



Pekeris approximation – another perspective



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ABSTRACT

Inspired on the Pekeris approximation for the centrifugal term, we elaborate a method of resolution for the Schrödinger equation subject to a potential $V(r)$ of a form more general than the exponential one. Generalizing the Pekeris approximation, we solve the Schrödinger equation with Rosen–Morse and Manning–Rosen potentials including the centrifugal term. The bound state energy eigenvalues for these potentials and for arbitrary values of n and l quantum numbers are presented.

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1. Introduction

In the last decade a large community of researchers have been involved a search of approximate solutions for wave equations (non-relativistic or relativistic) including the centrifugal term and subject to different potential functions $V(r)$. The main characteristic of these solutions lies in the substitution of the centrifugal term by an approximation, so that one can obtain an equation, normally hypergeometric, which is solvable.

Indeed, C.L. Pekeris [1] is the pioneer in the study, since, he managed to obtain analytic solutions for the radial Schrödinger equation with the Morse potential [2], through an expansion for the centrifugal term. For many molecules, the results obtained for the spectroscopic constant α_e were in excellent agreement with the experimental values.

Approximately forty years later, Greene and Aldrich [3] proposed another approximation for the centrifugal term, able to solve the Schrödinger equation. Using variational methods for the Hulthén potential [4], they obtained the energy levels for the states $2p$, $3p$, $3d$, $4p$, $4d$ and $4f$, in excellent agreement with the results of more elaborate methods [5].

Since then, most of the approximations proposed for the centrifugal term (generally, for potentials of the exponential type) were some variants of the approximations proposed by Pekeris, Greene and Aldrich. In particular, making use of an approximation very similar to those elaborated by Pekeris, Greene and Aldrich, bound state and scattering state solutions for the Schrödinger equation subject to the Manning–Rosen potential [6] was obtained

in [7–12] and [13,14], correspondingly, and through of the proper quantization rule in [15,16]. In the relativistic framework, the same kind of approximation for the centrifugal term was used in [17,18] to obtain solutions of the Dirac equation. Bound-state solutions of the Klein–Gordon equation have been studied in [19,20]. Analytical solutions for the Schrödinger equation and Dirac equation including the centrifugal term subject to Rosen–Morse potential [21] were obtained in [22] and [23,24], respectively.

The approximations proposed by Pekeris, Greene and Aldrich for the centrifugal term, as well as their modifications, have made it possible to find good results and represent a significant improvement. However, these approaches have been applied to a relatively narrow class allowed us treat of potential functions $V(r)$ of an exponential type. Moreover, in some cases, the approximation used for the centrifugal term is not convenient because it does not provide physically reasonable wave functions [13,22,25,26].

In the present Letter, we propose a generalization of the Pekeris approximation [1] for the centrifugal term, allowing potential functions of more general form to be treated. It provides physically reasonable wave functions.

The Letter is organized as follows. In Section 2, we present the generalized approximation for the centrifugal term, and discuss its role as head gear for the development of the new resolution method. In Sections 3 and 4 we solve the radial Schrödinger equation with Manning–Rosen and Rosen–Morse potentials and with a centrifugal term. The conclusions are given in Section 5.

2. General procedure

Observing closely the Pekeris approximation [1] for the centrifugal term

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$$\begin{aligned} \left(\frac{r_e}{r}\right)^2 &= \left(1 - \frac{\ln y}{ar_e}\right)^{-2} \\ &= 1 + \frac{2}{ar_e}(y-1) + \frac{1}{2!} \left[\frac{6}{(ar_e)^2} - \frac{2}{ar_e} \right] (y-1)^2 + \dots, \end{aligned} \quad (1)$$

where $y = \exp[-a(r-r_e)]$, r_e is the internuclear distance at equilibrium, and a is related to the potential range. We are going to show that it is possible to perform a generalization for the expansion (1) through an appropriate redefinition of the variable y .

Consider the function

$$F(y) = \left(\frac{r_e}{r}\right)^m = \left(1 \pm \frac{f^{-1}(y)}{ar_e}\right)^{-m}, \quad (2)$$

where $y = f[\pm a(r-r_e)]$, f and its inverse f^{-1} being analytical functions to be defined, a and r_e are the physical constants previously defined, and m a real number. The particular cases

$$\begin{aligned} F(y) &= \left(\frac{r_e}{r}\right)^2 = \left(1 + \frac{f^{-1}(y)}{ar_e}\right)^{-2}, \\ &\text{with } y = f[a(r-r_e)], \end{aligned} \quad (3)$$

and

$$\begin{aligned} F(y) &= \left(\frac{r_e}{r}\right)^2 = \left(1 - \frac{f^{-1}(y)}{ar_e}\right)^{-2}, \\ &\text{with } y = f[-a(r-r_e)], \end{aligned} \quad (4)$$

has physical importance and we will treat them in this work.

The Taylor expansion series for the function (3) or (4), is given by

$$F(y) = \sum_{n=0}^{\infty} c_n (y-\alpha)^n \quad \text{with } c_n = \frac{1}{n!} \left. \frac{d^n F(y)}{dy^n} \right|_{y=\alpha}. \quad (5)$$

Clearly we can realize that the expansion for the centrifugal term (1) proposed by Pekeris, can be obtained through (5) with $\alpha = 1$ and $y = \exp[-a(r-r_e)]$, the coefficients c_n can be obtained by (5) taking $F(y)$ in (4) with $f^{-1}(y) = \ln y$. The chosen value of $\alpha = 1$ isn't random, this value assures that the coefficients c_n will be calculated at $r = r_e$, since $\ln y = -a(r-r_e)$, being $y = \exp[-a(r-r_e)]$, then $\ln 1 = -a(r-r_e)$ leads to $r = r_e$, and belong to domain of the function $f^{-1}(y) = \ln y$.

Considering terms until $n = 2$ in (5), we have that

$$\begin{aligned} F(y) &= \left(\frac{r_e}{r}\right)^2 \approx c_0 + (y-\alpha)c_1 + \frac{c_2}{2!}(y-\alpha)^2 \\ &\approx c_0 - \alpha c_1 + \frac{\alpha^2}{2}c_2 + (c_1 - \alpha c_2)y + \frac{c_2}{2}y^2, \end{aligned} \quad (6)$$

substituting the approximation (6) into the radial Schrödinger equation

$$\frac{d^2 R}{dr^2} + \frac{2\mu}{\hbar^2} (E - V(r))R - \frac{l(l+1)}{r_e^2} \left(\frac{r_e}{r}\right)^2 = 0, \quad (7)$$

where E is the energy, μ is the reduced mass, $V(r)$ is an arbitrary potential, and $\Psi(r, \theta, \phi) = Y_l^m(\theta, \phi)R(r)/r$, we obtain

$$\frac{d^2 R}{dr^2} + \frac{2\mu}{\hbar^2} (W - V_{ef})R = 0 \quad (8)$$

with

$$W = E - \frac{l(l+1)\hbar^2}{2\mu r_e^2} \left(c_0 - \alpha c_1 + \frac{\alpha^2}{2} c_2 \right) \quad (9)$$

the renormalized energy, and

$$V_{ef} = V(r) + \frac{l(l+1)\hbar^2}{2\mu r_e^2} \left[(c_1 - \alpha c_2)y + \frac{c_2}{2}y^2 \right] \quad (10)$$

the effective potential.

In the case treated by Pekeris in [1] Eq. (7) with the Morse potential

$$\begin{aligned} \frac{d^2 R}{dr^2} + \frac{2\mu}{\hbar^2} (E - D_e \exp[-2a(r-r_e)] \\ + 2D_e \exp[-a(r-r_e)])R - \frac{l(l+1)}{r_e^2} \left(\frac{r_e}{r}\right)^2 R \\ = 0, \end{aligned} \quad (11)$$

after the substitution of approximation (1) with only the first three terms, has the form

$$\begin{aligned} \frac{d^2 R}{dr^2} + \frac{2\mu}{\hbar^2} \left[E - c + \frac{(2D_e - c_1)}{\exp[a(r-r_e)]} - \frac{(D_e - c_2)}{\exp[2a(r-r_e)]} \right] R \\ = 0, \end{aligned} \quad (12)$$

the renormalized energy is given by

$$W = E - A \left[1 - \frac{3}{ar_e} + \frac{3}{(ar_e)^2} \right], \quad \text{with } A = \frac{l(l+1)\hbar^2}{2\mu r_e^2},$$

and the effective potential

$$V_{ef} = (D_e - c_2) \exp[-2a(r-r_e)] - (2D_e - c_1) \exp[-a(r-r_e)],$$

being

$$\begin{aligned} c &= A - \frac{3A}{ar_e} + \frac{3A}{(ar_e)^2}, \quad c_1 = \frac{4A}{ar_e} - \frac{6A}{(ar_e)^2}, \quad \text{and} \\ c_2 &= \frac{3A}{(ar_e)^2} - \frac{A}{ar_e}, \end{aligned}$$

Eq. (12) is very similar to the equation obtained by Morse in [2] with ($l=0$).

In short, we will establish now the steps which will lead us to solve Eq. (7), subjected to a potential function $V(r)$ using the approximation (6), they are:

1. Given the potential function $V(r)$ in Eq. (7), we must define the function f in the general expression (3) or (4). The function f has to be chosen in such a way that, after the substitution of the approximation (6) in (7), the terms of the expression (6) to be absorbed by $V(r)$ generating a solvable effective potential V_{ef} .
2. With the choice of the functions f , we must perform the expansion in Taylor (or Maclaurin) series, keeping the terms until $n = 2$ in (5). The value chosen for α must belong to the domain of the inverse function f^{-1} .
3. After replacement of the approximation (6) into Eq. (7), the constant terms in the expansion (6) are absorbed in the expression for the renormalized energy W in (9) while the other terms are absorbed by the effective potential V_{ef} in the expression (10). So, the new Schrödinger equation obtained in (8) can be resolved by the same method used in the treatment of Eq. (7) without the centrifugal term (i. e., the equation for $l=0$).

In the following section we solve Eq. (7) with the Rosen-Morse and Manning-Rosen potentials. We will demonstrate that the wave function obtained possesses the same form that the solution of radial Schrödinger equation (7) with ($l=0$), i.e., disregarding the centrifugal term, as Pekeris has already pointed out in [1].

3. Rosen–Morse potential

The potential proposed by Rosen and Morse [21], in their study of the vibrational states of polyatomic molecules, with a special application for the molecule of ammonia, has the form

$$V(r) = B \tanh\left(\frac{r - r_e}{d}\right) - C \operatorname{sech}^2\left(\frac{r - r_e}{d}\right), \quad (13)$$

where B and C are the depth of the potential $1/d$ the range of the potential, and r_e equilibrium internuclear distance.

In [27] an equivalence was established of the Wei potential model and Tietz potential model for standard Morse, Rosen–Morse and Manning–Rosen potentials, when the parameter h in the Tietz potential has some special values. By employing the dissociation energy and the equilibrium bond length for a diatomic molecule as explicit parameters, in [28] improved expressions were generated for both versions of the Schiöberg potential energy function, which are the Rosen–Morse and Manning–Rosen potential functions.

Eq. (7) with the potential (13) is given by

$$\frac{d^2R}{dz^2} + \frac{2\mu d^2}{\hbar^2} (E - B \tanh z + C \operatorname{sech}^2 z) R - \frac{l(l+1)d^2}{r_e^2} \left(\frac{r_e}{r}\right)^2 R = 0, \quad (14)$$

where $z = (r - r_e)/d$.

According to the method described in the previous section, we must choose appropriate functions f and f^{-1} . So, let us consider $y = \tanh[(r - r_e)/d]$ and $f^{-1}(y) = \tanh^{-1} y$. Substituting this functions into (3), with $a = 1/d$, we obtain the following identity

$$\left(\frac{r_e}{r}\right)^2 = \left(1 + \frac{d \tanh^{-1} y}{r_e}\right)^{-2}.$$

The approximation (6) has the form

$$\left(\frac{r_e}{r}\right)^2 \approx c_0 - \alpha c_1 + \frac{c_2}{2} + \frac{\alpha^2}{2} c_2 + (c_1 - \alpha c_2) \tanh z - \frac{c_2}{2} \operatorname{sech}^2 z, \quad (15)$$

and the coefficients (5), with $n = 0, 1, 2$ are

$$\begin{aligned} c_0 &= \left(\frac{r_e + d \tanh^{-1} \alpha}{r_e}\right)^{-2}, \\ c_1 &= -\frac{2dr_e^2 (r_e + d \tanh^{-1} \alpha)^{-3}}{(1 - \alpha^2)}, \quad \text{and} \\ c_2 &= -\frac{4d\alpha r_e^2 (r_e + d \tanh^{-1} \alpha)^{-3}}{(1 - \alpha^2)^2} \\ &\quad + \frac{6(dr_e)^2 (r_e + d \tanh^{-1} \alpha)^{-4}}{(1 - \alpha^2)^2}, \end{aligned} \quad (16)$$

with α being a number limited to interval $|\alpha| < 1$, the domain of the function $f^{-1}(y) = \tanh^{-1} y$.

Substituting (15) into (14), we have that

$$\frac{d^2R}{dz^2} + (-W - \beta \tanh z + \gamma \operatorname{sech}^2 z) R = 0, \quad (17)$$

where

$$-W = \frac{2E\mu d^2}{\hbar^2} - \frac{l(l+1)d^2}{r_e^2} \left(c_0 - \alpha c_1 + \frac{c_2}{2} + \frac{\alpha^2}{2} c_2\right) \quad (18)$$

is the renormalized energy, and

$$V_{ef} = \beta \tanh z - \gamma \operatorname{sech}^2 z \quad (19)$$

is the effective potential, with

$$\begin{aligned} \beta &= \frac{2\mu B d^2}{\hbar^2} + \frac{l(l+1)d^2}{r_e^2} (c_1 - \alpha c_2) \quad \text{and} \\ \gamma &= \frac{2\mu C d^2}{\hbar^2} + \frac{l(l+1)d^2}{2r_e^2} c_2, \end{aligned} \quad (20)$$

being the renormalized coefficients of effective potential (19).

Eq. (17) is essentially the equation obtained by Rosen and Morse [21] for the case $l = 0$, but the coefficients β and γ are renormalized according to (20).

Following Rosen and Morse [21], we introduce the function $F(z)$ by $R(z) = e^{az} \cosh^{-b} z F(z)$, and, replacing it into Eq. (17), we obtain

$$\begin{aligned} \frac{d^2F}{dz^2} + 2(a - b \tanh z) \frac{dF}{dz} + (a^2 + b^2 - W) F(z) \\ - (2ab - \beta) \tanh z F(z) + [\gamma - a(b+1)] \operatorname{sech}^2 z F(z) \\ = 0. \end{aligned} \quad (21)$$

Imposing the conditions

$$2ab = \beta \quad \text{and} \quad a^2 + b^2 = W, \quad (22)$$

which can be satisfied if

$$\begin{aligned} a &= \frac{[(W - \beta)^{1/2} - (W + \beta)^{1/2}]}{2} \quad \text{and} \\ b &= \frac{[(W + \beta)^{1/2} + (W - \beta)^{1/2}]}{2}, \end{aligned} \quad (23)$$

one puts Eq. (21) into the form

$$\frac{d^2F}{dz^2} + 2(a - b \tanh z) \frac{dF}{dz} + [\gamma - b(b+1)] \operatorname{sech}^2 z F(z) = 0. \quad (24)$$

Then, performing the change of variables $u = \frac{1}{2}(1 + \tanh z)$ in (24), we obtain the hypergeometric equation

$$\begin{aligned} u(1-u) \frac{d^2F}{du^2} + [a+b+1 - 2(b+1)u] \frac{dF}{du} \\ + [\gamma - b(b+1)] F(u) \\ = 0, \end{aligned} \quad (25)$$

having as solution the hypergeometric function $F(u) = {}_2F_1(\zeta, \eta, \kappa, u)$ given by

$$F(u) = 1 + \frac{\zeta \cdot \eta}{1 \cdot \kappa} u + \frac{\zeta(\zeta+1)\eta(\eta+1)}{1 \cdot 2 \cdot \kappa(\kappa+1)} u^2 + \dots, \quad (26)$$

with parameters:

$$\begin{aligned} \zeta &= b + \frac{1}{2} - \left(\gamma + \frac{1}{4}\right)^{1/2}, \\ \eta &= b + \frac{1}{2} + \left(\gamma + \frac{1}{4}\right)^{1/2}, \quad \text{and} \quad \kappa = a + b + 1. \end{aligned} \quad (27)$$

It is clear from the definition (26) of the hypergeometric function that the parameter κ should never vanish or take a negative integer value. On the other hand, if some of the parameters ζ and η is equal to zero or to a negative integer, the series (26) will be truncated and the hypergeometric function will become a polynomial, according to [29]. So, if $\zeta = -n$, where $n = 0, 1, 2, \dots$, Eq. (27) for ζ leads to

$$b = \left(\gamma + \frac{1}{4}\right)^{1/2} - n - \frac{1}{2},$$

and from the first condition in (22) we can obtain the other constant a under the form

$$a = -\frac{\beta}{(4\gamma + 1)^{1/2} - 2n - 1}.$$

The allowed values for the energy are given through the second condition in (22) and the value for the renormalized energy (18), then

$$-E_n = \frac{(\beta\hbar)^2}{2\mu d^2[(4\gamma + 1)^{1/2} - 2n - 1]^2} + \frac{\hbar^2}{2\mu d^2} \left[\left(\gamma + \frac{1}{4}\right)^{1/2} - n - \frac{1}{2} \right]^2 - \frac{l(l+1)\hbar^2}{2\mu r_e^2} \left(c_0 - \alpha c_1 + \frac{c_2}{2} + \frac{\alpha^2}{2} c_2 \right). \tag{28}$$

The radial wavefunction is

$$R_n(z) = \sum_{n=0}^{\infty} N_n e^{az} \cosh^{-b} z {}_2F_1 \left[-n, \eta, \kappa, \frac{1}{2}(1 + \tanh z) \right],$$

and the normalization constant N_n will be calculated through the integral

$$d|N_n|^2 \int e^{2az} \cosh^{-2b} z \left({}_2F_1 \left[-n, \eta, \kappa, \frac{1}{2}(1 + \tanh z) \right] \right)^2 dz = 1. \tag{29}$$

Using the result of [30] for the integral (29), we have that the normalization constant is

$$N_n = \frac{d^{-1/2}}{2^{b-1/2}} \left[\frac{(\lambda + 1)\Gamma(n + k + 1)\Gamma(n + k + \lambda + 2)}{\Gamma(k + 1)^2\Gamma(n + \lambda + 2)} \right]^{1/2}, \tag{30}$$

being $k = a + b - 1$ and $\lambda = b - a - 1$.

4. Manning–Rosen potential

Let us consider the potential proposed by Manning and Rosen in [6]

$$V(r) = \frac{\hbar^2}{2\mu d^2} \left[\frac{\beta(\beta - 1) \exp[-2(r - r_e)/d]}{(1 - \exp[-(r - r_e)/d])^2} - \frac{A \exp[-(r - r_e)/d]}{1 - \exp[-(r - r_e)/d]} \right] \tag{31}$$

where A and β are dimensionless parameters, while d characterizes the range of the potential and has dimension of length, and r_e equilibrium internuclear distance.

It was determined in [31] that the Manning–Rosen potential, Schiöberg and Deng–Fan potential are the same solvable empirical potential energy function for diatomic molecules. Some values for the anharmonicity $\omega_e x_e$ and vibrational rotational coupling parameter α_e for 16 molecules have been calculated by choosing the experimental values of the dissociation energy D_e , equilibrium bond length r_e and vibrational frequency ω_e as inputs.

The potential (31) can also be written as

$$V(r) = \frac{\beta(\beta - 1)\hbar^2}{8\mu d^2} \operatorname{cosech}^2 \left[\frac{(r - r_e)}{2d} \right] - \frac{\nu\hbar^2}{2\mu d} \coth \left[\frac{(r - r_e)}{2d} \right] + \frac{\nu\hbar^2}{2\mu d} \tag{32}$$

according to Infeld and Hull in [32], with $\nu = [A + \beta(\beta - 1)]/2d$.

Substituting the potential (32) into Eq. (7), with $z = (r - r_e)/2d$, we have that

$$\frac{d^2 R}{dz^2} + \left[\frac{8\mu d^2}{\hbar^2} E - 4d\nu - 4d\nu \coth z - \beta(\beta - 1) \operatorname{cosech}^2 z - \frac{4l(l+1)d^2}{r_e^2} \left(\frac{r_e}{r} \right)^2 \right] R = 0. \tag{33}$$

Defining the functions $y = \coth[(r - r_e)/2d]$ and $f^{-1}(y) = \coth^{-1} y$ in (3), with $a = 1/2d$, we obtain the identity

$$\left(\frac{r_e}{r} \right)^2 = \left(1 + \frac{2d \coth^{-1} y}{r_e} \right)^{-2}.$$

The approximation (6) takes the form

$$\left(\frac{r_e}{r} \right)^2 \approx c_0 - \alpha c_1 + \frac{\alpha^2}{2} c_2 + \frac{c_2}{2} + (c_1 - \alpha c_2) \coth z + \frac{c_2}{2} \operatorname{cosech}^2 z, \tag{34}$$

with the coefficients

$$c_0 = \left(\frac{r_e + 2d \coth^{-1} \alpha}{r_e} \right)^{-2},$$

$$c_1 = -\frac{4d(r_e + 2d \coth^{-1} \alpha)^{-3}}{r_e^{-2}(1 - \alpha^2)}, \text{ and}$$

$$c_2 = -\frac{8d\alpha(r_e + 2d \coth^{-1} \alpha)^{-3}}{r_e^{-2}(1 - \alpha^2)^2} + \frac{24d^2(r_e + 2d \coth^{-1} \alpha)^{-4}}{r_e^{-2}(1 - \alpha^2)^2},$$

being α a number in the interval $|\alpha| > 1$ (the domain of the function $f^{-1}(y) = \coth^{-1} y$).

Substituting (34) into Eq. (33), we obtain

$$\frac{d^2 R}{dz^2} + (-W - B \coth z - A \operatorname{cosech}^2 z) R = 0, \tag{35}$$

with the renormalized energy

$$W = -\frac{8\mu d^2 E}{\hbar^2} + 4d\nu + \frac{4l(l+1)d^2}{r_e^2} \left(c_0 - \alpha c_1 + \frac{\alpha^2}{2} c_2 + \frac{c_2}{2} \right), \tag{36}$$

and the effective potential

$$V_{ef} = B \coth z + A \operatorname{cosech}^2 z, \tag{37}$$

being

$$A = \beta(\beta - 1) + \frac{4l(l+1)d^2}{r_e^2} c_2 \text{ and}$$

$$B = -4d\nu + \frac{4l(l+1)d^2}{r_e^2} (c_1 - \alpha c_2)$$

the renormalized coefficients of the effective potential (37).

Introducing the function $F(z)$ in (35) by mean $R(z) = e^{az} \sinh^{-b} z F(z)$, we obtain

$$\frac{d^2 F}{dz^2} + 2(a - b \coth z) \frac{dF}{dz} + (a^2 + b^2 - W) F(z) - \coth z (2ab - B) F(z) + [b(b + 1) - A] \operatorname{cosech}^2 z F(z) = 0. \tag{38}$$

Imposing the same conditions (22) and (23) as in the previous section, Eq. (38) reduces to

$$\frac{d^2 F}{dz^2} + 2(a - b \coth z) \frac{dF}{dz} + [b(b + 1) - A] \operatorname{cosech}^2 z F(z) = 0. \tag{39}$$

Now let $u = \frac{1}{2}(1 - \coth z)$, from this transformation Eq. (39) becomes the hypergeometric equation

$$u(1-u)\frac{d^2F}{du^2} + [-a+b+1-2(b+1)u]\frac{dF}{du} - [b(b+1)-A]F(u) = 0, \tag{40}$$

with solution given by (26) having parameters

$$\zeta = b + \frac{1}{2} - \left(A + \frac{1}{4}\right)^{1/2},$$

$$\eta = b + \frac{1}{2} + \left(A + \frac{1}{4}\right)^{1/2}, \quad \text{and} \quad \kappa = -a + b + 1. \tag{41}$$

As in the previous section, if $\zeta = -n$ Eq. (41) for ζ leads to

$$b = \left(A + \frac{1}{4}\right)^{1/2} - n - \frac{1}{2},$$

and, using the first condition in (22), we obtain

$$a = -\frac{B}{(4A+1)^{1/2} - 2n - 1}.$$

From the second condition in (22) and the expression for the renormalized energy (36), we obtain the energy spectrum

$$-E_n = \frac{(\hbar B)^2}{8\mu d^2[(4A+1)^{1/2} - 2n - 1]^2} + \frac{\hbar^2}{8\mu d^2} \left[\left(A + \frac{1}{4}\right)^{1/2} - n - \frac{1}{2} \right]^2 - \frac{l(l+1)\hbar^2}{2\mu r_e^2} \left(c_0 - \alpha c_1 + \frac{\alpha^2}{2} c_2 + \frac{c_2}{2} \right) - 2[A + \beta(\beta - 1)]. \tag{42}$$

The solution of Eq. (35) is the wave function

$$R_n(z) = \sum_{n=0}^{\infty} N_n e^{az} \sinh^{-b} z {}_2F_1\left(-n, \eta, \kappa, \frac{1}{2}(1 - \coth z)\right), \tag{43}$$

where the constant N_n is obtained from the normalization condition [30]

$$d|N_n|^2 \int e^{2az} \sinh^{-2b} z \left({}_2F_1\left[-n, \eta, \kappa, \frac{1}{2}(1 - \coth z)\right] \right)^2 dz = 1, \tag{44}$$

of the same form that in the previous sections, with $k = -a + b - 1$ and $\lambda = a + b - 1$, we have that the normalization constant will have the form

$$N_n = \frac{(-1)^{a-b-1}}{2^{b-1/2} d^{1/2}} \left[\frac{(\lambda+1)\Gamma(n+k+1)\Gamma(n+k+\lambda+2)}{\Gamma(k+1)^2\Gamma(n+\lambda+2)} \right]^{1/2}. \tag{45}$$

Mathematically nothing prevents us of use the expansion (5) with $n > 2$, this will depend on the particular shape of the potential $V(r)$ to be treated. For the potentials studied here, we could use any value of $n > 2$, as long as we eliminate the terms of order greater than y^2 , in the approximation (15) for Rosen–Morse potential and in the approximation (34) for Manning–Rosen potential.

The way as the method was developed in Section 2 requires α to be in the domain of the function f^{-1} . Due to this condition it would not always be possible to choose $r = r_e$ as the expansion point in the series (5).

In the case of Rosen–Morse potential if $\alpha = 0$ in (15), and using the fact that $\tanh y^{-1} = a(r - r_e)$, with $y = \tanh[a(r - r_e)]$, then $\tanh^{-1} 0 = a(r - r_e)$ lead us $r = r_e$. For this case the coefficients (16) in the approximation (15) can be estimated at $r = r_e$, so

$$\left(\frac{r_e}{r}\right)^2 \approx 1 + \frac{3d^2}{r_e^2} - \frac{2d}{r_e} \tanh z - \frac{3d^2}{r_e^2} \operatorname{sech}^2 z,$$

replacing this approximation in Eq. (14) and following the same steps we obtain for the energy spectrum the expression

$$-E_n = \frac{(\beta\hbar)^2}{2\mu d^2[(4\gamma+1)^{1/2} - 2n - 1]^2} + \frac{\hbar^2}{2\mu d^2} \left[\left(\gamma + \frac{1}{4}\right)^{1/2} - n - \frac{1}{2} \right]^2 + \frac{l(l+1)\hbar^2}{2\mu r_e^2} \left(1 + \frac{3d^2}{r_e^2} \right)$$

with the constants β and γ is given by

$$\beta = \frac{2\mu B d^2}{\hbar^2} - \frac{2l(l+1)d^3}{r_e^3} \quad \text{and} \quad \gamma = \frac{2\mu C d^2}{\hbar^2} + \frac{3l(l+1)d^4}{r_e^4}.$$

On the other side, for the Manning–Rosen potential isn't possible calculate the series (34) at $r = r_e$, the function $f^{-1}(y) = \coth^{-1} y$ hasn't the number zero in its image, i.e, there is no α such that $\coth^{-1} \alpha = a(r - r_e) = 0$.

5. Conclusion

In this Letter we propose a generalization to the centrifugal term, based on the Pekeris approximation, able to solve the Schrödinger equation with a potential $V(r)$ having a more general form. The eigenvalues for the bound state quantum number n and l were found to potential Rosen–Morse and Manning–Rosen. The wave functions obtained have the same form as in the case $l = 0$, but with renormalized values of the parameters.

From the expressions obtained for the energy (28) and (42), we can see that the value of α , which can be any number belonging to domain of the function f^{-1} in (3) or (4), can become a parameter correction for the energy spectrum, and its influence should be studied case by case.

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