Pekeris-type approximation for the $l$-wave in a Pöschl-Teller potential

Stoian I. Zlatev
Departamento de Física - CCET,
Universidade Federal de Sergipe
Av. Marechal Rondon, s/n, Jardim Rosa Elze
CEP 49100-000 - São Cristóvão/SE, Brasil

November 25, 2013

Abstract
An approximation for the centrifugal term which transforms the radial equation for a particle in a Pöschl-Teller potential into an exactly solvable approximate equation is proposed. In contrast to the approximations known in the literature, the new one can be used with the most general form of the central Pöschl-Teller potential. An approximate expression for the bound-state spectrum is obtained.

1 Introduction

The Pöschl-Teller functions [1] are among the one-dimensional potentials for which the discrete spectrum of the quantum-mechanical Hamiltonian is known, as well as the eigenfunctions [2]. Attracting less attention than Morse potential or Hulburt-Hirschfelder potential, the second Pöschl-Teller function has been successfully used for the description of the vibrational and rotational motion of diatomic molecules [3, 4].

A standard separation of variables reduces the bound-state problem for a particle in a Pöschl-Teller potential to an one-dimensional eigenvalue problem but the exact solutions of the latter are not known for non-zero values of the azimuthal quantum number $l$. A suitable approximation for the centrifugal term in the radial equation transforms the eigenvalue problem into one that can be solved analytically [5, 6, 7]. The approximations used are the Greene-Aldrich one [8] or its modifications [9, 10]. They lead to exactly solvable approximate equations only if one of the parameters in the Pöschl-Teller function, namely the parameter $r_0$ in eq. (1), is set equal to zero.

*Email address: zlatev@ufs.br
The aim of the present letter is to propose a new approximation for the centrifugal term that leads to an exactly solvable one-dimensional eigenvalue problem for the most general form of the Pöschl-Teller potential.

2 The Schrödinger equation with a Pöschl-Teller potential

In the Born-Oppenheimer approximation, the vibrational and rotational motion of a diatomic molecule is governed by a one-particle Hamiltonian

\[ H = -\frac{\hbar^2}{2M} \nabla^2 + V(r), \]

where \( M \) is the system reduced mass and the central potential \( V(r) \) satisfies some general requirements listed by Morse [11]. The second Pöschl-Teller potential [1],

\[ V(r) = \frac{A}{\sinh^2 \alpha (r - r_0)} - \frac{B}{\cosh^2 \alpha (r - r_0)}, \tag{1} \]

where the parameters \( A, B, \alpha \) are positive and \( r_0 \) is non-negative, satisfies all the requirements if \( A < B \), which we assume in the sequel. In this case, the potential has a minimum at

\[ r_e = r_0 + \frac{1}{\alpha} \text{artanh} \sqrt{\frac{A}{B}}. \tag{2} \]

The radial equation, obtained after the separation of the variables \( \psi(r, \theta, \phi) = r^{-l}R(r)Y(\theta, \phi) \), can be written as

\[ \frac{d^2 R}{dr^2} + \left[ -\alpha^2 \left( \frac{\nu(\nu - 1)}{\sinh^2 \alpha (r - r_0)} - \frac{\mu(\mu + 1)}{\cosh^2 \alpha (r - r_0)} \right) - \frac{l(l + 1)}{r^2} + \epsilon \right] R = 0, \tag{3} \]

where \( \epsilon \) is a spectral parameter related to the energy in an obvious way, \( l \) is the azimuthal quantum number and the parameters \( A \) and \( B \) have been changed for the positive solutions \( \nu \) and \( \mu \) of the equations

\[ \alpha^2 \nu(\nu - 1) = \frac{2M}{\hbar^2} A, \quad \alpha^2 \mu(\mu + 1) = \frac{2M}{\hbar^2} B. \tag{4} \]

For \( l = 0 \), the square-integrable solutions (on the interval \( r > r_0 \)) of eq. (3) are known and can be expressed in terms of elementary functions [2]. The number of the eigenvalues is finite and they are given by

\[ \epsilon_n = -\alpha^2 (\mu - \nu - 2n)^2, \quad n = 0, 1, \ldots < \frac{\mu - \nu}{2}. \tag{5} \]
The exact eigenvalues for \( l > 0 \) are not known, neither is known the exact form of the corresponding eigenfunctions. Therefore, it is natural to look for a suitable approximating function for the centrifugal term

\[
\frac{l(l+1)}{r^2} = \frac{l(l+1)}{r_e^2} \left( \frac{r_e}{r} \right)^2,
\]

which, replacing the centrifugal term in (3), yields an exactly solvable approximate equation.

3 Approximations for the centrifugal term used in the case \( r_0 = 0 \)

Such approximations have been proposed [6, 5, 7, 10] for the case when the adjustable parameter \( r_0 \) in the Pöschl-Teller function is set equal to zero. The approximation

\[
\frac{1}{r^2} \approx F_1(r, \alpha) = 4\alpha^2 \frac{e^{-2\alpha r}}{(1 - e^{-2\alpha r})^2} = \frac{\alpha^2}{\sinh^2(\alpha r)}
\]

introduced by Greene and Aldrich [8] has been used in Ref. [5] while an improved approximation [9]

\[
\frac{1}{r^2} \approx F_2(r, \alpha) = 4\alpha^2 \left[ \frac{1}{12} + \frac{e^{-2\alpha r}}{(1 - e^{-2\alpha r})^2} \right] = \frac{\alpha^2}{\sinh^2(\alpha r)} + \frac{\alpha^2}{3}
\]

has been used in Refs. [6, 7]. Both the approximations, and, especially, the improved one, are good “for small values of the parameter \( \alpha \)” [12], or, in other words, they are good approximations for the function \( 1/r^2 \) in the region \( r \lesssim \alpha^{-1} \). In the range where the centrifugal term “has any appreciable effect” [11], \( r - r_e \) is small, but not necessarily \( r \).

In the improved approximation (8), a quantity corresponding to the constant term in the Laurent expansion

\[
\frac{1}{\sinh^2 z} = \frac{1}{z^2} - \frac{1}{3} + \ldots
\]

is subtracted. This results in an improvement for small values of \( r \) at the price of a discrepancy for large values of \( r \) since \( F_2(r, \alpha) \rightarrow \alpha^2/3 \neq 0 \) when \( r \) goes to infinity.

The third approximation [10]

\[
\frac{1}{r^2} \approx F_3(r, \alpha) = \frac{\alpha^2}{\sinh^2(\alpha r)} + \frac{t\alpha^2}{\cosh^2(\alpha r)}
\]

replaces the \( r \)-independent term in \( F_2 \) by \( t\alpha^2/\cosh^2(\alpha r) \), where \( t \) is a parameter. For \( t = 1/3 \), the function \( F_3 \) shows the same behavior as \( F_2 \) for small values of \( r \), while the correct limit at infinity is recovered.
These approximations are useful if $r_0 = 0$ in the expression (1). However, the general form of the potential (1) is also of interest. For a large number of diatomic molecules, for example, the appropriate value of the parameter $r_0$ is different from zero [4].

4 A Pekeris-type approximation for the centrifugal term

The Pekeris approximation [13] for the centrifugal term has been successfully applied to the Schrödinger equation with the Morse potential. It has been shown recently [14, 15, 16] that similar schemes can be used with the Manning-Rosen and Rosen-Morse potentials.

A Pekeris-type approximation is based [13, 14, 15, 16] on the expansion of the centrifugal term (6) in powers of $y - y_e$, where $y = f(r)$ is a suitable function of $r$ and $y_e = f(r_e)$. The function $f$ is chosen in such a way that the replacement of the dimensionless quantity $(r_e/r)^2$ in the centrifugal term by the first three terms in the expansion

$$
\left( \frac{r}{r_e} \right)^2 = 1 + c_1 (y - y_e) + c_2 (y - y_e)^2 + O ((y - y_e)^3)
$$

yields an exactly solvable approximate radial equation. The higher order terms can be treated as a perturbation [13].

To obtain an approximation transforming eq. (3) into an exactly solvable approximate equation for any value of the azimuthal quantum number $l$, one can use the linear independence of the terms in the Pöschl-Teller potential (1). Let us put

$$
y = \frac{1}{\sinh^2 \alpha (r - r_0)} + \frac{C}{\cosh^2 \alpha (r - r_0)},
$$

where $C$ is a constant. While $y - y_e$ contains only terms proportional to $\sinh^{-2} \alpha (r - r_0)$, $\cosh^{-2} \alpha (r - r_0)$, and 1, this is not true regarding $(y - y_e)^2$, for any value of $C$. However, for a certain value of $C$, the coefficient $c_2$ in (10) vanishes. Indeed,

$$
c_2 = 1 \frac{d^2}{dy^2} \left( \frac{r_e}{r} \right)^2 \bigg|_{y=y_e}
$$

and the condition $c_2 = 0$ is equivalent to

$$
\left[ \frac{d^2y}{dr^2} + 3 \frac{dy}{dr} \right] \bigg|_{r=r_e} = 0
$$

4
as a simple calculation shows. Calculating the derivatives, substituting them into eq. (11), solving the equation obtained with respect to $C$, and taking into account eq. (2), one gets

$$C = - \left( \frac{b}{a} \right)^4 \frac{\alpha r_e (3b^2 - a^2) - 3ab}{\alpha r_e (3a^2 - b^2) - 3ab},$$

where

$$a = \sqrt[4]{\nu \nu - 1}, \quad b = \sqrt[4]{\mu \mu + 1}.$$ 

Then, calculating

$$c_1 = \frac{d}{dy} \left( \frac{r_e}{r} \right)^2 \bigg|_{y_e} = \frac{a^3 \left[ \alpha r_e (b^2 - 3a^2) + 3ab \right]}{4(\alpha r_e)^2 b(b^2 - a^2)^2},$$

$$y_e = 3 \left( \frac{b^2 - a^2}{a^4} \right)^2 \cdot \frac{\alpha r_e(a^2 + b^2) - ab}{\alpha r_e(b^2 - 3a^2) + 3ab},$$

and substituting it in (10), one obtains

$$\left( \frac{r_e}{r} \right)^2 = 1 + \frac{3}{4} \frac{ab - \alpha r_e(a^2 + b^2)}{(\alpha r_e)^2 ab} + \frac{1}{4(\alpha r_e)^2 (b^2 - a^2)^2} \left[ \frac{a^3}{b} \cdot \frac{3ab + \alpha r_e(b^2 - 3a^2)}{\sinh^2 \alpha (r - r_0)} - \frac{b^3}{a} \cdot \frac{3ab + \alpha r_e(a^2 - 3b^2)}{\cosh^2 \alpha (r - r_0)} \right] + O \left( (y - y_e)^3 \right).$$

5 The bound states

Replacing the function $(r/r_e)^2$ in the centrifugal term by the sum of the first two terms in the expansion (10), one obtains the (approximate) equation

$$\frac{d^2 R}{dr^2} - \alpha^2 \left[ \nu (\nu - 1) + \frac{c_1}{(\alpha r_e)^2} l(l + 1) \right] \frac{\sinh^2 \alpha (r - r_0)}{\cosh^2 \alpha (r - r_0)} R + \left[ \epsilon - \frac{l(l + 1) \nu C}{r_e^2 (1 - c_1 y_e)} \right] R = 0,$$

which has the form of eq. (3) with $l = 0$ and constants $\nu'$, $\mu'$, and $\epsilon'$ given by

$$\nu' (\nu' - 1) = \nu (\nu - 1) + \frac{c_1}{(\alpha r_e)^2},$$

$$\mu' (\mu' + 1) = \mu (\mu + 1) - \frac{c_1 C}{(\alpha r_e)^2},$$

$$\epsilon' = \epsilon - \frac{l(l + 1) \nu C}{r_e^2 (1 - c_1 y_e)}.$$
Solving these equations and substituting the values in the eq. (5), one obtains that the eigenvalues $\epsilon_{nl}$ for the equation (3) with azimuthal quantum number $l$ are (approximately) given by

$$\epsilon_{nl} = -\alpha^2 \left\{ 2 \left( n + \frac{1}{2} \right) \right. \right.$$  

$$+ \sqrt{\frac{1}{4} + a^4 + \frac{a^3 [3ab + \alpha r_e (b^2 - 3a^2)]}{4(\alpha r_e)^4 b(b^2 - a^2)^2} l(l + 1)} \right.$$  

$$- \sqrt{\frac{1}{4} + b^4 + \frac{b^3 [3ab + \alpha r_e (a^2 - 3b^2)]}{4(\alpha r_e)^4 a(b^2 - a^2)^2} l(l + 1)} \right. \right.$$  

$$- \left[ 1 - \frac{3}{4\alpha r_e} \left( \frac{a}{b} + \frac{b}{a} - \frac{1}{\alpha r_e} \right) \right] \frac{l(l + 1)}{(\alpha r_e)^2} \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \right. \r
7 Acknowledgment

The author thanks Flávio Jamil Souza Ferreira for useful discussions.

References

[1] G. Pöschl, E. Teller, Bemerkungen zur Quantenmechanik des anharmonischen Oszillators, Z. Phys. 83 (1933) 143–151.

[2] L. Infeld, T. E. Hull, The factorization method, Rev. Mod. Phys. 23 (1951) 21–68.

[3] M. Davies, Simple potential functions and the hydrogen halide molecules, J. Chem. Phys. 17 (1949) 374–379.

[4] C. L. Beckel, Superiority of Poeschl–Teller potential to that of Morse for diatomic molecules, Journ. Chem. Phys. 27 (1957) 998–1000.

[5] G.-F. Wei, S.-H. Dong, A novel algebraic approach to spin symmetry for Dirac equation with scalar and vector second Pöschl-Teller potentials, Eur. Phys. J. A 43 (2010) 185–190.

[6] Y. Xu, S. He, C.-S. Jia, Approximate analytical solutions of the Klein-Gordon equation with the Pöschl-Teller potential including the centrifugal term, Phys. Scr. 81 (2010) 045001.

[7] S. M. Ikhdair, M. Hamzavi, Approximate Dirac solutions of a complex parity-time-symmetric Pöschl-Teller potential in view of spin and pseudospin symmetries, Phys. Scr. 86 (2012) 045002.

[8] R. L. Greene, C. Aldrich, Variational wave functions for a screened Coulomb potential, Phys. Rev. A (1976) 2363–2366.

[9] C.-S. Jia, T. Chen, L.-G. Cui, Approximate analytical solutions of the Dirac equation with the generalized Pöschl-Teller potential including the pseudo-centrifugal term, Phys. Lett. A 373 (2009) 1621–1626.

[10] Y. You, F.-L. Lu, D.-S. Sun, C.-Y. Chen, S.-H. Dong, Solutions of the second Pöschl-Teller potential solved by an improved scheme to the centrifugal term, Few-Body Syst. 54 (2013) 2125–2132.

[11] P. M. Morse, Diatomic molecules according to the wave mechanics. II. vibrational levels, Phys. Rev. 34 (1929) 57–64.

[12] C.-S. Jia, J.-Y. Liu, P.-Q. Wang, X. Lin, Approximate analytical solutions of the Dirac equation with the hyperbolic potential in the presence of the spin symmetry and pseudo-spin symmetry, Int J. Theor. Phys. 48 (2009) 2633–2643.
[13] C. L. Pekeris, The rotation-vibration coupling in diatomic molecules, Phys. Rev. 45 (1934) 98–103.

[14] G.-F. Wei, S.-H. Dong, Pseudospin symmetry in the relativistic Manning-Rosen potential including a Pekeris-type approximation to the pseudo-centrifugal term, Physics Letters B 686 (2010) 288–292.

[15] G.-F. Wei, S.-H. Dong, Pseudospin symmetry in the relativistic Rosen-Morse potential including a Pekeris-type approximation to the pseudo-centrifugal term, Eur. Phys. J. A 47 (2010) 207–212.

[16] F. J. S. Ferreira, F. V. Prudente, Pekeris approximation - another perspective, Phys. Lett. A 377 (2013) 3027–3032.