ORIGINAL PAPER

Exact quantization rule to the Kratzer-type potentials: an application to the diatomic molecules

Sameer M. Ikhdair · Ramazan Sever

Abstract   For arbitrary values of n and l quantum numbers, we present a simple exact analytical solution of the D-dimensional ($D \geq 2$) hyperradial Schrödinger equation with the Kratzer and the modified Kratzer potentials within the framework of the exact quantization rule (EQR) method. The exact bound state energy eigenvalues (E_{nl}) are easily calculated from this EQR method. The corresponding normalized hyperradial wave functions ($\psi_{nl}(r)$) are also calculated. The exact energy eigenvalues for these Kratzer-type potentials are calculated numerically for a few typical LiH, CH, HCl, CO, NO, O_2, N_2 and I_2 diatomic molecules for various values of n and l quantum numbers. Numerical tests using the energy calculations for the inter dimensional degeneracy ($D = 2 - 4$) for I_2, LiH, HCl, O_2, NO and CO are also given. Our results obtained by EQR are in exact agreement with those obtained by other methods.

Keywords   Bound states · Modified Kratzer potential · Exact quantization rule · Diatomic molecules

1 Introduction

It is well-known that the exact analytical solution of the hyperradial Schrödinger equation, in any arbitrary spatial dimension ($D \geq 2$), for its bound state energy levels, is fundamental to understanding of molecular spectrum of a diatomic molecules in a nonrelativistic quantum mechanics, since the resulting wave function contains all

S. M. Ikhdair
Department of Physics, Near East University, Nicosia, Northern Cyprus, Turkey
e-mail: sameer@neu.edu.tr

R. Sever (✉)
Department of Physics, Middle East Technical University, 06531 Ankara, Turkey
e-mail: sever@metu.edu.tr

the necessary information to describe a quantum system fully. There are only a few potentials for which the radial Schrödinger equation can be solved explicitly for all n and all l quantum numbers. So far, some useful methods have been developed, such as supersymmetry (SUSY) [1], the Nikiforov-Uvarov method (NU) [2], the Pekris approximation [3], asymptotic iteration method (AIM) [4], variational [5], the hyper-virial perturbation [6], the shifted $1/N$ expansion (SE) and the modified shifted $1/N$ expansion (MSE) [7], exact quantization rule (EQR) [8], perturbative formalism [9], polynomial solution [10] and wave function ansatz method [11] to solve the radial Schrödinger equation exactly or quasi-exactly for $l \neq 0$ within a given potential.

The kratzer and modified Kratzer-type potentials [12] that we study in the present work are important molecular potentials describe the interaction between two atoms and have attracted a great of interest for some decades in the history of quantum chemistry. Until now, these potentials have been used extensively to describe the molecular structure and interactions [13]. In this work, we attempt to apply the recently proposed EQR method [8], as an alternative approach, to obtain analytically ($l \neq 0$) exact energy levels and the corresponding wave functions of the D-dimensional ($D \geq 2$) Schrödinger equation with the Kratzer-type potentials. Further, we calculate numerically these bound state energy levels for LiH, CH, HCl, CO, NO, O_2, N_2 and I_2 diatomic molecules for different values of n and l quantum numbers. Further, we give numerical tests using energy calculations for interdimensional degeneracy, i.e., $(n, l, D) \rightarrow (n, l \pm 1, D \mp 2)$ corresponding to the confined $D = 2$–4 dimensional Kratzer's potential.

This paper is organized as follows. In Sect. 2 the EQR method is reviewed. In Sect. 3, the D-dimensional ($D \geq 2$) Schrödinger equation is solved by this method with $l \neq 0$ quantum numbers to obtain the energy eigenvalues and the corresponding hyperradial wave functions of the Kratzer-type potential. In Sect. 4 the interdimensional degeneracy is introduced. Numerical calculations of the energy levels and test of interdimensional degeneracy for a few typical CO, NO, CH, HCl, LiH, N_2, O_2, and I_2 diatomic molecules are performed for various values of n and l quantum numbers to compare with those obtained by other methods in Sect. 5. Finally, we make a few concluding remarks in Sect. 6.

2 Exact quantization rule method

A brief outline to the EQR method is presented with an extension to the D-dimensional space ($D \geq 2$). The details can be found in [8]. The EQR has recently been proposed to solve the one-dimensional ($1D$) Schrödinger equation:

$$\frac{d^2}{dx^2}\psi(x) + k(x)^2\psi(x) = 0, \quad k(x) = \frac{1}{\hbar}\sqrt{2\mu\left[E - V(x)\right]}, \tag{1}$$

where μ represents the reduced mass of the two interacting particles, $k(x)$ is the momentum and the potential $V(x)$ is a piecewise continuous real function of x. Equation 1 can be reduced into the Riccati equation:

$$\frac{d}{dx}\phi(x) + \phi(x)^2 + k(x)^2 = 0, \tag{2}$$

where $\phi(x) = \psi(x)^{-1}d\psi(x)/dx$ is the logarithmic derivative of wave function $\psi(x)$. Due to the Sturm-Liouville theorem, the $\phi(x)$ decreases monotonically with respect to x between two turning points, where $E \geq V(x)$. Specifically, as x increases across a node of the wave function $\psi(x)$, where $E \geq V(x)$, $\phi(x)$ decreases to $-\infty$, jumps to $+\infty$, and then decreases again. By carefully studying the $1D$ Schrödinger equation, Ma and Xu [8] obtained the EQR as

$$\int_{x_a}^{x_b} k(x)dx = N\pi + \int_{x_a}^{x_b} \phi(x)\left[\frac{dk(x)}{dx}\right]\left[\frac{d\phi(x)}{dx}\right]^{-1}dx, \tag{3}$$

where x_a and x_b are two turning points determined by letting $E = V(x)$, N is the number of nodes of $\phi(x)$ in the region $E \geq V(x)$ and it is larger by one than the number of nodes of wave function $\psi(x)$, i.e. $N = n + 1$. Further, Ma and Xu [8] have generalized the EQR to $3D$ radial Schrödinger equation with a spherically symmetric potential. Here, we extend the $3D$-generalization of the EQR given by [8] into the D-dimensional ($D \geq 2$) Schrödinger equation. It is well-known that in the D-dimensional hyperradial Schrödinger equation, for any arbitrary spherically symmetric potential, can be simply written as [14]

$$\left[\frac{d^2}{dr^2} + \frac{(D-1)}{r}\frac{d}{dr} - \frac{l(l+D-2)}{r^2} + \frac{2\mu}{\hbar^2}(E - V(r))\right]\psi_{n,l,m}(r, \Omega_D) = 0,$$

$$\psi_{n,l,m}(r, \Omega_D) = \psi_{n,l}(r)Y_l^m(\Omega_D), \tag{4}$$

where l denotes the orbital angular momentum quantum number, μ is the reduced mass, $\psi_{n,l}(r)$ is the hyperradial part of the wave function and $Y_l^m(\Omega_D)$ is the hyperspherical harmonics. Furthermore, to remove the first derivative from the above equation, we define a new radial wave function $R(r)$ by means of equation

$$\psi_{n,l}(r) = r^{-(D-1)/2}R(r), \tag{5}$$

which will give the radial wave function $R(r)$ satisfying the wave equation

$$\left\{\frac{d^2}{dr^2} - \frac{[4l(l+D-2) + (D-1)(D-3)]}{4r^2} + \frac{2\mu}{\hbar^2}(E - V(r))\right\}R(r) = 0. \tag{6}$$

Further, the hyperradial Eq. 6 can be written into a simple analogy of the $2D$ and $3D$ radial Schrödinger equation given in [8] as [15]

$$\frac{d^2}{dr^2}R(r) = -\frac{2\mu}{\hbar^2}[E - V_{\text{eff}}(r)]R(r), \quad V_{\text{eff}}(r) = \frac{(\eta^2 - 1/4)\hbar^2}{2\mu r^2} + V(r), \tag{7}$$

with the parameter

$$\eta = l + \frac{1}{2}(D - 2),\qquad(8)$$

which is a linear combination of the spatial dimensions D and the angular momentum quantum number l. Thus, the EQR can be generalized to the D-dimensional ($D \geq 2$) hyperradial Schrödinger equation, with the new effective potential form given by (7) as

$$\int_{r_a}^{r_b} K(r)dr = N\pi + Q_c, \quad K(r) = \frac{2\mu}{\hbar^2}[E - V_{\text{eff}}(r)],\qquad(9)$$

where

$$Q_c = \int_{r_a}^{r_b} \phi(r)\left[\frac{dk(r)}{dr}\right]\left[\frac{d\phi(r)}{dr}\right]^{-1} dr,\qquad(10)$$

is called the quantum correction, $N\pi$ is the contribution from the nodes of wave function and $K(r)$ being the momentum between the two turning points r_a and r_b. It has also been found that this quantum correction is independent of the number of nodes of wave function for solvable quantum system. Thus, the quantum correction in Eq. 10 can be replaced by the ground-state calculations:

$$Q_c = \int_{r_a}^{r_b} \phi_0(r)\left[\frac{dk_0(r)}{dr}\right]\left[\frac{d\phi_0(r)}{dr}\right]^{-1} dr = \pi q.\qquad(11)$$

3 Solutions of the Kratzer and modified Kratzer-type potentials

Considerable interest has recently been shown in the Kratzer-Fues [12,16–19] as a model to describe internuclear vibration of a diatomic molecule [20–23]. This potential can be expressed in the form

$$V(r) = -D_e\left(\frac{2r_e}{r} - \frac{r_e^2}{r^2}\right),\qquad(12)$$

where D_e is the dissociation energy between two atoms in a solid and r_e is the equilibrium internuclear length. This type of the potential in (12) has been studied through the smooth transformation [16], the algebraic approach [17], and the AIM [18]. The standard Kratzer's potential has been recently modified by adding a D_e term to the potential [24]. A new type of this potential is called the modified Kratzer potential:

$$V(r) = D_e \left(\frac{r - r_e}{r} \right)^2,$$ (13)

which is shifted in amount of D_e. The above potential has been studied in D-dimensions through the polynomial solutions [25] and also the selection of a suitable wave function ansatz [15]. The modified Kratzer potential has also been studied before in the $3D$ through the NU method [24]. This potential can be simply taken as

$$V(r) = \frac{A}{r^2} - \frac{B}{r} + C,$$ (14)

where $A = D_e r_e^2$, $B = 2D_e r_e$ and $C = D_e$ [15,25,26]. For this spherically symmetric modified Kratzer potential, the effective potential in Eq. 7 can be arranged to

$$V_{\text{eff}}(r) = \frac{2\mu A + \frac{1}{4}\left[(M-2)^2 - 1\right]\hbar^2}{2\mu r^2} - \frac{B}{r} + C, \quad M = D + 2l.$$ (15)

Further, by introducing the notation

$$\Lambda(\Lambda + 1)\hbar^2 = 2\mu A + \frac{1}{4}\left[(M-2)^2 - 1\right]\hbar^2,$$ (16)

from which we obtain a physically acceptable solution

$$\Lambda = \frac{-1 + \sqrt{(M-2)^2 + 8\mu A/\hbar^2}}{2},$$ (17)

and finally the effective potential becomes

$$V_{\text{eff}}(r) = \frac{\Lambda(\Lambda + 1)\hbar^2}{2\mu r^2} - \frac{B}{r} + C.$$ (18)

On the other hand, by taking $\phi(r) = R(r)^{-1}dR(r)/dr$, the Riccati equation reads

$$\frac{d}{dr}\phi(r) + \phi(r)^2 = -\frac{2\mu}{\hbar^2}\left[E - C - \frac{\Lambda(\Lambda + 1)\hbar^2}{2\mu r^2} + \frac{B}{r}\right].$$ (19)

Now, we apply the EQR [8,26,27] given by (9) to solve the above Riccati equation. At first, we must determine the turning points r_a and r_b from solving the relation $E = V_{\text{eff}}(r)$ with $r_a < r_b$. Thus, we find

$$r_a = \frac{1}{-2(E-C)}\left[B - \sqrt{B^2 + \frac{2\Lambda(\Lambda + 1)(E-C)\hbar^2}{\mu}}\right],$$ (20)

$$r_b = \frac{1}{-2(E-C)} \left[B + \sqrt{B^2 + \frac{2\Lambda(\Lambda+1)(E-C)\hbar^2}{\mu}} \right]. \tag{21}$$

The momentum between two turning points r_a and r_b can be calculated by $k(r) = \sqrt{2\mu[E_0 - V_{\text{eff}}(r)]}/\hbar$ as

$$k(r) = \frac{1}{\hbar r} \sqrt{-2\mu(E-C)(r-r_a)(r_b-r)}. \tag{22}$$

Since the phase angle $\phi(r)$ decreases as r increases, then the solution with one node and no pole only has a unique solution $\phi_0(r) = \alpha_1 r^{-1} + \alpha_2$ with $\alpha_1 > 0$ due to the monotonic property. Substituting this solution into the Riccati equation (19), we find the ground-state solution as

$$\phi_0(r) = \frac{\Lambda+1}{r} - \frac{\mu B}{(\Lambda+1)\hbar^2}, \quad \text{with} \quad E_0 = C - \frac{\mu B^2}{2(\Lambda+1)^2\hbar^2}. \tag{23}$$

Evidently $\phi_0(r)$ is negative when $r \to \infty$, so that the solution satisfies the physically admissible boundary condition. In order to obtain the energy levels of all the bound-states, making use of the integrals given in Appendix A, we are able to calculate the quantum correction from Eq. 11 as

$$Q_c = \frac{\sqrt{-2\mu(E_0-C)}}{2(\Lambda+1)^2\hbar^3} \int_{r_a}^{r_b} \frac{[(\Lambda+1)^2\hbar^2 - \mu Br]}{r\sqrt{(r-r_a)(r_b-r)}} [(r_a+r_b)r - 2r_ar_b]\,dr \tag{24}$$

$$= \left[\Lambda - \sqrt{\Lambda(\Lambda+1)} \right] \pi,$$

where the following formulas

$$r_a + r_b = -\frac{B}{(E_0-C)}, \quad r_ar_b = -\frac{\Lambda(\Lambda+1)\hbar^2}{2\mu(E_0-C)}, \quad \sqrt{-2\mu(E_0-C)} = \frac{\mu B}{(\Lambda+1)\hbar}, \tag{25}$$

have been used in finding Eq. 24. On the other hand, for any n state, we calculate the left hand side of Eq. 9 for $V_{\text{eff}}(r)$ given in Eq. 18 using Eq. 22 as

$$\int_{r_a}^{r_b} K(r)\,dr = \left[\frac{\mu B}{\sqrt{-2\mu(E_n-C)}\hbar} - \sqrt{\Lambda(\Lambda+1)} \right] \pi. \tag{26}$$

Further, the substitution of Eqs. 24, and 26, into Eq. 9, enables us to obtain the energy levels of all bound states in any arbitrary dimension $D \geq 2$ as

$$E_{nl}^{(D)} = C - \left(\frac{2\mu}{\hbar^2}B^2\right)\left[2n+1+\sqrt{(D+2l-2)^2+\frac{8\mu}{\hbar^2}A}\right]^{-2}$$

$$= C - \frac{\mu}{2\hbar^2}\left(\frac{B}{\tilde{n}}\right)^2, \quad \tilde{n} = N + \Lambda, \quad n, l = 0, 1, 2, \ldots \quad (27)$$

where $N = n + 1$ was used with n is the number of nodes in the wave functions $R(r)$.

Therefore, for the D-dimensional Kratzer's potential ($C = 0$), the energy spectra become

$$E_{nl}^{(D)} = -\left(\frac{2\mu}{\hbar^2}D_e^2 r_e^2\right)\left[n+\frac{1}{2}+\sqrt{\left(l+\frac{D}{2}-1\right)^2+\frac{2\mu}{\hbar^2}D_e r_e^2}\right]^{-2}, \quad (28)$$

and also for the modified Kratzer-type ($C = D_e$) potential read

$$E_{nl}^{(D)} = D_e - \left(\frac{2\mu}{\hbar^2}D_e^2 r_e^2\right)\left[n+\frac{1}{2}+\sqrt{\left(l+\frac{D}{2}-1\right)^2+\frac{2\mu}{\hbar^2}D_e r_e^2}\right]^{-2}, \quad E_{nl}^{(D)} < D_e,$$

$$(29)$$

where $n = 0, 1, 2, \ldots$ and l signify the usual radial and angular momentum quantum numbers, respectively. In what follows, we want to obtain the corresponding normalized hyperwave function. At first, we define

$$\nu(\nu + D - 2) = l(l + D - 2) + \frac{2\mu A}{\hbar^2}, \quad (30)$$

$$\rho = 2\kappa r, \quad \tau = \frac{\mu B}{\hbar^2 \kappa}, \quad \kappa = \sqrt{-2\mu(E-C)/\hbar^2}, \quad (31)$$

where for bound state case, states with $E < C$, we have real numbers for the parameters κ and τ. Thus, the hyperradial Eq. 4 transforms to a standard form given by

$$\psi_{n,l}''(\rho) + \frac{(D-1)}{\rho}\psi_{n,l}'(\rho) + \left[-\frac{1}{4}+\frac{\tau}{\rho}-\frac{\nu(\nu+D-2)}{\rho^2}\right]\psi_{n,l}(\rho) = 0, \quad (32)$$

$$\nu = -\frac{(D-2)}{2} + \frac{1}{2}\sqrt{(2l+D-2)^2+\frac{8\mu A}{\hbar^2}}, \quad (33)$$

whose solutions are given as [19,25]

$$\psi_{n,l}(\rho) = N(n,l)\rho^\nu e^{-\rho/2} {}_1F_1\left(-\tau + \nu + \frac{D-1}{2}, 2\nu + D - 1; \rho\right) \tag{34}$$

from which we can obtain the quantum condition as $-\tau + \nu + \frac{D-1}{2} = -n$, $n = 0, 1, 2, \ldots$ [28,29]. Furthermore, we can renormalize the bound state solutions in (34) since these solutions are finite and convergent for both $\rho = 0$ ($r = 0$) and $\rho \to \infty$.

On the other hand, using the following relationship between the associated Laguerre function and the hypergeometric function:

$$L_n^\alpha(z) = \frac{\Gamma(\alpha + n + 1)}{n!\Gamma(a + 1)} {}_1F_1(-n, \alpha + 1; z), \tag{35}$$

we may further rewrite the wave functions as

$$\psi_{n,l}(\rho) = \mathcal{N}(n,l)\rho^\nu e^{-\rho/2} L_n^{(2\nu+D-2)}(\rho), \tag{36}$$

where $\mathcal{N}(n, l)$ is the normalization factor has to be determined by the renormalization condition

$$\int\limits_0^\infty |\psi_{n,l}(\rho)|^2 r^{(D-1)} dr = 1. \tag{37}$$

To find the normalizing factor, let us review the generalized Coulomb-like integral $J_{n,\alpha}^{(\beta)}(z)$ for noninteger α and β derived in [30] as

$$J_{n,\alpha}^{(\beta)}(z) = \int\limits_0^\infty e^{-z} z^{\alpha+\beta} \left[L_n^{(\alpha)}(z)\right]^2 dz = \frac{\Gamma(\alpha + n + 1)}{\Gamma(n + 1)} \sum_{j=0}^n (-1)^j \frac{\Gamma(n - j - \beta)}{\Gamma(-j - \beta)}$$

$$\times \frac{\Gamma(\alpha + \beta + j + 1)}{\Gamma(\alpha + j + 1)} \frac{1}{\Gamma(j + 1)\Gamma(n - j + 1)}, \quad \mathcal{R}e(\alpha + \beta + 1) > 0. \tag{38}$$

In the present case, we have $\beta = 1$. This $J_{n,\alpha}^{(1)}$ has only two nonzero contributions (for $j = n - 1$ and n) in the sum (38) because of the gamma functions of negative integers. The result $J_{n,\alpha}^{(1)} = \frac{(2n+\alpha+1)\Gamma(\alpha+n+1)}{\Gamma(n+1)}$ enables us to write for our case

$$J_{n,2\nu+D-2}^{(1)} = \frac{(2\nu + 2n + D - 1)(2\nu + n + D - 2)!}{n!}, \tag{39}$$

which gives the normalization factor

$$
\mathcal{N}(n,l) = \left[\frac{n!(2\kappa)^D}{(2\nu + 2n + D - 1)(2\nu + n + D - 2)!} \right]^{1/2},
$$
$$
\kappa = \frac{\mu B}{\hbar^2(n + \Lambda + 1)}, \quad \Lambda = \nu + \frac{(D-3)}{2}.
\tag{40}
$$

Therefore, we can finally obtain the re-normalized hyper wave function for the modified Kratzer potential as

$$
\psi_{n,l,m}(r, \Omega_D) = \left[\frac{n!}{(\nu_1 + 2n + 1)(\nu_1 + n)!} \right]^{1/2} (2\kappa)^{\nu_2} r^\nu e^{-\kappa r} L_n^{(\nu_1)}(2\kappa r) Y_l^m(\Omega_D),
\tag{41}
$$

with

$$
2\kappa = \frac{8\mu D_e r_e}{\hbar^2(2n + \nu_1 + 1)}, \quad \nu_1 = \sqrt{(2l + D - 2)^2 + \frac{8\mu}{\hbar^2} D_e r_e},
\tag{42}
$$

$$
\nu_2 = \frac{\nu_1 + 2}{2}, \quad \nu = \frac{\nu_1 - (D-2)}{2}.
\tag{43}
$$

which is found to be consistent with our previous findings in [25] using the polynomial solution.

4 Interdimensional degeneracy

From Eq. 27, it can be seen that two interdimensional states are degenerate whenever [31]

$$
(n, l, D) \rightarrow (n, l \pm 1, D \mp 2).
\tag{44}
$$

Thus, a knowledge of $E_{nl}^{(D)}$ for $D = 2$ and $D = 3$ provides the information necessary to find $E_{nl}^{(D)}$ for other higher dimensions.

Table 1 Reduced masses and spectroscopically determined properties of various diatomic molecules in the ground electronic state

Parameters[a]	LiH	I_2	O_2	HCl	NO	CO
D_0 (in eV)	2.515283695	1.581791863	5.156658828	4.619061175	8.043782568	10.84514471
r_0 (in A°)	1.5956	2.662	1.208	1.2746	1.1508	1.1282
μ (in amu)	0.8801221	63.45223502	7.997457504	0.9801045	7.468441000	6.860586000

[a] The data listed in this table are taken from [34–37]

Table 2 Comparison of the energy levels, E_{nl} (in eV), corresponding to the $3D$ Kratzer's potential for the various n and l quantum numbers for the diatomic molecules LiH, I$_2$, and O$_2$, where $\hbar c = 1973.29$ eV A°

n	l	LiH [EQR]	I$_2$ [EQR]	I$_2$ [AIM]	O$_2$ [EQR]	O$_2$ [AIM]
0	0	−2.467310304097	−1.579082576525	−1.579082577	−5.126358620071	−5.126358625
1	0	−2.375819214406	−1.573687150333	−1.573687151	−5.066641146718	−5.066641151
	1	−2.374107972668	−1.573677924919	−1.573677925	−5.066292321402	−5.066292323
2	0	−2.289324266253	−1.568319329698	−1.568319330	−5.007961110233	−5.007961116
	1	−2.287705602815	−1.568310151445	−1.568310152	−5.007618327191	−5.007618329
	2	−2.284475215373	−1.568291795200	−1.568291796	−5.006932902380	−5.006932904
3	0	−2.207468200275	−1.562978926616	−1.562978927	−4.950294618656	−4.950294624
	1	−2.205935555783	−1.562969795203	−1.562969796	−4.949957739138	−4.949957740
	2	−2.202876749755	−1.562951532697	−1.562951533	−4.949284118344	−4.949284119
	3	−2.198304679122	−1.562924139740	−1.562924140	−4.948274032620	−4.948274034
4	0	−2.129925128672	−1.557665754681	−1.557665755	−4.893618463868	−4.893618469
	1	−2.128472514560	−1.557656669790	−1.557656670	−4.893287353086	−4.893287355
	2	−2.125573350591	−1.557638500327	−1.557638501	−4.892625266816	−4.892625268
	3	−2.121239701434	−1.557611246928	−1.557611247	−4.891632475505	−4.891632476
	4	−2.115489505754	−1.557574910549	−1.557574911	−4.890309384483	−4.890309388
5	0	−2.056397286593	−1.552379629069	−1.552379630	−4.837910098245	−4.837910103
	1	−2.055019226505	−1.552370590385	−1.552370591	−4.837584625235	−4.837584627
	2	−2.052268785922	−1.552352513333	−1.552352514	−4.836933811639	−4.836933812
	3	−2.048157264859	−1.552325398546	−1.552325399	−4.835957922172	−4.835957923
	4	−2.042701466576	−1.552289246974	−1.552289248	−4.834657353568	−4.834657357
	5	−2.035923524667	−1.552244059882	−1.552244060	−4.833032634174	−4.833032637

Table 3 Comparison of the energy levels, E_{nl} (in eV), corresponding to the $3D$ Kratzer's potential for the various n and l quantum numbers for the diatomic molecules HCl, NO,and CO, where $\hbar c = 1973.29$ eV A°

n	l	HCl [EQR]	NO [EQR]	NO [AIM]	CO [EQR]	CO [AIM]
0	0	−4.541848211101	−8.002659419493	−8.002659417	−10.794315323	−10.79431532
1	0	−4.393727956046	−7.921456840689	−7.921456839	−10.693839925	−10.69383992
	1	−4.391293850595	−7.921043829925	−7.921043834	−10.693371229	−10.69337123
2	0	−4.252737112329	−7.841483958093	−7.841483956	−10.594760890	−10.59476089
	1	−4.250419208735	−7.841077185904	−7.841077188	−10.594298692	−10.59429869
	2	−4.245791052967	−7.840263768523	−7.840263771	−10.593374417	−10.59337441
3	0	−4.118425371585	−7.762716067159	−7.762716066	−10.497052462	−10.49705246
	1	−4.116216389518	−7.762315408528	−7.762315413	−10.496596643	−10.49659664
	2	−4.111805631214	−7.761514215884	−7.761514218	−10.495685124	−10.49568512
	3	−4.105207449232	−7.760312738370	−7.760312744	−10.494318144	−10.49431814
4	0	−3.990377425087	−7.685129080626	−7.685129079	−10.400689478	−10.40068947
	1	−3.988270645562	−7.684734413653	−7.684734417	−10.400239921	−10.40023992
	2	−3.984063879462	−7.683945202003	−7.683945203	−10.399340924	−10.39934092
	3	−3.977770657506	−7.682761690175	−7.682761696	−10.397992722	−10.39799272
	4	−3.969411138650	−7.681184244677	−7.681184246	−10.396195666	−10.39619567
5	0	−3.868209749404	−7.608699510108	−7.608699509	−10.305647347	−10.30564735
	1	−3.866198963636	−7.608310715917	−7.608310719	−10.305203938	−10.30520394
	2	−3.862183802008	−7.607533247563	−7.607533248	−10.304317236	−10.30431723
	3	−3.856177032746	−7.606367345012	−7.606367349	−10.302987469	−10.30298747
	4	−3.848197679994	−7.604813367976	−7.604813368	−10.301214985	−10.30121499
	5	−3.838270872139	−7.602871795644	−7.602871795	−10.299000242	−10.29900024

Table 4 Numerical tests using the energy calculations (in eV) for the interdimensional degeneracy corresponding to the confined $D = 2$–4 dimensional Kratzer potential for various n, l quantum numbers for the diatomic molecules I_2, LiH, and HCl, where $\hbar c = 1973.29$ eV A$°$

D	l	n	I_2 [EQR]	LiH [EQR]	HCl [EQR]
2	0	0	−1.579083735645	−2.467536868725	−4.542168190064
		1	−1.573688303518	−2.376033294347	−4.394032410177
		2	−1.568320476987	−2.289526762193	−4.253027029918
	1	0	−1.579079099175	−2.466630860376	−4.540888545222
		1	−1.573683690790	−2.375177207655	−4.392814848343
		2	−1.568315887840	−2.288716995880	−4.251867599163
	2	0	−1.579065189928	−2.463916832438	−4.537053942242
		1	−1.573669852770	−2.372612671616	−4.389166233568
		2	−1.568302120561	−2.286291171344	−4.248393136578
	3	0	−1.579042008394	−2.459406732177	−4.530677339114
		1	−1.573646789943	−2.368350817764	−4.383098743943
		2	−1.568279175633	−2.282259674365	−4.242615099462
3	0	0	−1.579082576525	−2.467310304097	−4.541848211101
		1	−1.573687150333	−2.375819214406	−4.393727956046
		2	−1.568319329698	−2.289324266254	−4.252737112328
	1	0	−1.579073303626	−2.465499287366	−4.539290004878
		1	−1.573677924919	−2.374107972668	−4.391293850595
		2	−1.568310151445	−2.287705602815	−4.250419208735
	2	0	−1.579054758153	−2.461885237093	−4.534182246350
		1	−1.573659474414	−2.370692927106	−4.386433772612
4	0	0	−1.579079099175	−2.466630860376	−4.540888545222
		1	−1.573683690790	−2.375177207655	−4.392814848343
		2	−1.568315887840	−2.288716995880	−4.251867599163
	1	0	−1.579065189928	−2.463916832438	−4.537053942242
		1	−1.573669852770	−2.372612671616	−4.389166233568
		2	−1.568302120561	−2.286291171344	−4.248393136578
	2	0	−1.579042008394	−2.459406732177	−4.530677339114
		1	−1.573646789943	−2.368350817764	−4.383098743943
		2	−1.568279175633	−2.282259674365	−4.242615099462

For example, $E_{0,4}^{(2)} = E_{0,3}^{(4)} = E_{0,2}^{(6)} = E_{0,1}^{(8)}$. This is the same transformational invariance described for bound states of free atoms and molecules [32,33] and demonstrates the existence of interdimensional degeneracies among states of the confined Kratzer potential.

5 Numerical applications

In this work, we have given numerical calculations for a few known typical diatomic molecules to compare with those obtained by other numerical exact methods given by the AIM [18] and the NU method [24]. In this regard, we have calculated the bound state energy eigenvalues with Eq. 28 using the Kratzer's potential for a few CO, NO, HCl, LiH, O_2 and I_2 diatomic molecules for selected n, l quantum numbers with parameter values given in Table 1. These parameters values are taken from [34–37]. Therefore, we give the explicit values of Kratzer's energy levels for different values of n and l in Tables 2 and 3. We further compare these results with those obtained by

Table 5 Numerical tests using the energy calculations (in eV) for the interdimensional degeneracy corresponding to the confined $D = 2$–4 dimensional Kratzer potential for various n, l quantum numbers for the diatomic molecules O_2, NO, and CO, where $\hbar c = 1973.29$ eV $A°$

D	l	n	O_2 [EQR]	NO [EQR]	CO [EQR]
2	0	0	−5.126402999836	−8.002711844782	−10.794374740920
		1	−5.066684753267	−7.921508470069	−10.693898515189
		2	−5.008003961426	−7.841534807595	−10.594818667644
	1	0	−5.126225485390	−8.002502147751	−10.794137074251
		1	−5.066510331583	−7.921301956595	−10.693664159142
		2	−5.007832561073	−7.841331413560	−10.594587561016
	2	0	−5.125693015861	−8.001873122635	−10.793424137068
		1	−5.065987138736	−7.920682480901	−10.692961152734
		2	−5.007318430661	−7.840721294966	−10.593894301796
	3	0	−5.124805812601	−8.000824967303	−10.792236117812
		1	−5.065115391268	−7.919650237110	−10.691789681130
		2	−5.006461782057	−7.839704642277	−10.592739071948
3	0	0	−5.126358620071	−8.002659419493	−10.794315323271
		1	−5.066641146718	−7.921456840689	−10.693839925213
		2	−5.007961110233	−7.841483958093	−10.594760890040
	1	0	−5.126003609633	−8.002240041928	−10.793840005639
		1	−5.066292321402	−7.921043829925	−10.693371228552
		2	−5.007618327191	−7.841077185904	−10.594298691949
	2	0	−5.125293736355	−8.001401418731	−10.792889496018
		1	−5.065594815162	−7.920217937834	−10.692433958691
4	0	0	−5.126225485390	−8.002502147751	−10.794137074251
		1	−5.066510331583	−7.921301956595	−10.693664159142
		2	−5.007832561073	−7.841331413560	−10.594587561016
	1	0	−5.125693015861	−8.001873122635	−10.793424137068
		1	−5.065987138736	−7.920682480901	−10.692961152734
		2	−5.007318430661	−7.840721294966	−10.593894301796
	2	0	−5.124805812601	−8.000824967303	−10.792236117812
		1	−5.065115391268	−7.919650237110	−10.691789681130
		2	−5.006461782057	−7.839704642277	−10.592739071948

Table 6 Reduced masses and spectroscopically determined properties of N_2, CO, NO and CH diatomic molecules in the ground electronic state

Parameters[a]	N_2	CO	NO	CH
D_0 (cm^{-1})	96288.03528	87471.42567	64877.06229	31838.08149
r_0 (A°)	1.0940	1.1282	1.1508	1.1198
μ (amu)	7.00335	6.860586	7.468441	0.929931

[a] The data listed in this table are taken from [24]

the AIM [18]. In Tables 4 and 5, we have also tested the interdimensional degeneracy ($D = 2 - 4$) using the energy calculations for a few CO, NO, HCl, LiH, O_2, and I_2 diatomic molecules. On the other hand, for the recently proposed modified Kratzer potential, we have used the parameters for CO, NO, CH and N_2 diatomic molecules given in Table 6 to compare with the NU method [24]. For this case, in Tables 7–8, we give the energy levels for CO, NO, CH and N_2 diatomic molecules for various n, l quantum numbers by using Eq. 29.

Table 7 Comparison of the energy eigenvalues, E_{nl} (in eV), corresponding to the $3D$ modified Kratzer potential for the various n and l quantum numbers for the diatomic molecules N_2 and CO, where $\hbar c = 1973.29\,eV\,A^\circ$

n	l	N_2 [EQR]	N_2 [NU]	CO [EQR]	CO [NU]
0	0	0.054436738370	0.054430	0.050829386733	0.050823
1	0	0.162076974947	0.162057	0.151304784801	0.151287
	1	0.162565552668	0.162546	0.151773481462	0.151755
2	0	0.268261347644	0.268229	0.250383819984	0.250354
	1	0.268743332192	0.268711	0.250846018075	0.250816
	2	0.269707181517	0.269675	0.251770292931	0.251744
3	0	0.373015993195	0.372972	0.348092247640	0.348051
	1	0.373491502668	0.373447	0.348548066746	0.348507
	2	0.374442403850	0.374398	0.349459585720	0.349418
	3	0.375868461286	0.375823	0.350826566166	0.350785
4	0	0.476366464424	0.476313	0.444455232045	0.444403
	1	0.476835614288	0.476779	0.444904789014	0.444852
	2	0.477773798215	0.477717	0.445803785755	0.445751
	3	0.479180784677	0.479124	0.447151987956	0.447099
	4	0.481056226559	0.480999	0.448949044337	0.448895
5	0	0.578337745829	0.578269	0.539497362596	0.539434
	1	0.578800648986	0.578732	0.539940771611	0.539877
	2	0.579726341424	0.579658	0.540827474443	0.540764
	3	0.581114595455	0.581046	0.542157240772	0.542093
	4	0.582965069724	0.582896	0.543929725307	0.543865
	5	0.585277309425	0.585208	0.546144468004	0.546082

Table 8 Comparison of the energy eigenvalues, E_{nl} (in eV), corresponding to the $3D$ modified Kratzer potential for the various n and l quantum numbers for the diatomic molecules NO and CH, where $\hbar c = 1973.29\,eV\,A^\circ$

n	l	NO [EQR]	NO [NU]	CH [EQR]	CH [NU]
0	0	0.041123148507	0.041118	0.083224106534	0.083214
1	0	0.122325727312	0.122311	0.241151342060	0.241123
	1	0.122738738076	0.122724	0.244409651454	0.244381
2	0	0.202298609907	0.202274	0.389591252689	0.389547
	1	0.202705382097	0.202681	0.392655829482	0.392611
	2	0.203518799478	0.203494	0.398768962343	0.398722
3	0	0.281066500842	0.281033	0.529288818460	0.529229
	1	0.281467159473	0.281434	0.532174721830	0.532115
	2	0.282268352117	0.282235	0.537931662876	0.537870
	3	0.283469829631	0.283436	0.546530102918	0.546467
4	0	0.358653487375	0.358611	0.660917306208	0.660844
	1	0.359048154348	0.359006	0.663638151412	0.663565
	2	0.359837365998	0.359795	0.669066052612	0.668992
	3	0.361020877826	0.360978	0.677173530261	0.677098
	4	0.362598323324	0.362555	0.687919851051	0.687842
5	0	0.435083057893	0.435032	0.785086396757	0.785001
	1	0.435471852084	0.435421	0.787654550920	0.787569
	2	0.436249320438	0.436198	0.792778001145	0.792692
	3	0.437415222989	0.437364	0.800431194100	0.800343
	4	0.438969200025	0.438917	0.810576203106	0.810487
	5	0.440910772357	0.440858	0.823163201411	0.823071

6 Concluding remarks

In this study, we have used a different approach to find the $l \neq 0$ analytical and numerical solutions to the D-dimensional hyperradial Schrödinger equation with Kratzer-type potentials for various diatomic molecules within the framework of the exact quantization rule. For such potentials, the problem is simply reduced to a Coulomb potential plus an inverse quadratic potential term. The exact eigensolutions for this particular case have been obtained, in a similar way as the Hydrogenic solutions [30]. Further, we have calculated the exact bound state energy eigenvalues and the corresponding normalized hyper wave functions for various diatomic molecules for any l angular momentum quantum number bound by an exactly solvable Kratzer-type potential. The advantage of the present method is that it enables one to find the energy eigenvalues directly in a simple way. The method presented in this work can be applied to find the energy eigenvalues and the corresponding eigenfunctions of the Schrödinger equation within a given potential for various diatomic molecules.

It is obvious that Eqs. 27 and 36 (with Eqs. 31 and 40) reduce to the well-known eigenvalues and eigenfunctions for the $3D$ Kratzer-Fues potential when $D = 3$ [38, 39]. Further, they reduce to the Coulomb-like solutions in D-dimensions if $A = C = 0$ [40]. Similarly, for $B = 2Z > 0$ and $A = \lambda$, Z and λ are real constants [41].

Appendix A: Some helpful formulas

Here we list some helpful integrals, which are not available in the integral table, used in the present work to calculate the momentum integral and the quantum correction terms [26,27]:

$$\int_{r_a}^{r_b} \frac{r}{\sqrt{(r - r_a)(r_b - r)}} dr = \frac{\pi}{2}(r_a + r_b), \tag{A1}$$

$$\int_{r_a}^{r_b} \frac{1}{r\sqrt{(r - r_a)(r_b - r)}} dr = \frac{\pi}{\sqrt{r_a r_b}}, \tag{A2}$$

$$\int_{r_a}^{r_b} \frac{1}{\sqrt{(r - r_a)(r_b - r)}} dr = \pi, \tag{A3}$$

$$\int_{r_a}^{r_b} \frac{1}{r}\sqrt{(r - r_a)(r_b - r)} dr = \left[\frac{1}{2}(r_a + r_b) - \sqrt{r_a r_b}\right]\pi. \tag{A4}$$

References

1. F. Cooper, A. Khare, U. Sukhatme, Phys. Rep. **251**, 267 (1995); D.A. Morales, Chem. Phys. Lett. **394**, 68 (2004)
2. A.F. Nikiforov, V.B. Uvarov, *Special Functions of Mathematical Physics*. (Birkhaauser, Basel, 1988); S.M. Ikhdair, Chinese J. Phys. **46**(3), 291 (2008); S.M. Ikhdair, R. Sever, Ann. Phys. (Leibzig) **16**, 218 (2007); S.M. Ikhdair, R. Sever, Int. J. Theor. Phys. **46**, 1643 (2007); S.M. Ikhdair, R. Sever, Int. J. Theor. Phys. **46**, 2384 (2007); J. Math. Chem. **42**, 461 (2007); quant-ph/0605045 to appear in Int. J. Mod. Phys. E; arXiv:0704.0489 to appear in Cent. Eur. J. Phys.; quant-ph/0703131 to appear in Cent. Eur. J. Phys.; quant-ph/0703008 to appear in Int. J. Mod. Phys. C; arXiv:0801.3518; arXiv:0801.4271; arXiv:080.14857
3. C.L. Pekeris, Phys. Rev. **45**, 98 (1934)
4. O. Bayrak, I. Boztosun, J. Phys. A: Math. Gen. **39**, 6955 (2006); H. Ciftci, R.L. Hall, N. Saad, J. Phys. A: Math. Gen. **36**, 11807 (2003); H. Ciftci, R.L. Hall, N. Saad, Phys. Lett. A **340**, 388 (2005)
5. E.D. Filho, R.M. Ricotta, Phys. Lett. A **269**, 269 (2000)
6. J.B. Killingbeck, A. Grosjean, G. Jolicard, J. Chem. Phys. **116**, 447 (2002)
7. M. Bag, M.M. Panja, R. Dutt, Phys. Rev. A **46**, 6059 (1992)
8. Z.Q. Ma, B.W. Xu, Europhys Lett. **69**, 685 (2005)
9. B. Gonul, K. Koksal, E. Bakir, Phys. Scr. **73**, 279 (2006); S.M. Ikhdair, R. Sever, Int. J. Mod. Phys. A **21**, 6465 (2006); S.M. Ikhdair, R. Sever, J. Mol. Struc.-Theochem **809**, 103 (2007); S.M. Ikhdair, R. Sever, J. Math. Chem. **41**, 329 (2007); S.M. Ikhdair, R. Sever, J. Math. Chem. **41**, 343 (2007)
10. S.M. Ikhdair, R. Sever, J. Mol. Struc.:Theochem. **806**, 155 (2007); S.M. Ikhdair, R. Sever, J. Mol. Struc.:Theochem. **855**, 13 (2008)
11. S.H. Dong, Int. J. Theor. Phys. **39**, 1119 (2000); S.H. Dong, Int. J. Theor. Phys. **40**, 569 (2001); S.H. Dong, Phys. Scr. **65**, 289 (2002)
12. A. Kratzer, Z. Phys. **3**, 289 (1920); S.M. Ikhdair, R. Sever, Int. J. Mod. Phys. C **19**, 221 (2008); S.M. Ikhdair, R. Sever, Cent. Eur. J. Phys. **6**, 141 (2008)
13. R.J. Le Roy, R.B. Bernstein, J. Chem. Phys. **52**, 3869 (1970)
14. S.M. Ikhdair, R. Sever, Z. Phys. C **56**, 155 (1992); S.M. Ikhdair, R. Sever, Z. Phys. C **58**, 153 (1993); S.M. Ikhdair, R. Sever, Z. Phys. D **28**, 1 (1993); S.M. Ikhdair, R. Sever, Hadronic J. **15**, 389 (1992); S.M. Ikhdair, R. Sever, Int. J. Mod. Phys. A **18**, 4215 (2003); S.M. Ikhdair, R. Sever, Int. J. Mod. Phys. A **19**, 1771 (2004); S.M. Ikhdair, R. Sever, Int. J. Mod. Phys. A **20**, 4035 (2005); S.M. Ikhdair, R. Sever, Int. J. Mod. Phys. A **20**, 6509 (2005); S.M. Ikhdair, R. Sever, Int. J. Mod. Phys. A **21**, 2191 (2006); S.M. Ikhdair, R. Sever, Int. J. Mod. Phys. A **21**, 3989 (2006); Int. J. Mod. Phys. A **21**, 6699 (2006); S.M. Ikhdair, R. Sever, Int. J. Mod. Phys. E **17**, 669 (2008); S. Ikhdair et al., Tr. J. Phys. **16**, 510 (1992); S. Ikhdair et al., Tr. J. Phys. **17**, 474 (1993)
15. S.M. Ikhdair, R. Sever, Cent. Eur. J. Phys. **5**, 516 (2007); S.M. Ikhdair, R. Sever, Cent. Eur. J. Phys. **6**, 697 (2008).
16. R.L. Hall, N. Saad, J. Chem. Phys. **109**, 2983 (1998)
17. M.R. Setare, E. Karimi, Phys. Scr. **75**, 90 (2007)
18. O. Bayrak, I. Boztosun, H. Ciftci, Int. J. Quant. Chem. **107**, 540 (2007)
19. K. Oyewumi, J. Found. Phys. Lett. **18**, 75 (2005)
20. G. van Hooydonk, J. Mol. Struc.-Theochem. **109**, 84 (1984)
21. D. Secrest, J. Chem. Phys. **89**, 1017 (1988)
22. A. Requena, J. Zuniga, L.M. Fuentes, A. Hidolgo, J. Chem. Phys. **85**, 3939 (1986)
23. J.M. Frances, J. Zuifga, M. Alacid , A. Requena, J. Appl. Phys. **90**, 5536 (1989)
24. C. Berkdemir, A. Berkdemir, J. Han, Chem. Phys. Lett. **417**, 326 (2006)
25. S.M. Ikhdair, R. Sever, J. Mol. Struct.-Theochem. **855**, 13 (2008)
26. S.H. Dong, D. Morales, J. Garcia-Ravelo, Int. J. Mod. Phys. E **16**, 189 (2007)
27. W.C. Qiang, S.H. Dong, Phys. Lett. A **363**, 169 (2007)
28. E. Merzbacher, *Quantum Mechanics*, 3rd edn. (Wiley, New York, 1998)
29. M. Abramowitz, I.A. Stegun, *Handbook of Mathematical Functions with Formula, Graphs and Mathematical Tables* (Dover, New York, 1970)
30. M.M. Nieto, L.M. Simmons Jr., Phys. Rev. A **19**, 438 (1979); M.M. Nieto, Am. J. Phys. **47**, 1067 (1979)
31. H.E. Montgomery Jr., N.A. Aquino, K.D. Sen, Int. J. Quant. Chem. **107**, 798 (2007)
32. D.R. Herrick, J. Math. Phys. **16**, 281 (1975); D.R. Herrick, F.H. Stillinger, Phys. Rev. **11**, 42 (1975)

33. D.D. Fratz, D.R. Herschbach, J. Chem. Phys. **92**, 6668 (1990)
34. L.E. Sutton, *Tables of Interatomic Distance and Configuration in Molecules and Ions* (Chemical Society of London, London, 1958)
35. M. Karplus, R.N. Porter, *Atoms and Molecules: An Introduction For Students of Physical Chemistry* (Benjamin, Menlo Park, CA, 1970)
36. L. Brewer, G.M. Rosenblatt, Adv. High Temp. Sci. **2**, 1 (1969)
37. A. Kant, J. Chem. Phys. **49**, 5144 (1968)
38. I.I. Gol'dman, V.D. Krivchenkov, V.I. Kogan, V.M. Galitskii, *Problems in Quantum Mechanics* (Academic, New York, 1960), p. 308
39. S. Flügge, *Practical Quantum Mechanics*, vol. 1 (Springer, Berlin, 1994), p. 178
40. S. Al-Jaber, Int. J. Theor. Phys. **37**, 1289 (1998)
41. F.M. Fernández, A.López Piñeiro, B. Moreno, J. Phys.: Math. Gen. **27**, 5013 (1994)