

Mie-type potential from a class of multiparameter exponential-type potential: Bound state solutions in D dimensions

J. J. Peña¹, A. Menéndez², J. García-Ravelo² and J. Morales¹

¹Universidad Autónoma Metropolitana - Azcapotzalco, CBI -
Area de Física Atómica Molecular Aplicada, Av. San Pablo 180,
02200 México, D.F., MEXICO.

²Escuela Superior de Física y Matemáticas, Instituto
Politécnico Nacional - Zacatenco, Edificio 9, Unidad Profesional
Adolfo López Mateos, 07738 México, D.F.

Corresponding author: jjpg@correo.azc.uam.mx

Abstract. The Mie potential is a model of molecular interaction, very useful in the study of diatomic molecules because allows one to describe the softness/hardness of the repulsive interactions as well as the range of attraction. As a consequence, the Mie potential and one of their particular cases, the Lennard-Jones potential, have been extensively used in many branches of physics and chemistry. In this work, the exact bound state solutions of the D-dimensional Schrödinger equation with the Mie-type potential are presented. These eigen-functions/values are obtained as a particular case of the exactly solvable Schrödinger equation for a class of multiparameter exponential-type potential. Furthermore our approach does not need any approximation to the centrifugal term. As an example of the usefulness of our proposition, we show how the bound state solutions of the Kratzer-Fues and Coulomb potentials in D-dimensions are particular cases from the proposal.

1. Introduction

The molecular vibrational and rotational spectroscopy is one of the most important fields of research due that it is a valuable tool in practically all the areas of scientific sciences. At this regard, numerous molecular interaction models have been proposed to describe the behavior of diatomic molecules as well as different approaches to the treatment of the centrifugal term. Specifically, the Mie (n,m) potential [1] has been advantageously used in many branches of physics and chemistry because this model of molecular interaction comprises a repulsive term at short distances and an attractive part for large distances. This feature has been exploited in the investigation of the effect of Mie-type potential range on the cohesive energy of metallic nanoparticles using the size-dependent potential parameters method [2]. Also, the thermodynamic properties of the Mie n-6 potential has been studied by means of a comparison between the statistical associating fluid theory of variable range approach and molecular dynamics results [3]. In the same way, the particular case (n=12, m=6), the Lennard-Jones



potential [4], is one of the most celebrated interaction potential models used to get thermodynamic properties [5], phase diagrams of fluids [6], Molecular dynamics calculations [7] and so on. On the other hand, from the theoretical point of view different methods have been employed in the search of bound states solutions of Mie potential in the non relativistic and relativistic cases. For example, the Nikiforov-Uvarov method has been used in the search of the exact solution of Dirac equation for the Mie-type potential under pseudospin and spin symmetry limit [8-9] as well as for the Mie-type potential including a Coulomb-like tensor potential [10]. Similarly, the Laplace transform approach was used to find the exact solutions of the Schrödinger equation for the Mie-type potential [11-12] and for relativistic studies of spin-1/2 particles [13]. Also, the factorization method has been employed to obtain the exact solution of Schrödinger equation for the Mie-type potential [14] as well as the SU(1,1) dynamical algebra to built their corresponding ladder operators. [15]. However, as far as we know, all works dedicated to the Mie interaction potential model, have as common characteristic the selection of a specific method to solve the corresponding Schrödinger and/or Dirac equations. In this work, we are showing how the Mie-type potential can be solved as a particular case of a class of multiparameter exponential-type potential [16] in D-dimensions without using any approximation to the centrifugal term as will be seen next.

2. A class of multiparameter exponential-like potential.

Recently, Peña et al [17] have proposed a canonical transformation approach applied to the Schrödinger equation to identify those exactly solvable exponential-type potentials with hypergeometric wavefunctions. Accordingly to their results, the radial potential

$$V(r) = \frac{Gqe^{-r/k} + Hq^2e^{-2r/k}}{(1 - qe^{r/k})^2} \quad (1)$$

with

$$G = [4ab - 2c(a + b + 1)]/4k^2 \quad \text{and} \quad H = [(a - b)^2 - (c - 1)^2]/4k^2 \quad (2)$$

where a , b , and c are the parameters of the hypergeometric function, has physically acceptable wavefunctions

$$\psi_n = (e^{-r/k})^{(c-1)/2} (1 - e^{-r/k})^{(h+1)/2} {}_2F_1(-n, b; c; qe^{-r/k}) \quad (3)$$

and energy spectra given by

$$E_n = -\frac{1}{4k^2} \left[\frac{\left(n + \frac{h+1}{2}\right)^2 - k^2 H}{n + \frac{h+1}{2}} \right]^2 \quad (4)$$

where

$$b = \frac{(h+1)(h-a) - 2k^2 G}{h+1-2a} \quad \text{and} \quad c = \frac{2a(h-a) - 2k^2 G}{h+1-2a} \quad (5)$$

such that

$$c = a + b - h \quad \text{with} \quad h = \sqrt{1 + 4k^2(G + H)}, \quad (6)$$

on condition that $a = -n$ where $n = 0, 1, 2, \dots$

To obtain the D-dimensional form of the above potential [18], we consider $q = 1$ and the redefinition of parameters

$$G = k^{-2}(\mathbf{G} + L(L + 1)) + k^{-1}A \quad \text{and} \quad H = k^{-2}\mathbf{H} - k^{-1}A \quad (7)$$

that allows rewrite

$$V(r) = \frac{1}{k^2} \left(\frac{G e^{-r/k} + H e^{-2r/k}}{(1 - e^{r/k})^2} + \frac{L(L+1) e^{-r/k}}{(1 - e^{r/k})^2} \right) \quad (8)$$

with

where $L = \ell + (D-3)/2$ such that $L(L+1) = \ell_D(\ell_D+1) - (D-1)(3-D)/4$ being $\ell_D = \sqrt{1/4 + \ell(\ell+D-2)} - 1/2$ with ℓ the usual angular momentum. In this new situation the energy spectra is given by

$$E_n = -\frac{1}{4k^2} \left[\frac{\left(n + \frac{h+1}{2}\right)^2 - H + kA}{n + \frac{h+1}{2}} \right]^2 \quad (9)$$

with eigenfunctions

$$\psi_{nL}(r) = (e^{-r/k})^{(c_L-1)/2} (1 - e^{-r/k})^{(h_L+1)/2} {}_2F_1(-n, b_L; c_L; e^{-r/k}) \quad (10)$$

where

$$b_L = \frac{(h_L+1)(h_L+n) - 2(G+kA+L(L+1))}{h_L+1+2n}, \quad (11)$$

$$c_L = \frac{-2n(h_L+n) - 2(G+kA+L(L+1))}{h_L+1+2n} \quad (12)$$

and

$$h_L = \sqrt{(2L+1)^2 + 4(H+G)}. \quad (13)$$

3. Bound state solutions of the Mie-Type potential in D-dimensions.

As well known, the Mie intermolecular pair potential has the standard form [1]

$$V_M(r) = \left(\frac{n}{n-m}\right) \left(\frac{n}{m}\right)^{\frac{m}{n-m}} \varepsilon \left[\left(\frac{\sigma}{r}\right)^n - \left(\frac{\sigma}{r}\right)^m \right] \quad (14)$$

where $r = |r_1 - r_2|$, σ is the value of r at $V(r)$ and ε is the well depth; we notice the particular case ($n = 12, m = 6$) refers to the Lennard-Jones. With the aim to obtain the above $V_M(r)$ form the D-dimensional multiparameter exponential-type potential given in Eq.(8), we consider the limit $k \rightarrow \infty$ leading to

$$V_{M-t}(r) = \frac{A}{r} + \frac{G+H}{r^2} + \frac{L(L+1)}{r^2} \quad (15)$$

with energy spectra

$$E_{nL} = -\frac{A^2}{(1+2n+h_L)^2} \quad (16)$$

which indicates that the new potential $V_{M-t}(r)$ is of Mie-type (M-t) for the case $n = 2, m = 1$. At this point it is important to notice that despite of the divergences in the parameters b_L and c_L when

$k \rightarrow \mathbb{N}$ the wavefunctions can be written without divergences. To show that, we begin by using Eq.(11) and Eq.(12) along with the value of h_L given in Eq.(13) to find

$$b_L = \frac{h_L+1}{2} + \nu + \xi k \quad \text{and} \quad c_L = -n - \frac{h_L-1}{2} + \nu + \xi k \quad (17)$$

where

$$\nu = \frac{2H}{2n+h_L+1} \quad \text{with} \quad \xi = -\frac{2A}{2n+h_L+1}. \quad (18)$$

With this new definitions, the corresponding wave functions for $V_{M-t}(r)$ are given by

$$\begin{aligned} \psi_{nL} &= e^{-\xi r} (e^{-r/k})^{(\nu-n)/2} (e^{-r/k})^{\frac{h_L+1}{4}} (1 - e^{-r/k})^{\frac{h_L+1}{2}} {}_2F_1 \left(-n, b_L; c_L; e^{-r/k} \right) \\ &= e^{-\xi k} (e^{-r/k})^{(\nu-n)/2} (e^{r/2k} - e^{-r/2k})^{\frac{h_L+1}{2}} {}_2F_1 \left(-n, b_L; c_L; e^{-r/k} \right) \\ &= \left(\frac{1}{2k} \right)^{\frac{h_L+1}{2}} e^{-\xi r} (e^{-r/k})^{(\nu-n)/2} r^{(h_L+1)/2} \left[\frac{\sinh(r/2k)}{r/2k} \right]^{\frac{h_L+1}{2}} {}_2F_1 \left(-n, b_L; c_L; e^{-r/k} \right). \end{aligned} \quad (19)$$

Furthermore, using the relationship between the hypergeometric function and Jacobi polynomials

$${}_2F_1 \left(-n, \alpha + \beta + n + 1, \alpha + 1; \frac{1-z}{2} \right) = \frac{n!}{(\alpha+1)_n} P_n^{\alpha, \beta}(z) \quad (20)$$

along with

$$P_n^{\alpha, \beta}(z) = (-1)^n P_n^{\beta, \alpha}(-z), \quad (21)$$

the wavefunctions of Eq.(19) can be written as

$$\psi_{nL}(r) = C_{nk} e^{-\xi r} \left(e^{-\frac{r}{k}} \right)^{\frac{\nu-n}{2}} r^{\frac{h_L+1}{2}} \left[\frac{\sinh\left(\frac{r}{2k}\right)}{\frac{r}{2k}} \right]^{\frac{h_L+1}{2}} P_n^{h_L, \xi k + \nu - n - \frac{h_L-1}{2}} \left(2e^{-\frac{r}{k}} - 1 \right) \quad (22)$$

where

$$C_{nk} = \frac{\left(\frac{1}{2k} \right)^{\frac{h_L+1}{2}} n! (-1)^n}{\left(-\xi k + \nu - n - \frac{h_L-1}{2} \right)_n}. \quad (23)$$

At this point, we want to mention that the function

$$\begin{aligned} \varphi_{nL}(r) &= (C_{nk})^{-1} \psi_{nL}(r) \\ &= e^{-\xi r} \left(e^{-\frac{r}{k}} \right)^{\frac{\nu-n}{2}} r^{\frac{h_L+1}{2}} \left[\frac{\sinh\left(\frac{r}{2k}\right)}{\frac{r}{2k}} \right]^{\frac{h_L+1}{2}} P_n^{h_L, \xi k + \nu - n - \frac{h_L-1}{2}} \left(2e^{-\frac{r}{k}} - 1 \right) \end{aligned} \quad (24)$$

is also solution of the Schrödinger equation for the potential given in Eq.(8). Consequently, in order to apply the limit $k \rightarrow \mathbb{N}$ to the function $\varphi_{nL}(r)$ we make use of the identities [19]

$$\lim_{k \rightarrow \mathbb{N}} P_n^{\alpha, 2\beta k + \gamma} \left(1 - \frac{z}{k} \right) = L_n^{\alpha}(\beta z) \quad (25)$$

$$P_n^{\alpha, \beta}(z) = (-1)^n P_n^{\beta, \alpha}(z) \quad (26)$$

to obtain

$$R_{nL}(r) = \lim_{k \rightarrow \infty} \varphi_{nL}(r) = e^{-\xi r} r^{\frac{h_L+1}{2}} L_n^{h_L}(\xi r), \quad (27)$$

for the wavefunction of the potential $V_{M-t}(r)$ given in Eq.(15). At this regard, we notice that the calculation of the above limit was possible after using the expansion ($k \gg 1$)

$$1 - 2e^{-\frac{r}{k}} = 1 - \frac{2r}{k} + \frac{r^2}{k^2} - \frac{r^3}{3k^3} + \frac{r^4}{12k^4} \dots \dots \dots 1 - 2r/k \quad (28)$$

4. Applications

In this section, some useful examples of potentials derived directly from our proposal $V_{M-t}(r)$ are shown next.

a) Coulomb potential.

Straightforward, by choosing the values $A = -Ze^2$ and $\mathbf{G} + \mathbf{H} = 0$ in Eq.(15) one gets

$$V_C(r) = -\frac{Ze^2}{r^2} + \frac{L(L+1)}{r^2} \quad (29)$$

that is the D-dimensional Coulomb potential. Consequently, from Eq.(16) the corresponding energy spectra results as

$$E_{nL} = -\frac{Z^2 e^4}{4(n+L+1)^2}, \quad (30)$$

in agreement with Eq.(18) of Abgoola [20]. Furthermore, accordingly to Eq.(27) the respective wavefunctions are given by

$$R_{nL}(r) = e^{-\xi r} r^{L+1} L_n^{2L+1}(\xi r) \quad (31)$$

where $\xi = \frac{Ze^2}{n+L+1}$.

b) Kratzer-Fues potential

Another particular case comes from the choice $A = -2aD_e$, $\mathbf{G} = 0$ and $\mathbf{H} = a^2 D_e$ in Eq.(15) to obtain the potential

$$V_{MK}(r) = -\frac{2aD_e}{r^2} + \frac{a^2 D_e}{r^2} + \frac{L(L+1)}{r^2} \quad (32)$$

that corresponds to the Kratzer potential with energy spectra given, through Eq.(16), by

$$\begin{aligned} E_{nL} &= -\frac{4a^2 D_e}{\left[1+2n+\sqrt{(2L+1)^2+4a^2 D_e}\right]^2} \\ &= -\frac{a^2 D_e}{\left[n+1/2+\sqrt{(L+1/2)^2+a^2 D_e}\right]^2} \end{aligned} \quad (33)$$

in agreement with the exact analytical solution obtained by Bayrak *et al* [21] using the asymptotic iteration method. Similarly, from Eq.(27) the corresponding wavefunction becomes

$$R_{nL}(r) = e^{-\xi r} r^{\frac{h_L+1}{2}} L_n^{h_L}(\xi r) \quad (34)$$

where

$$h_L = \sqrt{(2L+1)^2 + 4a^2 D_e} \quad (35)$$

c) A non-central potential

A class of non-central potential that can be solved with the approach given before, is

$$V(r, \theta) = V_1(r) + \frac{1}{r^2} V(\theta) \quad (36)$$

where

$$V_1(r) = \frac{A}{r} + \frac{B}{r^2} \quad \text{and} \quad V_2(\theta) = \frac{C+D \cos \theta}{\sin^2 \theta}, \quad (37)$$

which, although has dependence on the polar angle θ , the D-dimensional Schrödinger equation can be solved via the separation variables method. In fact, following the procedure given by Ikhaier and Sever [22] and using the notation of reference [18] for $(r, \Omega) = (r, \theta_1, \theta_2, \theta_3 \dots \theta_{D-2}, \phi)$, the radial equation is given by

$$\left(-\frac{d^2}{dr^2} + V_1(r) + \frac{L(L+1)}{r^2} \right) u(r) = Eu(r). \quad (38)$$

Similarly, the angular part becomes

$$\left(\frac{1}{\sin^{D-2}\theta_1} \frac{d}{d\theta_1} \left(\sin^{D-2}\theta_1 \frac{d}{d\theta_1} \right) + \ell_D(\ell_D + 1) - \frac{\Lambda_{D-2}}{\sin^{D-2}\theta_1} - V_2(\theta_1) \right) H_1(\theta_1) = 0 \quad (39)$$

until

$$\left(\frac{1}{\sin^{j-1}\theta_j} \frac{d}{d\theta_j} \left(\sin^{j-1}\theta_j \frac{d}{d\theta_j} \right) + \Lambda_j - \frac{\Lambda_{j-1}}{\sin^2\theta_j} \right) H_j(\theta_j) = 0, \quad (40)$$

$$\left(\frac{d^2}{d\phi^2} + \Lambda_D \right) H_\phi = 0 \quad (41)$$

where $j = 2, 3, \dots, D-2$ and Λ_j are separation constants. Since the angular part has been already solved [22], in the following we consider only the radial equation. Thus, by comparing the potential $V_1(r)$ with $V_{M-t}(r)$ given in Eq.(15), it becomes $\mathbf{G} = 0$ and $\mathbf{H} = B$ to have the corresponding energy spectra

$$E_{nL} = -\frac{A^2}{(2n+h_L+1)^2} \quad (42)$$

as well as the wavefunctions

$$u_{nL}(r) = e^{-\xi r} r^{\frac{h_L+1}{2}} L_n^{h_L}(-\xi r) \quad (43)$$

where $h_L = \sqrt{(2L+1)^2 + 4B}$, in good agreement with Eq.(16) of reference [20].

5. Concluding remarks

This work is devoted to obtain the bound state solutions of the Mie-type potential in D-dimensions. The proposal is direct because the corresponding solution is found as a particular case of the exactly solvable multiparameter exponential-type potential under the action of the limit $k \rightarrow \mathbb{N}$. With this approach, our proposal does not need any approximation of the centrifugal term as usually is done. In addition, the eigenvalues and wavefunctions of the Kratzer, Coulomb and a class of non-central potentials are derived as particular cases from our proposition. Advantageously, instead of solving the Schrödinger equation for a specific potential with a particular solution method, we are offering a procedure that consider the general solution of a class of multiparameter exponential-type potential from where particular or specific potentials can be derived. Beyond the case considered, by selecting different possibilities of the involved parameters A , B and C the proposed method can be also applied directly to other kinds of potentials.

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