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WKB Energy Expression for the Radial Schrödinger Equation with a Generalized Pseudoharmonic **Potential**

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Authors' contributions

This work was carried out in collaboration among all authors. Author EO designed the study, performed the statistical analysis, wrote the protocol and wrote the first draft of the manuscript. Authors OEO and IBO managed the analyses of the study. All authors read and approved the final manuscript.

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ABSTRACT

In this paper, we applied the semi-classical quantization approximation method to solve the radial Schrödinger equation with a generalized Pseudoharmonic potential. The four turning points problem within the framework of the Wentzel-Kramers-Brillouin (WKB) method was transformed into two turning points and subsequently, the energy spectrum was obtained. Some special cases of the generalized Pseudoharmonic potential are presented. The WKB approximation approach reproduces the exact energy expression obtained with several analytical methods in the literature. The values of the energy levels for some selected diatomic molecules (N_2 , CO, NO, CH) obtained numerically are in excellent agreement with those from previous works in the literature.

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1. INTRODUCTION

The Schrödinger equation (SE) plays a significant role in quantum mechanics in that its solution can be used to investigate the eigenstates of guantum mechanical systems. The knowledge of the bound states solutions and the wave functions are crucial to understanding the electronic state of atoms and molecules. The SE has been solved for several potentials of interest. Some of these potentials are exactly solvable while the non-exactly solvable potentials can be approximated by using a numerical approach and appropriate analytical methods. Some methods that are routinely used to estimate the bound states solutions of the SE are the Asymptotic iterative method [1-4]. Nikiforov-Uvarov method [5-9], supersymmetric quantum mechanics approach [10,11] analytical exact iterative method [12], I/N expansion approach [13], Artificial neural network scheme [14], the WKB approximation method [15-22] and so on.

In this paper, we considered the radial SE with a generalized Pseudoharmonic potential (PHP) modeled as

$$V(r) = (a_1 + a_2)r^2 + \frac{(b_1 + b_2)}{r^2} + c_1 + c_2,$$
(1)

where a_1, a_2, b_1, b_2, c_1 and c_2 are arbitrary potential parameters. The PHP is used in chemical and molecular physics to study the rovibrational states and spectra of diatomic molecules including nuclear rotations and vibrations [23,24]. Several methods have been applied to obtain the eigenenergies and wave functions of the radial SE with the PHP. The Laplace transform approach was applied to the radial SE with a generalized PHP [23,24]. Das and Arda [23] presented the special cases of the reduced generalized PHP such as the isotropic harmonic oscillator, isotropic plus inverse quadratic potentials. Rani et al. [25] presented the solutions of the radial SE with Kratzer and PHP molecular potentials using a series expansion approach. They obtained the energy states for some diatomic molecules such as CO, NO, N₂, and CH. Ikhdair and Sever [26] used a polynomial method to obtain the energy spectrum and wave function for the PHP and computed the energy states for some selected diatomic molecules such as N₂, CO, NO and CH. The Nikiforov-Uvarov method was applied to obtain the eigensolutions of the PHP [8,27]. Ovewumi and Sen [28] solved the radial SE for the PHP using the SU (1, 1) spectrum generating algebra method. They obtained the energy states. expectation values and Heisenberg uncertainty product of some diatomic molecules such as CO, NO, O₂, N₂, CH, H₂ and ScH. Furthermore, Oyewumi et al. [29] studied the effects of external magnetic field on the bound states of the two-dimensional radial SE with a PHP. Using different Larmor frequencies and potential the energy parameters. they obtained fluctuations both in the presence and absence of a magnetic field. Ikhdair and Sever [30] applied the eigenfunction ansatz method to solve the two-dimensional SE with the PHP and Kratzer potentials. The approach used in Ikhdair and Sever [30], was also applied to the threedimensional SE for the PHP and Mie-type potentials [31]. The supersymmetric [32] and algebra methods [33] have been used to obtain exact bound states solutions of the PHP. The dynamical algebra of the PHP was also studied [34] in which the ladder operators were constructed directly from the wave function. Dong [34] using factorization, showed that the ladder operators satisfied the commutation relation of the dynamical SU (1, 1) group generators.

The remaining part of the paper is structured as follows. In section two, we present a brief review of the WKB approximation approach. Section three contains the bound states solutions of the radial SE with the PHP given in (1) using the WKB approximation approach. Furthermore, special cases of the modeled potential are discussed in section four. The obtained energy expression is applied to some selected diatomic molecules (N₂, CO, NO, CH). The article is finally concluded in section five.

2. THE WKB APPROXIMATION METHOD

The WKB approximation method offers a way of finding approximate solutions of linear differential equations including the SE. For the SE, it is used to investigate tunneling rates through a potential barrier and also for the calculation of the bound states of potentials of interest [35]. Omugbe [35] stated that the WKB method yield accurate energy eigenvalues for large values of the radial quantum number and also suitable for slow varying potential functions. Hruska et al. [36] stated that the WKB bound states accuracies may vary substantially for the ground and other low lying states depending on the potential energy function. Furthermore, the leading order WKB approximation scheme does not yield an exact eigenvalue of the radial SE [19]. To overcome this problem, the centrifugal barrier term $l(l+1)\hbar^2/2\mu r^2$ in the radial SE has to be replaced with the term $\left(l + \frac{1}{2}\right)^2 \hbar^2/2\mu r^2$. This modification is known as the Langer correction [37]. Sergeenko [21] stated that the Langer correction regularizes the WKB wave function at the origin and ensures correct asymptotic behaviour at large radial quantum numbers. Thus at l = 0, the orbital centrifugal term is nonvanishing. This gives the contribution of the quantum fluctuation of the angular momentum to the ground state energy [19].

The three-dimensional time-independent SE with a reduced mass μ and wave-function $\psi(r, \theta, \phi)$ is given as

$$-\frac{\hbar^{2}}{2\mu} \left[\frac{1}{r^{2}} \frac{\partial}{\partial r} \left(r^{2} \frac{\partial}{\partial r} \right) + \frac{1}{r^{2} \sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial}{\partial \theta} \right) + \frac{1}{r^{2} \sin^{2} \theta} \frac{\partial^{2}}{\partial \phi^{2}} \right] \psi(r, \theta, \phi) + V(r) \psi(r, \theta, \phi) = E \psi(r, \theta, \phi)$$

$$(2)$$

Substituting $\psi(r, \theta, \phi) = \frac{R(r)Y(\theta, \phi)}{r}$ into (2), with the appropriate separation constant, we obtain the radial SE as

$$\frac{d^2 R(r)}{dr^2} + \frac{2\mu}{\hbar^2} \left[E - V_{eff}(r) \right] R(r) = 0.$$
(3)

where the effective potential is given as

$$V_{eff}(r) = V(r) + \frac{\left(l + \frac{1}{2}\right)^2 \hbar^2}{2\mu r^2}$$
(4)

We can recast Eq. (3) as

$$\left[\left(-i\frac{d}{dr}\right)^{2}\right]R(r) = \frac{2\mu}{\hbar^{2}}\left[E - V(r) - \frac{\left(l + \frac{1}{2}\right)^{2}\hbar^{2}}{2\mu r^{2}}\right]R(r).$$
 (5)

From (5) the classical momentum is given by

$$P(r) = \left\{ \frac{2\mu}{\hbar^2} \left[E - V(r) - \frac{\left(l + \frac{1}{2}\right)^2 \hbar^2}{2\mu r^2} \right] \right\}^{\frac{1}{2}}.$$
 (6)

The standard WKB quantization condition [21,36] for two turning point (r_1 , r_2) problem is given as

$$\int_{r_1}^{r_2} P(r) dr = \pi \left(n + \frac{1}{2} \right), r_1 < r < r_2 \quad n = 0, 1, 2 \cdots$$
(7)

The turning points are gotten from Eq. (6) by setting P(r) = 0. The semi-classical wave

function in the leading \hbar approximation has the form of

$$\psi^{WKB}(r) = \frac{N}{\sqrt{P(r)}} exp\left[\pm \frac{i}{\hbar} \int P(r) dr\right].$$
(8)

3. SOLUTION OF THE RADIAL SE

To obtain the energy eigenvalues, we substitute (6) into (7) with the PHP given in (1)

$$\int_{r_1}^{r_2} \left\{ \frac{2\mu}{\hbar^2} \left[E - (a_1 + a_2)r^2 - \frac{(b_1 + b_2)}{r^2} - c_1 - c_2 - \frac{(b_1 + b_2)^2}{2\mu r^2} - c_1 - c_2 \right] \right\}^{\frac{1}{2}} dr = \pi \left(n + \frac{1}{2} \right),$$
(9)

That is

$$\int_{r_1}^{r_2} \frac{1}{r} \left\{ -\frac{2\mu}{\hbar^2} (a_1 + a_2) r^4 + \frac{2\mu}{\hbar^2} [E - (c_1 + c_2)] r^2 - \frac{2\mu}{\hbar^2} (b_1 + b_2) + \left(l + \frac{1}{2} \right)^2 \right\}^{\frac{1}{2}} dr$$

$$= \pi \left(n + \frac{1}{2} \right)$$
(10)

Equation (10) is further reduced to

$$\sqrt{\frac{2\mu}{\hbar^2}(a_1+a_2)} \int_{r_1}^{r_2} \frac{1}{r} \Biggl\{ -r^4 + \frac{\frac{2\mu}{\hbar^2}[E-(c_1+c_2)]}{\frac{2\mu}{\hbar^2}(a_1+a_2)} r^2 - \frac{\frac{2\mu}{\hbar^2}(b_1+b_2) + \left(l+\frac{1}{2}\right)^2}{\frac{2\mu}{\hbar^2}(a_1+a_2)} \Biggr\}^{\frac{1}{2}} dr = \pi \left(n + \frac{1}{2}\right),$$
(11)

With

$$\bar{A} = \frac{2\mu}{\hbar^2}(a_1 + a_2),$$
 (12a)

$$B = \frac{\frac{2\mu}{\hbar^2} [E - (c_1 + c_2)]}{\bar{A}}$$
(12b)

and

$$C = \frac{\frac{2\mu}{\hbar^2}(b_1 + b_2) + \left(l + \frac{1}{2}\right)^2}{\bar{A}},$$
 (12c)

Equation (11) can be written as

$$\sqrt{\bar{A}} \int_{r_1}^{r_2} \frac{1}{r} \sqrt{-r^4 + Br^2 - C} \, dr = \pi \left(n + \frac{1}{2} \right) \tag{13}$$

We obtained the turning points by equating the momentum term to zero

$$-r^4 + Br^2 - C = 0 \tag{14}$$

Equation (14) yield four turning points r_1 , r_2 , r_3 and r_4 . Sergeenko [19,22] stated that the four

turning points problem can either be solved in the complex plane for r < 0 or in the physical axis (r > 0) provided that the potential function is symmetric. The generalized PHP is a symmetric function and using the transformation $r^2 = t$ reduces the four turning points problem to a two turning points one [19,22].

Using the transformation $r^2 = t$ in (14) implies that

$$-t^2 + Bt - C = 0 (15)$$

The roots of (15) are

$$t_1 = \frac{B - \sqrt{B^2 - 4C}}{2}$$
 (16a)

$$t_2 = \frac{B + \sqrt{B^2 - 4C}}{2}$$
 (16b)

Next we substitute the turning points with the transformation $r^2 = t$ into the WKB quantization condition in (13) to obtain

$$\frac{\sqrt{A}}{2} \int_{t_1}^{t_2} \frac{1}{t} \sqrt{-t^2 + Bt - C} dt = \pi \left(n + \frac{1}{2} \right).$$
(17)

We can write (17) in a regular form to obtain

$$\frac{\sqrt{A}}{2} \int_{t_1}^{t_2} \frac{1}{t} \sqrt{(t-t_1)(t_2-t)} dt = \pi \left(n + \frac{1}{2}\right).$$
(18)

Using the standard integral in the literature [36, 38], we evaluated (18) and obtained

$$\frac{\sqrt{\bar{A}}}{2} \left[\frac{1}{2} (t_1 + t_2) - \sqrt{t_1 t_2} \right] = n + \frac{1}{2}$$
(19)

Substituting the turning points in (16a) and (16b) with the constants A, B and C in (12a), (12b) and (12c) into (19) yields

$$E_{nl} = \sqrt{\frac{8(a_1+a_2)\hbar^2}{\mu}} \left[n + \frac{1}{2} + \frac{1}{4} \sqrt{\frac{8\mu(b_1+b_2)}{\hbar^2}} + (2l+1)^2 \right] + c_1 + c_2$$
(20)

Equation (20) is the exact energy spectrum of the radial SE with the generalized PHP. In the next section we now consider some special cases of the generalized PHP given by (1).

4. RESULTS AND DISCUSSION

Case 1. If we set $a_1 = b_1 = c_1 = 0$, $a_2 = \frac{D_e}{r_e^2}$, $b_2 = D_e r_e^2$, $c_2 = -2D_e$ in (1), where $D_e = \frac{1}{8}k_e r_e^2$ is the dissociation energy with force constant k_e and r_e is an equilibrium constant, then we obtain a molecular PHP. The plots of the potential energy variation with radial distance for (N₂, CO, NO and CH) are shown in Fig. 1.

In this case, the exact energy equation for the molecular PHP is given as

$$E_{nl} = \sqrt{\frac{8\left(\frac{D_e}{r_e^2}\right)\hbar^2}{\mu}} \left[n + \frac{1}{2} + \frac{1}{4}\sqrt{\frac{8\mu(D_e r_e^2)}{\hbar^2} + (2l+1)^2} \right] - 2D_e$$
(21)



Fig. 1. Potential energy variation with radial distance for selected diatomic molecules

Equation (21) is identical to the eigenvalue equations obtained by other analytical methods in the literature [23-28,31-33]. Using the given in spectroscopic parameters [27] the Table 1 with conversion $\hbar c = 1973.29 \text{ eVÅ}, 1 \text{amu} = 931.494028 \text{ Mev}/c^2$, we applied (21) to generate the eigenvalues for any arbitrary n and l quantum numbers of some selected diatomic molecules as shown in Table 2 and Table 3. In comparison, our numerical results for the selected molecules N₂, CO, NO and CH are in good agreement with the results reported by Ikhdair and Sever [26].

Case 2. For
$$a_1 = \frac{V_0}{R^2}$$
, $c_2 = -V_0$, $a_2 = b_1 = 0$, $b_2 = 0$, $c_1 = 0$,

where *R* represents a quantum dot radius and V_0 is a positive potential parameter, (1) reduces to the parabolic or shifted isotropic harmonic potential used as a model to study electron states in semiconductor quantum dots [39,40]. The energy spectrum is given as

$$E_{nl} = \sqrt{\frac{2V_0\hbar^2}{\mu R^2}} \left(2n + l + \frac{3}{2}\right) - V_0.$$
 (22)

For (22) is similar to the respective (4) and (10) in the literature [39,40].

Case 3. $a_1 = \frac{1}{2}\mu\omega^2$, $b_1 \neq 0$, $a_2 = b_2 = c_2 = c_1 = 0$. The generalized PHP reduces to the isotropic harmonic oscillator potential plus the inverse quadratic potential. The obtained eigenenergy equation becomes

$$E_{nl} = \frac{\hbar\omega}{2} \left[4n + 2 + \sqrt{\frac{8\mu(b_1)}{\hbar^2} + (2l+1)^2} \right],$$
 (23)

where μ and ω are the respective reduced mass and angular frequency. Equation (23) is equivalent to the respective expression (41), (38) and (30) obtained in the literature [23,41,42]

If we set $b_1 = 0$ in (23) we obtain the energy spectrum of the 3D isotropic harmonic oscillator given as

$$E_{nl} = \hbar\omega \left(2n + l + \frac{3}{2}\right) \tag{24}$$

Table 1. Potential parameters for selected diatomic molecules taken from Sever et al. [27]

Molecules	D_e (in eV)	<i>r_e</i> (in Å)	μ (in amu)
N ₂	11.938193820	1.0940	7.00335000
CO	10.845073641	1.1283	6.86058600
NO	8.043729855	1.1508	7.468441000
CH	3.947418665	1.1198	0.929931000

Table 2. Bound state energies E	E_{nl} (in eV) for N ₂ and CO	molecules in comparison v	with previous
	work [26]		

Sta	ate	N ₂		CO	
n	l	Present	[26]	Present	[26]
0	0	0.1091850	0.1091559	0.1019487	0.1019306
1	0	0.3274303	0.3273430	0.3057266	0.3056722
	1	0.3279290	0.3278417	0.3062052	0.3061508
2	0	0.5456756	0.5455302	0.5095044	0.5094137
	1	0.5461744	0.5460288	0.5099830	0.5098923
	2	0.5471718	0.5470260	0.5109402	0.5108495
4	0	0.9821663	0.9819045	0.9170601	0.9168969
	1	0.9826650	0.9824031	0.9175387	0.9173755
	2	0.9836624	0.9834003	0.9184958	0.9183327
	3	0.9851585	0.9848961	0.9199316	0.9197684
	4	0.9871530	0.9868903	0.9218457	0.9216825
5	0	1.2004116	1.2000916	1.1208379	1.1206384
	1	1.2009103	1.2005902	1.1213165	1.1211170
	2	1.2019077	1.2015875	1.1222737	1.1220742
	3	1.2034038	1.2030832	1.1237094	1.1235099
	4	1.2053983	1.2050774	1.1256235	1.1254240
	5	1.2078913	1.2075699	1.1280160	1.1258165

Sta	ate	NC)	CH	
n	l	Present	[26]	Present	[26]
0	0	0.0825103	0.0824883	0.1686793	0.1686344
1	0	0.2474251	0.2473592	0.5051418	0.5050072
	1	0.2478477	0.2477817	0.5087256	0.5085903
2	0	0.4123400	0.4122301	0.8416042	0.8413800
	1	0.4127626	0.4126526	0.8451881	0.8449631
	2	0.4136078	0.4134977	0.8523508	0.8521246
4	0	0.7421697	0.7419718	1.5145292	1.5141255
	1	0.7425923	0.7423944	1.5181130	1.5177087
	2	0.7434376	0.7432395	1.5252759	1.5248701
	3	0.7447053	0.7445070	1.5360079	1.5356002
	4	0.7463955	0.7461969	1.5502946	1.5498843
5	0	0.9070845	0.9068427	1.8509917	1.8504983
	1	0.9075072	0.9072653	1.8545756	1.8540815
	2	0.9083524	0.9081104	1.8617383	1.8612429
	3	0.9096202	0.9093779	1.8724703	1.8719729
	4	0.9113104	0.9110678	1.8867571	1.8862571
	5	0.9134229	0.9131799	1.9045795	1.9040761

Table 3. Bound state energies E_{nl} (in eV) for NO and CH molecules in comparison with
previous work [26]

Case 4
$$a_2 = \frac{D_e}{r_e^2}, \ b_2 = D_e r_e^2, \ c_2 = -2D_e$$

 $a_1 = \frac{1}{2}\omega_L^2, \ b_1 = 0, \ c_1 = m\omega_L.$

With $m = \left(l + \frac{1}{2}\right)$ in (3), the radial SE reduces to a two-dimensional problem. The constants D_e and r_e have their usual meanings while mand ω_L are the respective eigenvalues of the angular momentum and Larmor frequency [29]. The eigenvalue equation in this case using (20) is

$$E_{nm} = \sqrt{\frac{\left(\omega_L^2 + \frac{2D_e}{r_e^2}\right)\hbar^2}{\mu}} \left[(2n+1) + \sqrt{\frac{2\mu(D_e r_e^2)}{\hbar^2} + m^2} \right] + m\omega_L - 2D_e$$
(25)

Equation (25) gives the exact analytical energy expression of the two-dimensional radial SE with the PHP in the presence of magnetic field [29]. Also if we set $\omega_L = 0$, we will obtain similar result of the energy eigenvalue equation given in the literature [30,42].

$$E_{nm} = \sqrt{\frac{\left(\frac{2D_e}{r_e^2}\right)\hbar^2}{\mu}} \left[(2n+1) + \sqrt{\frac{2\mu(D_e r_e^2)}{\hbar^2} + m^2} \right] - 2D_e$$
(26)

5. CONCLUSION

The WKB approximation scheme offers a direct and simple way of obtaining the solutions of the bound states of the wave equation if the momentum of a quantum system is known. We applied this scheme to the radial SE and obtained the analytical energy expression of the modeled generalized PHP. This potential with other molecular potentials such as the Morse, Kratzer-Fues, Mie-type potentials, etc is used as a model in chemical and molecular physics for studying the rovibrational states and spectra states of diatomic molecules. Furthermore the potential can be applied to study bound state energies of guarkonia and guantum dots systems [25,39]. The WKB approximation method reproduces equivalent energy eigenvalues equations obtained with other analytical methods [23-28,31-33]. The energy eigenvalues of selected diatomic molecules such as N2, CO, NO, and CH, obtained numerically are in excellent agreement with the results in previous analytical works [23-28,32].

COMPETING INTERESTS

Authors have declared that no competing interests exist.

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