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ORIGINAL PAPER

Non-central potentials, exact solutions and Laplace transform approach

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Abstract Exact bound state solutions and the corresponding wave functions of the Schrödinger equation for some non-central potentials including Makarov potential, modified-Kratzer plus a ring-shaped potential, double ring-shaped Kratzer potential, modified non-central potential and ring-shaped non-spherical oscillator potential are obtained by using the Laplace transform approach. The energy spectrums of the Hartmann potential, modified-Kratzer potential and ring-shaped oscillator potential are also briefly studied as special cases. It is seen that our analytical results for all these potentials are consistent with those obtained by other works. We also give some numerical results obtained for the modified non-central potential for different values of the related quantum numbers.

Keywords Exact solution · Laplace transform · Non-central potential · Schrödinger equation

1 Introduction

An important part of chemistry based on quantum mechanics and also of nuclear physics include to study ro-vibrational energy levels of molecules and atoms having multi-electrons, the distorted nucleus and the correlation states of quantum fluid systems [1]. Describing ring-shaped molecules (like benzene) and interactions between

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deformed pairs of nuclei have received many applications in the above areas of physics [2]. Because of the above statements, the non-central potentials have been extensively studied in literature. Moreover, these potentials provide a useful theoretical ground describing the interaction between the ring-shaped molecules and the interaction between distorted nucleus [1,2].

Non-central potentials including also ring-shaped molecular potentials include two parts: The spherical harmonic oscillator potentials and angular dependent potentials as a second part. Such potentials studying in non-relativistic and/or relativistic quantum mechanical viewpoints by using different methods could be listed as: Hartmann [3] and Makarov potential [4] within the supersymmetric approach [5,6], algebraic investigation of the ring-shaped potential [7], a new anharmonic oscillator potential studying in terms of hypergeometric functions [8], investigation of a non-central potential parameterizing with $\hat{C}, C, C_0$ based on L^2-series solution [9], the Coulombic ring-shaped [10] and Makarov potential [11] within the Nikiforov-Uvarov formalism, relativistic searching of Makarov potential by factorization method [12], double ring-shaped oscillator potential within the supersymmetric formalism [13], the Hartmann potential via Laplace transforms [14], searching of some non-central potentials by using exact quantization rule [15], etc.

The non-central potentials are needed to obtain better results than those given of central potentials about the dynamical properties of the molecular structures and interactions [16]. Meanwhile, these potentials make it possible to obtain algebraic exact solutions of the Schrödinger equation (SE). To obtain the exact solutions of the SE for molecular potentials is one of the basic problems in quantum physics [17]. In this manner, we search in the present work the exact bound state solutions of the SE for some non-central potentials including the ring-shaped non-spherical oscillator potential, the Makarov potential, the modified Kratzer plus a ring-shaped potential and the double ring-shaped Kratzer potential. The Laplace transform approach (LTA) will be used to find the energy levels and the corresponding wave functions of the above potentials.

The LTA has been widely used to obtain the exact solutions of central and non-central potentials in the non-relativistic domain [14,18–20]. This approach is also used to find some recursion relations in terms of step-up and step-down operators for the harmonic oscillator [21]. The LTA describes a simple way for obtaining the solutions of the SE by reducing it to a first-order differential equation meaning that whose solutions may be obtained easily.

The organization of this letter is as follows. In Sect. 2, the time-independent SE in spherical coordinates is separated into radial and angular equations for a particle subjected to a non-central potential. In Sect. 3, the LTA is applied to the radial SE to obtain the energy spectrum of the above non-central potentials and the results are compared with those obtained before.

2 Equations in spherical coordinates

Time-independent SE in spherical coordinates is written [22]

$$\left\{\vec{\nabla}^2 - MV(r,\theta,\phi) + ME_{n\ell}\right\}\Psi(r,\theta,\phi) = 0\,, \tag{1}$$

where $M = \frac{2m}{\hbar^2}$, $E_{n\ell}$ is the particle energy and $V(r, \theta, \phi)$ is the potential field giving

$$V(r, \theta, \phi) = V(r) + \frac{V(\theta)}{r^2} + \frac{V(\phi)}{r^2 sin^2\theta}. \tag{2}$$

Writing the total wave function as

$$\Psi(r, \theta, \phi) = \mathcal{R}(r)\Theta(\theta)(sin\theta)^{-1/2}\Phi(\phi)\ ; \mathcal{R}(r) = \frac{R(r)}{r} \tag{3}$$

and using the method of separation of variables gives the following Eqs. [14,23]

$$\left\{\frac{d^2}{d\phi^2} - MV(\phi) + m^2\right\}\Phi(\phi) = 0, \tag{4a}$$

$$\left\{\frac{d^2}{d\theta^2} - MV(\theta) - \frac{\xi}{sin^2\theta} + \ell^2\right\}\Theta(\theta) = 0; \quad \xi = m^2 - \frac{1}{4}, \tag{4b}$$

$$\left\{\frac{d^2}{dr^2} - MV(r) - \frac{L}{r^2} + ME_{n\ell}\right\}R(r) = 0; \quad L = \ell^2 - \frac{1}{4}. \tag{4c}$$

where m^2 and ℓ^2 are separation constants. Throughout this paper $V(\phi)$ will be $V(\phi) = 0$, then Eq. (4a) becomes

$$\left\{\frac{d^2}{d\phi^2} + m^2\right\}\Phi(\phi) = 0\,, \tag{5}$$

and its solution

$$\Phi(\phi) = a_n e^{\pm im\phi}, \quad m = 0, 1, 2, \ldots \tag{6}$$

Now we use the LTA applied to Eq. (4c) to find the bound state solutions and the corresponding wave functions of the non-central potentials. It is well known that the contributions coming from the angular part of the potential are placed in the parameter ℓ in Eq. (4b). So, these contributions are taken from related literature while we are looking for the solutions of Eq. (4c).

3 Bound state solutions

3.1 Makarov potential

Inserting the Makarov potential [4]

$$V(r, \theta) = \frac{\alpha}{r} + \frac{\beta}{r^2 sin^2\theta} + \frac{\gamma cos\theta}{r^2 sin^2\theta}\,, \tag{7}$$

into Eq. (4b) we obtain the polar angle equation

$$\left\{\frac{d^2}{d\theta^2}-\frac{1}{sin^2\theta}\left(\xi+\frac{M}{r^2}\,(\beta+\gamma cos\theta)\right)+\ell^2\right\}\Theta(\theta)=0, \tag{8}$$

where the parameter ℓ is obtained as $\ell=\{\frac{1}{2}\,[\beta+m^2+\sqrt{(\beta+m^2)^2-\gamma^2}\,]\}^{1/2}+s+\frac{1}{2}$ in Ref. [15] and s is a positive integer.

The radial Eq. (4c) becomes for the Makarov potential

$$\left\{\frac{d^2}{dr^2}-\frac{M\alpha}{r}-\frac{L}{r^2}+ME_{n\ell}\right\}R(r)=0, \tag{9}$$

Rewriting the radial wave function as $\psi(r)=r^{-\frac{1}{2}}R(r)$ and inserting it into Eq. (9) we get

$$\left\{\frac{d^2}{dr^2}+\frac{1}{r}\frac{d}{dr}-\left(\mu_1^2+\frac{\mu_2^2}{r}+\frac{\mu_3^2}{r^2}\right)\right\}\psi(r)=0, \tag{10}$$

where

$$\mu_1^2=-ME_{n\ell};\quad \mu_2^2=M\alpha;\quad \mu_3^2=\frac{1}{4}+L \tag{11}$$

In order to obtain an equation suitable for applying the Laplace transform approach, we take the wave function as $\psi(r)=r^{\delta}g(r)$ with δ is a constant in Eq. (10) and then obtain

$$r^2\frac{d^2g(r)}{dr^2}+(2\delta+1)r\frac{dg(r)}{dr}-\left(\mu_1^2r^2+\mu_2^2r+\mu_3^2-\delta^2\right)g(r)=0\,, \tag{12}$$

Physically acceptable wave function has to be finite when $r\to\infty$ in Eq. (12), so the parameter δ should be $\delta=-\mu_3$ and we get

$$\left\{\frac{d^2}{dr^2}-(2\mu_3-1)\,\frac{1}{r}\,\frac{d}{dr}-\mu_1^2r-\mu^2\right\}g(r)=0\,, \tag{13}$$

By applying the Laplace transform defined as [24]

$$\mathcal{L}\{g(r)\}=f(t)=\int_0^{\infty}dre^{-tr}g(r), \tag{14}$$

to Eq. (13), we obtain

$$\left(t^2-\mu_1^2\right)\frac{df(t)}{dt}+\left\{(2\mu_3+1)\,t+\mu_2^2\right\}f(t)=0. \tag{15}$$

which is a first-order differential equation and its solution is written as

$$f(t) = a'(t+\mu_1)^{-(2\mu_3+1)} \left(\frac{t+\mu_1}{t-\mu_1}\right)^{\frac{\mu_2^2}{2\mu_1}+\frac{2\mu_3+1}{2}}. \tag{16}$$

In order to get single-valued wave functions, it should be

$$\frac{\mu_2^2}{2\mu_1} + \frac{2\mu_3+1}{2} = -n, \quad n = 0, 1, 2, \ldots \tag{17}$$

With the help of this condition, the function in Eq. (16) could be expended into series as

$$f(t) = a'' \sum_{k=0}^{n} \frac{(-1)^k n!}{(n-k)!k!} (2\mu_1)^k (t+\mu_1)^{-(2\mu_3+1)-k}, \tag{18}$$

where a'' is another constant. The solution of Eq. (13) is immediately obtained by applying the inverse-Laplace transformation [24]

$$g(r) = a''' r^{2\mu_3} e^{-\mu_1 r} \sum_{k=0}^{n} \frac{(-1)^k n!}{(n-k)!k!} \frac{\Gamma(2\mu_3+1)}{\Gamma(2\mu_3+1+k)} (2\mu_1 r)^k \tag{19}$$

which gives finally the eigenfunctions of the Makarov potential

$$R(r) = a_n r^{\mu_3+\frac{1}{2}} e^{-\mu_1 r} \, {}_1F_1(-n, 2\mu_3+1, 2\mu_1 r). \tag{20}$$

where a_n is normalization constant and used the following properties of hypergeometric functions [25]

$${}_1F_1(-n, \sigma, z) = \sum_{m=0}^{n} \frac{(-1)^m n!}{(n-m)!m!} \frac{\Gamma(\sigma)}{\Gamma(\sigma+m)} z^m. \tag{21}$$

Equation (17) with Eq. (11) gives us the following algebraic expression of the bound state of the Makarov potential

$$E_{n\ell} = -\frac{M\alpha^2}{4\left(n+\frac{1}{2}+\ell\right)^2}. \tag{22}$$

which is the same result with the ones given in Ref. [15].

Setting in Eq. (7) $\gamma = 0$ gives the Hartmann potential and Eq. (22) turns into

$$E_{n\ell} = -\frac{M\alpha^2}{(2n+\ell'+1)^2} \; ; \quad \ell' = 2\sqrt{\beta+m^2} + 2s + 1. \tag{23}$$

which is the exact energy states of the Hartmann potential [11,15].

3.2 Modified Kratzer plus a ring-shaped potential

This potential has the form

$$V(r,\theta) = D_0\left(1-\frac{r_0}{r}\right)^2 + \frac{\beta}{r^2}\left(\frac{cos\theta}{sin\theta}\right)^2, \tag{24}$$

where D_0 is the association energy and r_0 is the equilibrium distance of the molecule. Inserting this into Eqs. (4b) and (4c), we obtain the angular dependent and radial equations as

$$\left\{\frac{d^2}{d\theta^2} + \beta M - \frac{\xi+\beta M}{sin^2\theta} + \ell^2\right\}\Theta(\theta) = 0, \tag{25a}$$

$$\left\{\frac{d^2}{dr^2} - \frac{MD_0r_0^2+L}{r^2} + \frac{2MD_0r_0}{r} + M(E_{n\ell}-D_0)\right\}R(r) = 0. \tag{25b}$$

where the parameter ℓ is obtained as $\ell^2 = (\sqrt{\beta+m^2}+s+1/2)^2 - \beta$ in Ref. [15].

We apply the LTA to Eq. (25b) to obtain the exact bound state solutions and the corresponding eigenfunctions of the modified Kratzer plus a ring-shaped potential. We follow the same procedure in the above section, since the radial equations in Eq. (10) and Eq. (25b) have the same form. In the present case, the parameters in Eq. (11) become

$$\mu_1^2 = M(D_0 - E_{n\ell}); \quad \mu_2^2 = -2MD_0r_0; \quad \mu_3^2 = L + MD_0r_0^2 + \frac{1}{4} \tag{26}$$

Using the same transformations in the above section on the wave functions and requirements, we obtain the radial eigenfunctions of the modified Kratzer plus a ring-shaped potential as

$$R(r) = b_n r^{\mu_3+\frac{1}{2}} e^{-\mu_1 r}\, {}_1F_1(-n, 2\mu_3+1, 2\mu_1 r), \tag{27}$$

where b_n is normalization constant.

In order to get a single-valued wave functions the parameters must be satisfied an equation like Eq. (17) which gives the energy spectrum of the modified Kratzer plus a ring-shaped potential as

$$E_{n\ell} = D_0 - \left[\frac{2n+1+\sqrt{MD_0r_0^2+\ell^2}}{2MD_0r_0}\right]^{-2}, \tag{28}$$

which is the same result with the one given in Ref. [15]. If $\beta = 0$ in Eq. (24), we have the modified Kratzer potential whose energy spectrum is obtained from the last equation

$$E_{n\ell} = D_0 - \left[\frac{2MD_0r_0}{2n+1+\sqrt{MD_0r_0^2+\mathcal{L}(\mathcal{L}+1)+\frac{1}{4}}} \right]^2 . \tag{29}$$

where the parameter $\mathcal{L}$ is defined as $\mathcal{L}(\mathcal{L}+1) = \ell^2(\beta \to 0) - \frac{1}{4}$. This spectrum is exactly of the modified Kratzer potential [26].

3.3 Double ring-shaped Kratzer potential

This potential is given [27]

$$V(r,\theta) = -2D_0 \left\{ \frac{r_0}{r} - \frac{1}{2}\left(\frac{r_0^2}{r^2}\right) \right\} + \frac{1}{r^2}\left(\frac{\beta}{sin^2\theta} + \frac{\gamma}{cos^2\theta} \right), \tag{30}$$

which gives for $\beta = \gamma = 0$ the Kratzer potential. For this potential, Eqs. (4b) and (4c) gives the following equations

$$\left\{ \frac{d^2}{d\theta^2} - \frac{M\gamma}{cos^2\theta} - \frac{\xi+\beta M}{sin^2\theta} + \ell^2 \right\} \Theta(\theta) = 0\,, \tag{31a}$$

$$\left\{ \frac{d^2}{dr^2} + ME_{n\ell} - \frac{2MD_0r_0}{r} - \frac{MD_0r_0^2+L}{r^2} \right\} R(r) = 0. \tag{31b}$$

where the parameter ℓ is obtained as $\ell = \sqrt{\beta^2+m} + \sqrt{\frac{1}{4}+\gamma} + 2s + 1$ in Ref. [15].

Following the same procedure in last two sections we obtain the energy levels of the double ring-shaped Kratzer potential and the corresponding eigenfunctions, respectively,

$$E_{n\ell} = -M \left\{ \frac{D_0r_0}{n+\frac{1}{2}+\sqrt{\ell^2+MD_0r_0^2}} \right\}^2 , \tag{32}$$

and

$$R(r) = c_n r^{\mu_3+\frac{1}{2}} e^{-\mu_1 r}\, {}_1F_1(-n, 2\mu_3+1, 2\mu_1 r). \tag{33}$$

where c_n is normalization constant and the parameters in Eq. (11) have the values in the present case

$$\mu_1^2 = -ME; \quad \mu_2^2 = 2MD_0r_0; \quad \mu_3^2 = L + MD_0r_0^2 + \frac{1}{4} \tag{34}$$

It is seen that the result given in Eq. (32) is consistent with the one obtained in Ref. [27].

3.4 Modified non-central potential

The modified non-central potential is written [28]

$$V(r,\theta) = D\left(1-\frac{a}{r}\right)^2 + \frac{\beta}{r^2 sin^2\theta} + \frac{\gamma cos\theta}{r^2 sin^2\theta}, \tag{35}$$

where the parameter D corresponds to the association energy and a corresponds to the equilibrium distance of the molecule. The radial part of this potential is similar to that of the potential in Eq. (24). By inserting Eq. (35) into Eqs. (4b) and (4c) we obtain the following angular dependent and radial equations, respectively,

$$\left\{\frac{d^2}{d\theta^2} - \frac{M\beta+\xi+M\gamma cos\theta}{sin^2\theta} + \ell^2\right\}\Theta(\theta) = 0, \tag{36a}$$

$$\left\{\frac{d^2}{dr^2} + M(E_{n\ell} - D) + \frac{2MDa}{r} - \frac{MDa^2+L}{r^2}\right\}R(r) = 0. \tag{36b}$$

where the parameter ℓ is given as $\ell = \sqrt{\frac{1}{2}}\sqrt{M\beta + m^2 + \sqrt{(m^2+M\beta)^2 - (M\gamma)^2}} + s$ in Ref. [16]. In the present case, applying the LTA as in the above subsections gives the energy spectrum and the corresponding eigenfunctions of the modified non-central potential

$$E_{n\ell} = D - \left(\frac{2\sqrt{M}\,Da}{2n+1+\sqrt{4MDa^2+4\ell(\ell+1)+1}}\right)^2, \tag{37}$$

and

$$R(r) = d_n r^{\mu_3+\frac{1}{2}} e_1^{-\mu_1 r} F_1(-n, 2\mu_3+1, 2\mu_1 r). \tag{38}$$

where d_n is normalization constant and

$$\mu_1^2 = -M(E_{n\ell} - D); \quad \mu_2^2 = -2MDa; \quad \mu_3^2 = L + MDa^2 + \frac{1}{4}. \tag{39}$$

Now we give the results our numerical analysis for the diatomic molecule N_2 in Table 1 where the energy eigenvalues are given for different values of quantum numbers and the parameters of β and γ. Our parameter values for N_2 molecule are as follows: $D = 11.9384$ eV, $\mu = 7.00335$ amu and $a = 1.0940$ Å [26]. From Table 1, we see that the contributions coming from angular dependent part of the potential in Eq. (37) are negligible than the results obtained for the pure Kratzer potential ($\beta = \gamma = 0$).

Table 1 Energy eigenvalues of the modified non-central potential for different values of quantum numbers in eV for N_2 molecule

			$E_{n\ell}$		Ref. [26]
n	s	m	$\beta=\gamma=0.1$	$\beta=\gamma=0$	
0	0	0	11.93837780671	0.05443703	0.054430
1	0	0	11.93837780698	0.16207785	0.162057
	1	1	11.93837780740	0.16354346	0.162546
2	0	0	11.93837780726	0.26826281	0.268229
	1	1	11.93837778077	0.26970864	0.268711
	2	2	11.93837780810	0.27308086	0.269675
3	0	0	11.93837780754	0.37301804	0.372972
	1	1	11.93837780800	0.37444445	0.373447
	2	2	11.93837780840	0.37777137	0.374398
	3	3	11.93837780880	0.38299550	0.375823

3.5 Ring-shaped non-spherical oscillator potential

As final potential, we search the energy levels and the corresponding wave functions of the ring-shaped oscillator potential which is given [29]

$$V(r,\theta)=\kappa r^2+\frac{\omega}{r^2}+\frac{1}{r^2}\,\beta cosec^2\theta, \tag{40}$$

Inserting this potential to the SE gives the following two equations

$$\left\{\frac{d^2}{d\theta^2}-\frac{\xi+\beta M}{sin^2\theta}+\ell^2\right\}\Theta(\theta)=0, \tag{41a}$$

$$\left\{\frac{d^2}{dr^2}-M\kappa r^2-\frac{L+M\omega}{r^2}+ME_{n\ell}\right\}R(r)=0. \tag{41b}$$

where the parameter ℓ is given as $\ell=\sqrt{\beta+m^2}+\frac{1}{2}+s$ [15].

Defining a new variable $r^2=u$, taking a trial wave function as $R=u^{-\tau/2}\phi(u)$ and using the following abbreviations

$$\mu_1^2=-M\kappa;\quad \mu_2^2=ME_{n\ell};\quad \tau(\tau+1)=L+M\omega \tag{42}$$

Equation (41b) turns into

$$u\frac{d^2\phi(u)}{du^2}-\left(\tau-\frac{1}{2}\right)\frac{d\phi(u)}{du}-\frac{1}{4}\left(\mu_1^2u-\mu_2^2\right)\phi(u)=0, \tag{43}$$

Applying the Laplace transform to Eq. (43) we obtain a first-order differential equation

$$\left(t^2-\frac{\mu_1^2}{4}\right)\frac{df(t)}{dt}+\left\{\left(\tau+\frac{3}{2}\right)t-\frac{\mu_2^2}{4}\right\}f(t)=0\,, \tag{44}$$

whose solution is

$$f(t) = e' \left(t + \frac{\mu_1}{2}\right)^{-\frac{\mu_2^2}{4\mu_1} - \frac{1}{2}\left(\tau + \frac{3}{2}\right)} \left(t - \frac{\mu_1}{2}\right)^{\frac{\mu_2^2}{4\mu_1} - \frac{1}{2}\left(\tau + \frac{3}{2}\right)}, \tag{45}$$

where e' is a constant determining later.

We find a physically acceptable wave function (finite) only if

$$\frac{\mu_2^2}{4\mu_1} - \frac{1}{2}\left(\tau + \frac{3}{2}\right) = n, \quad n = 0, 1, 2, \ldots \tag{46}$$

By using this requirement and expanding the function in Eq. (45) into series, we get

$$f(t) = e'' \sum_{k=0}^{n} \frac{(-1)^k n!}{(n-k)!k!} \left(t + \frac{\mu_1}{2}\right)^{-(\tau + \frac{3}{2} + k)}, \tag{47}$$

where e'' is another constant. Using the inverse Laplace transform we obtain the solution of Eq. (43)

$$\phi(u) = e''' e^{-\mu_1 u/2} u_1^{\tau + 1/2} F_1\left(-n, \tau + \frac{3}{2}, u\right), \tag{48}$$

where e''' is a constant and used the property of the hypergeometric functions given in Eq. (21). The radial wave functions of the ring-shaped oscillator is

$$R(u) = e_n e^{-\mu_1 u/2} u^{(\tau+1)/2}\, {}_1F_1\left(-n, \tau + \frac{3}{2}, u\right), \tag{49}$$

where e_n is normalization constant. Equation (46) with the help of Eq. (42) gives the energy spectrum of the ring-shaped non-spherical oscillator potential

$$E_{n\ell} = 2\sqrt{\frac{\kappa}{M}}\left[2n + \sqrt{\ell^2 + M\omega} + 1\right]. \tag{50}$$

The ring-shaped oscillator potential [7] is obtained by setting $\omega = 0$ in Eq. (40) which gives from last equation

$$E_{n\ell} = \sqrt{\frac{16\kappa}{M}}\left(n + \ell' + \frac{1}{2}\right). \tag{51}$$

where $\ell' = \ell/2$ and last equation is the same result with the ones obtained in Ref. [30] if setting $\kappa = \frac{\omega^2}{4}$ and $M = 1$.

4 Conclusions

We have obtained the exact energy spectrum of some non-central potentials such as Makarov potential, modified-Kratzer plus a ring-shaped potential, double ring-shaped Kratzer potential, modified non-central potential and ring-shaped non-spherical oscillator potential by applying the Laplace transform approach to the related part of the Schrödinger equation in spherical coordinates. We have also obtained the corresponding eigenfunctions of the above diatomic potentials. We have discussed briefly some special cases of the potentials and observed that our analytical results and also the results for the special cases are the same with the ones obtained in literature. It is shown that the Laplace transform approach is an applicable formalism to obtain the energy spectrum and the eigenfunctions of some non-central potentials.

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