilde{\tau}(s)}{2}\right)^2-\tilde{\sigma}(s)+k\sigma(s)}, \tag{12}$$

where k is constant as defined after Eq. (9). The function y(s) is a hyper geometric type function. In Rodrigues relation form this function is written as,

$$y_n(s)=\frac{B_n}{\rho(s)}\frac{d^n}{ds^n}\left[\sigma^n(s)\rho(s)\right] \tag{13}$$

Where B_n is the normalization constant and the function ρ(s) is obtained as bellow

$$\left(\sigma(s)\rho(s)\right)'=\tau(s)\rho(s) \tag{14}$$

By looking at the Eq. (12), it is clear that the only unknown parameter or function in this relation, is the parameter k. On the other hand the function $\pi(s)$ is at most a first order polynomial. Hence using of this condition is suitable to obtain the parameter k. Therefore, the sum of the all expression under the squire root must be a squire of a first order polynomial. In order to take into account this condition, the discriminant of the expression under the root sign must be zero, namely $\Delta = b^2 - 4ac$. After that, the k parameter is obtained well clearly. And then the function $\pi(s)$ is obtained from the Eq. (12). To obtain $\tau(s)$ and λ using of the Eq. (11) and $\lambda = k + \pi'$ is suitable respectively. Unfortunately, the energy eigenvalues relation for the Schrodinger equation can be written as bellow:

$$\lambda = \lambda_n = -n\tau' - \frac{n(n-1)}{2}\sigma'', \qquad (n = 0,1,2,3,\ldots) \tag{15}$$

4 Solving of the Schrodinger equation with the Morse Potential

The Morse potential can be written as

$$V(r) = C_e\left[e^{-2a(r-r_e)} - 2e^{-a(r-r_e)}\right] \qquad C_e > 0,\ a > 0,\ r_e > 0 \tag{16}$$

where C_e is the dissociation energy, re is the equilibrium internuclear distance and a is a parameter controlling the width of the potential well. If anyone wants to modify this potential, shifting through the positive axis, it would be quite enough to insert an additional C_e into the potential. So the potential would be called the modified Morse potential. The vibrations and rotations of a two-atomic molecule can be exactly described by this potential in the case of $\ell = 0$. If we want to obtain the solution for $l \neq 0$, the centrifugal term has to be approximated in terms of exponential variables. In order to calculate the bound state energy spectrum and the corresponding radial wavefunction, the potential function given by Eq. (16) is inserted into the radial Schrodinger equation (SE)

$$\frac{d^2\psi_{nl}}{dr^2} + \frac{2m}{\hbar^2}\left[E_{nl} - C_e\left(e^{-2a(r-r_e)} - 2e^{-a(r-r_e)}\right) - \frac{\hbar^2\tilde{l}(\tilde{l}+1)}{2mr^2}\right]\psi_{nl} = 0 \tag{17}$$

An analytical solution of this differential equation cannot be obtained without an approximation because Eq. (17) includes both exponential and radial terms. For this reason, we outline a procedure given by Pekeris to suggest an approximation to the solution of SE given in Eq. (17).

The approximation is based on the expansion of the centrifugal term in a series of exponential depending on the internuclear distance, keeping terms up to second order. In this way, the centrifugal term can be rearranged by keeping the parameters in the Morse potential.

However, by construction, this approximation is valid only for the low vibrational energy states. Therefore, we can take into account the rotational term in the following way, using the Pekeris approximation. We first simplify the centrifugal part of Eq. (17) by changing the coordinates $x = (r - r_e)/r_e$ around $x = 0$. Hence, it may be expanded into a series of powers as

$$V_{rot}(r) = \frac{\lambda}{(1+x)^2} = \lambda(1 - 2x + 3x^2 - 4x^3 + \cdots) \tag{18}$$

with

$$\lambda = \frac{\hbar^2 \tilde{l}(\tilde{l}+1)}{2mr_e^2} \tag{19}$$

the first few terms should be quite sufficient. Instead, we now replace the centrifugal term by Eq. (20)

$$\frac{\hbar^2 \tilde{l}(\tilde{l}+1)}{2mr^2} = \frac{\lambda}{(1+x)^2} = \lambda(C_0 + C_1 e^{-\delta x} + C_2 e^{-2\delta x}) \tag{20}$$

$$C_0 = 1 - 3\delta^{-1} + 3\delta^{-2} \tag{21}$$

$$C_1 = 4\delta^{-1} - 6\delta^{-2} \tag{22}$$

$$C_2 = -\delta^{-1} + 3\delta^{-2} \tag{23}$$

We now can take the Eq. (20) instead of the exact rotational potential $\frac{\hbar^2 \tilde{l}(\tilde{l}+1)}{2mr^2}$ and solve the Schrodinger equation in Eq. (17). In order to apply the NU method, we rewrite Eq. (17) by using a new variable of the form $z = \exp(-\delta x)$,

$$\frac{d^2\psi}{dz^2} + \frac{1}{z}\frac{d\psi}{dz} + \frac{1}{z^2}\Big[-\gamma z^2 + \beta z - \alpha\Big]\psi = 0 \tag{24}$$

$$\alpha = -\frac{2mr_e^2(E - \lambda C_0)}{\hbar^2\delta^2} \tag{25}$$

$$\beta = \frac{2mr_e^2(2C_e - \lambda C_1)}{\hbar^2\delta^2} \tag{26}$$

$$\gamma = \frac{2mr_e^2(C_e - \lambda C_2)}{\hbar^2\delta^2} \tag{27}$$

After the comparison of Eq. (7) with Eq. (24), we obtain the corresponding polynomials as

$$\tilde{\tau}(z) = 1,$$
$$\sigma(\mathrm{z}) = \mathrm{z},$$
$$\tilde{\sigma}(z) = -\gamma z^2 + \beta z - \alpha \tag{28}$$

Substituting these polynomials into Eq. (12), we obtain the polynomial $\pi(z)$;

$$\pi(z) = \pm\sqrt{\gamma z^2 + (k-\beta)z + \alpha} \tag{29}$$

taking $\sigma'(z) = 1$. The discriminant of the upper expression under the square root has to be zero. Hence, the expression becomes the square of a polynomial of first degree;

$$(k-\beta)^2 - 4\alpha\beta = 0 \tag{30}$$

When the required arrangements are prepared with respect to the constant k, its double roots are derived as $k_{\pm} = \beta \pm 2\sqrt{\alpha\gamma}$. Substituting $k_{\pm}$ into Eq. (29), the following four possible forms of the $\pi(z)$ are obtained

$$\pi(z) = \pm\begin{cases} \sqrt{\gamma}z + \sqrt{\alpha} & \text{for } k_{+} = \beta + 2\sqrt{\alpha\gamma} \\ \sqrt{\gamma}z - \sqrt{\alpha} & \text{for } k_{-} = \beta - 2\sqrt{\alpha\gamma} \end{cases} \tag{31}$$

In general Eq. (12) for $\pi(z)$ has four possible forms, but in Eq. (31) it has two possible forms. We just select one of two possible forms of the π(s), i.e, $\pi(z) = -\sqrt{\gamma}z + \sqrt{\alpha}$ for $k_{-} = \beta - 2\sqrt{\alpha\gamma}$, because it would be provided a negative derivative of $\tau(z)$ given in Eq. (11). Hence,

The $\tau(z)$ satisfies the requirement below

$$\tau(z) = +1 + 2\sqrt{\alpha} - 2\sqrt{\gamma}z \tag{32}$$

From $\lambda = k - \pi'(z)$ Eq.(17) we obtain

$$\lambda = \beta - 2\sqrt{\alpha\gamma} - \sqrt{\gamma} \tag{33}$$

and from Eq. (15) we also get

$$\lambda_n = 2n\sqrt{\gamma} \tag{34}$$

remembering the expression $\lambda = \lambda_n$ (Eq. (15)) therefore

$$2n\sqrt{\gamma} = \beta - 2\sqrt{\alpha\gamma} - \sqrt{\gamma}. \tag{35}$$

Substituting the values of α, β and γ into Eq. (35), we can determine the energy spectrum E as

$$E=\frac{\hbar^2}{2mr_e^2}\left(l+\tfrac{D-3}{2}\right)\left(l+\tfrac{D-1}{2}\right)\left[1-\frac{3}{ar_e}+\frac{3}{ar_e^2}\right]-\frac{\hbar^2a^2}{2m}\left[\frac{\beta}{2\sqrt{\gamma}}-\left(n+\tfrac{1}{2}\right)\right] \quad (36)$$

where

$$\beta=\frac{4mC_e}{\hbar^2a^2}-\frac{1}{a^2r_e^2}\left(l+\tfrac{D-3}{2}\right)\left(l+\tfrac{D-1}{2}\right)\left[\frac{4}{ar_e}-\frac{6}{a^2r_e^2}\right] \quad (37)$$

$$\gamma=\frac{2mC_e}{\hbar^2a^2}+\frac{1}{a^2r_e^2}\left(l+\tfrac{D-3}{2}\right)\left(l+\tfrac{D-1}{2}\right)\left[-\frac{1}{ar_e}+\frac{3}{a^2r_e^2}\right] \quad (38)$$

Here D is the dimension of space and therefore the energy spectrum in three-dimension will be

$$E=\frac{\hbar^2}{2mr_e^2}l\left(l+1\right)\left[1-\frac{3}{ar_e}+\frac{3}{ar_e^2}\right]-\frac{\hbar^2a^2}{2m}\left[\frac{\beta}{2\sqrt{\gamma}}-n-\frac{1}{2}\right] \quad (39)$$

And in two-dimension will be

$$E=\frac{\hbar^2}{2mr_e^2}\left(l^2-\tfrac{1}{4}\right)\left[1-\frac{3}{ar_e}+\frac{3}{ar_e^2}\right]-\frac{\hbar^2a^2}{2m}\left[\frac{\beta}{2\sqrt{\gamma}}-n-\frac{1}{2}\right] \quad (40)$$

Let us now find the corresponding wavefunction of the Morse potential. A simple calculation reveals that $\varphi(z)$ can be calculated by recalling Eq. (10) and submitting the $\sigma(z)=z$ and the $\pi(z)=-\sqrt{\gamma}z+\sqrt{\alpha}$, then;

$$\varphi(z)=z^{\sqrt{\alpha}}e^{-\sqrt{\gamma}z} \quad (41)$$

which is one of the separable parts of the wave function $\psi(z)=\phi(z)y(z)$. The polynomial solution of the hyper geometric-type function $y_n(z)$ depends on the determination of the weight function $\rho(z)$ ($\left[\sigma(z)\rho(z)\right]'=\tau(z)\rho(z)$). Thus, $\rho(z)$ is calculated as

$$\rho(z)=z^{2\sqrt{\alpha}}e^{-2\sqrt{\gamma}z}. \quad (42)$$

Substituting Eq. (42) into the Rodrigues' formula given in Eq. (13), the other separable part of the wavefunction $\psi(z)$ is given in the following form

$$y(z)=B_nz^{-2\sqrt{\alpha}}e^{2\sqrt{\gamma}z}\frac{d^n}{dz^n}\left[z^{n+2\sqrt{\alpha}}e^{-2\sqrt{\gamma}z}\right] \quad (43)$$

The polynomial solution of $y_n(z)$ in Eq. (43) is expressed in terms of the associated Laguerre

Polynomials, which is one of the orthogonal polynomials, that is

$$y(z) = L_n^{2\sqrt{\alpha}}(2\sqrt{\gamma}z) \tag{44}$$

Combining the Laguerre polynomials and $\varphi(z)$ in Eq. (41), the radial wave functions are constructed as

$$\psi(z) = N_{n,l} z^{\sqrt{\alpha}} e^{-\sqrt{\gamma}z} L_n^{2\sqrt{\alpha}}(2\sqrt{\gamma}z) \tag{45}$$

where $N_{n,l}$ is the normalization constant.

5 Conclusions

We have presented an approximation for the Morse potential which leads to analytic calculations for the energy spectrums and wave functions. In these calculations, we have used a new method which is developed by Nikiforov–Uvarov and applied the Pekeris approximation. Our main results are summarized in Eqs. (39) and (45). This new method is used to solve a D-dimension Schrodinger equation and through that we get the solution of 3-dimension Schrodinger equation. It also gives us the energy spectrum and wave function of 2-dimensional Schrodinger equation, which can be considered as a solution of the Schrodinger equation in cylindrical coordinates.

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