Research article

Nonrelativistic treatment of inversely quadratic Hellmann-Kratzer potential and thermodynamic properties

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A B S T R A C T

The study presents approximate analytical solutions of the Schrödinger equation with a newly proposed potential model called Inversely Quadratic Hellmann-Kratzer potential (IQHKP). This potential is a superposition of Inversely Quadratic Hellman potential and Kratzer potential. The energy eigenvalues and corresponding wavefunction are calculated via the formula method. We applied our results to evaluate thermodynamic functions such as vibrational free energy, F, vibrational internal energy, U, vibrational entropy, S, and vibrational specific heat, C. We also reported special cases of importance.

1. Introduction

The interaction of two or more potential models in describing quantum systems is interesting due to increased applications. Many known potential models have been combined recently in the framework of the Schrödinger equation with great success [1, 2, 3, 4, 5, 6, 7]. As a motivation, in the present study, a superposition of the inversely quadratic Hellmann and Kratzer potentials (IQHKP) is studied within the concept of non-relativistic quantum mechanics. The proposed Inversely quadratic Hellmann-Kratzer potential (IQHKP) reads:

$$V(r) = -\frac{A}{r} + \frac{Be^{-\alpha r}}{r^2} - 2D_e\left(\frac{r_e}{r} - \frac{1}{2}\frac{r_e^2}{r^2}\right), \tag{1}$$

where A and B are parameters associated with the height of the potential. α, D_e, r_e, r are respectively, the screening parameter, dissociation energy, equilibrium internuclear distance, and internuclear separation. The inversely quadratic Hellmann potential has drawn research interest over the years [8, 9, 10]. Very recently, the inversely quadratic Hellmann potential was applied to the study of the optical properties of GaAs quantum dots [11]. The Kratzer potential itself has been studied in its various forms [12, 13, 14, 15, 16, 17, 18, 19]. Recently, Ikot et al. [20], proposed a modified form of Kratzer potential by including an exponential term that includes the screening parameter. Several studies on the

combination of potentials involving the Hellmann and Kratzer potentials have also been reported [21, 22, 23, 24, 25, 26]. The potential models discussed in this work are useful in some branches of physics such as chemical physics, atomic physics, and nuclear physics. Therefore, it is of importance to find solutions to the Schrödinger equation for a particle under such potentials.

For a particle under influence of a potential field, the thermodynamic effects must be considered. Many authors have studied thermodynamic properties in various potential. For example, Dong and Cruz-Irrison [27], solved the Schrödinger equation and evaluated thermodynamic properties with modified Rosen-Morse potential using a quantization approach. Njoku et al. [28] investigated thermodynamic properties of Hua potential via the Nikiforov-Uvarov method. Oyewumi et al. [29] studied thermodynamic properties of Shifted Deng-Fan potential. Thermodynamic properties with Poschl Teller potential have been studied [30]. Other works on thermodynamic properties in various systems can be found in recent articles [31, 32, 33, 34].

To study the thermodynamic properties of a system, one needs to establish the partition function which is known as the starting point in statistical physics. We first present the Schrödinger equation with IQHKP. Next, by applying the Formula method, we derive the energy eigenvalues and corresponding wave function. Further, we try to evaluate the thermodynamic quantities such as vibrational free energy, F, vibrational

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internal energy, *U*, vibrational entropy, *S*, and vibrational specific heat, *C* for the Schrodinger equation with the IQHKP model.

This paper is outlined as follows: In section 2, we calculate the solutions of the Schrödinger equation using the formula [35]. Thermodynamic properties are discussed in section 3. Discussion of results and special cases of IQHKP are contained in sec.4. Finally, the conclusion is given in sec.5.

2. Non relativistic solution of Schrödinger equation with IQHKP

Given the radial Schrödinger equation [36, 37, 38, 39, 40].

$$\frac{d^2 R_{nl}(r)}{dr^2} + \frac{2}{r}\frac{dR_{nl}(r)}{dr}\left[\frac{2\mu}{\hbar^2}(E_{nl} - V(r)) - \frac{l(l+1)}{r^2}\right]R_{nl}(r) = 0, \quad (2)$$

where µ is the reduced mass, *V(r)* is the potential function and E_{nl} is the energy. If we expand Eq. (1) by Taylor series expansion and neglect terms above r^2, the potential becomes

$$V(r) = \left(-\frac{A}{r} - \frac{\alpha B}{r} - \frac{2D_e r_e}{r}\right) + \left(\frac{B}{r^2} + \frac{D_e r_e^2}{r^2}\right) + \frac{B\alpha^2}{2}. \quad (3)$$

Substituting Eq. (3) in (2) and simplifying yields

$$\frac{d^2 R_{nl}(r)}{dr^2} + \frac{2}{r}\frac{dR_{nl}(r)}{dr} + \frac{Qr^2 + Xr + P}{r^2}R_{nl}(r) = 0, \quad (4)$$

where,

$$Q = \frac{2\mu}{\hbar^2}\left(E_{nl} - \frac{\alpha^2 B}{2}\right); \ X = \frac{2\mu}{\hbar^2}(A + \alpha B + 2D_e r_e); P = -\frac{2\mu}{\hbar^2}\left(B + D_e r_e^2\right)$$
$$- l(l+1) \quad (5)$$

To solve Eq. (4), we apply the formula method proposed by Falaye et al. [35]. The formula method is applied to solve problems of relativistic and non-relativistic wave equations. The method is gaining popularity because it is considered simple, accurate, and easy in applications. Recently, some authors have applied this method in various studies [34, 41, 42]. We consider the differential equation [43] of the form

$$\frac{d^2\psi(s)}{ds^2} + \frac{c_1 - c_2 s}{s(1 - c_3 s)}\frac{d\psi(s)}{ds} + \frac{\xi_1 s^2 + \xi_2 s + \xi_3}{s^2(1 - c_3 s)^2}\psi(s) = 0, \quad (6)$$

where ξ_1, ξ_2, ξ_3 are constants. According to Falaye et al. [35], the energy equation is determined using

$$\left[\frac{c_4^2 - c_5^2 - \left[\frac{1-2n}{2} - \frac{1}{2c_3}\left(c_2 - \sqrt{(c_3 - c_2)^2 - 4\xi_1}\right)\right]^2}{2\left[\frac{1-2n}{2} - \frac{1}{2c_3}\left(c_2 - \sqrt{(c_3 - c_2)^2 - 4\xi_1}\right)\right]}\right]^2 - c_5^2 = 0, c_3 \neq 0, \quad (7)$$

where,

$$\left.\begin{array}{l} c_4 = \frac{(1 - c_1) + \sqrt{(1 - c_1)^2 - 4\xi_3}}{2} \\[3mm] c_5 = \frac{1}{2} + \frac{c_1}{2} - \frac{c_2}{2c_3} + \sqrt{\left(\frac{1}{2} + \frac{c_1}{2} - \frac{c_2}{2c_3}\right)^2 - \left(\frac{\xi_1}{c_3^2} + \frac{\xi_2}{c_3} + \xi_3\right)} \end{array}\right\}. \quad (8)$$

The wave function in terms of generalized hypergeometric functions can be derived using

$$\psi(s) = N_n s^{c_4}(1 - c_3 s)^{c_5} {}_2F_1\left(-n, n + 2(c_4 + c_5) + \frac{c_2}{c_3} - 1; 2c_4 + c_1; c_3 s\right), \quad (9)$$

where N_n is a normalizing factor.

For a case where $c_3 \rightarrow 0$ Eq. (7) reduces to

$$\left[\frac{B - c_4 c_2 - nc_2}{2c_4 + c_1 + 2n}\right]^2 - c_5^2 = 0. \quad (10)$$

And the wave function becomes

$$\psi(s) = N_n s^{c_4}\exp(-c_5 s){}_1F_1(-n, 2c_4 + c_1, 2(c_5 + c_2)s). \quad (11)$$

Comparing Eq. (4) and Eq. (6), it is obvious that $c_1 = 2, c_2 = c_3 = 0$, thus, using Eq. (8), the constants are deduced as follows

$$\left.\begin{array}{l} c_4 = -\frac{1}{2} + \frac{\sqrt{1 - 4P}}{2} \\[3mm] c_5 = \sqrt{-Q} \end{array}\right\}. \quad (12)$$

Using Eqs. (10) and (11), the energy and wave function are calculated respectively as

$$E_{nl} = \frac{\alpha^2 B}{2} - \frac{\hbar^2}{2\mu}\left(\frac{\frac{\mu}{\hbar^2}(A + \alpha B + 2D_e r_e)}{\frac{1}{2} + n + \sqrt{\left(l + \frac{1}{2}\right)^2 + \frac{2\mu}{\hbar^2}\left(B + D_e r_e^2\right)}}\right)^2, \quad (13)$$

and

$$R_{nl}(r) = N_{nl}\, r^{c_4} e^{-r\sqrt{-Q}} L_n^{2c_4 + 1}\left(2\sqrt{-Q}\, r\right). \quad (14)$$

The normalization factor is obtained using the condition $\int_0^\infty r^2 |R_{nl}(r)|^2 dr = 1$ as

$$N_{nl} = \sqrt{\frac{\left(2\sqrt{-Q}\right)^{2c_4 + 2}}{\sum\limits_{i=0}^{n}\frac{\Gamma(2c_4 + 3 + i)}{\Gamma(1+i)(\Gamma(2 - n + i)\Gamma(n - i + 1))^2}}}. \quad (15)$$

3. Thermodynamic properties of the IQHKP

The partition function is usually the first consideration in thermodynamic properties. The partition function of a system can be written as [28, 44].

$$Z(\beta) = \sum_{n=0}^{\eta} e^{-\beta E_n}, \beta = \frac{1}{k_B T}, \quad (16)$$

where k_B is the Boltzmann constant and T is the temperature. η is the upper bound quantum number obtained from $\left.\frac{dE_n}{dn}\right|_{n=\eta} = 0$.

By setting *l = 0*, the energy expression in Eq. (13) can be simplified as

$$E_n = \gamma - q\left(\frac{\Omega}{n + \sigma}\right)^2, \quad (17)$$

where,

$$q = \frac{\hbar^2}{2\mu}; \ \Omega = \frac{\mu}{\hbar^2}(A + \alpha B + 2D_e r_e); \sigma = \frac{1}{2} + \sqrt{\frac{1}{4} + \frac{2\mu}{\hbar^2}\left(B + D_e r_e^2\right)}; \gamma = \frac{\alpha^2 B}{2}. \quad (18)$$

Substituting Eq. (17) in Eq. (16) gives

$$Z(\beta) = \sum_{n=0}^{\eta} e^{-\beta\left(\gamma - \frac{q\Omega^2}{(n+\sigma)^2}\right)}. \quad (19)$$

In the classical limit, the summation turns to an integration, thus, setting $\rho = n + \sigma$ gives

$$Z(\beta) = \int_{\sigma}^{\sigma+\eta} e^{-\gamma\beta + \frac{M}{\rho^2}\beta} d\rho, \tag{20}$$

where $M = \frac{\hbar^2 \Omega^2}{2\mu}$. Using Maple software, Eq. (20) is evaluated as

$$Z(\beta) =$$

$$\frac{-M\beta\sqrt{\pi}erf\left(\frac{\sqrt{-M\beta}}{\sigma+\eta}\right) + M\beta\sqrt{\pi}erf\left(\frac{\sqrt{-M\beta}}{\sigma}\right) - \sqrt{-M\beta}\left((-\sigma-\eta)e^{\frac{M\beta}{(\sigma+\eta)^2}} + \sigma e^{\frac{M\beta}{\sigma^2}}\right)}{\sqrt{-M\beta}e^{\beta D_e}},$$

$$\tag{21}$$

where the error function is stated as

$$erf(z) = \frac{2}{\pi} \int_0^z e^{-t^2} dt. \tag{22}$$

Thermodynamic properties of IQHKP are obtained as:

i. Vibrational Internal Energy

$$U(\beta) = -\frac{\partial \ln Z(\beta)}{\partial \beta}. \tag{23}$$

ii. Vibrational Free Energy

$$F(\beta) = -\frac{1}{\beta} \ln Z(\beta). \tag{24}$$

iii. Vibrational Entropy

$$S(\beta) = k \ln Z(\beta) - k\beta \frac{\partial \ln Z(\beta)}{\partial \beta}. \tag{25}$$

iv. Vibrational Specific Heat Capacity

$$C(\beta) = k\beta^2 \frac{\partial^2 \ln Z(\beta)}{\partial \beta^2}. \tag{26}$$
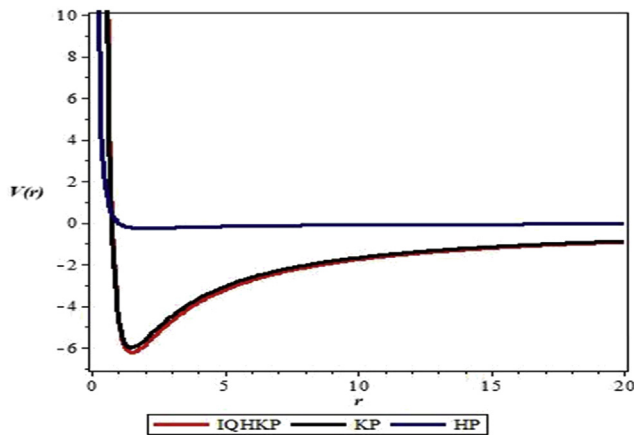

Figure 1. Variation of the Inversely quadratic Hellmann-Kratzer potential, Kratzer potential and the Inversely quadratic Hellmann potential with internuclear distance.
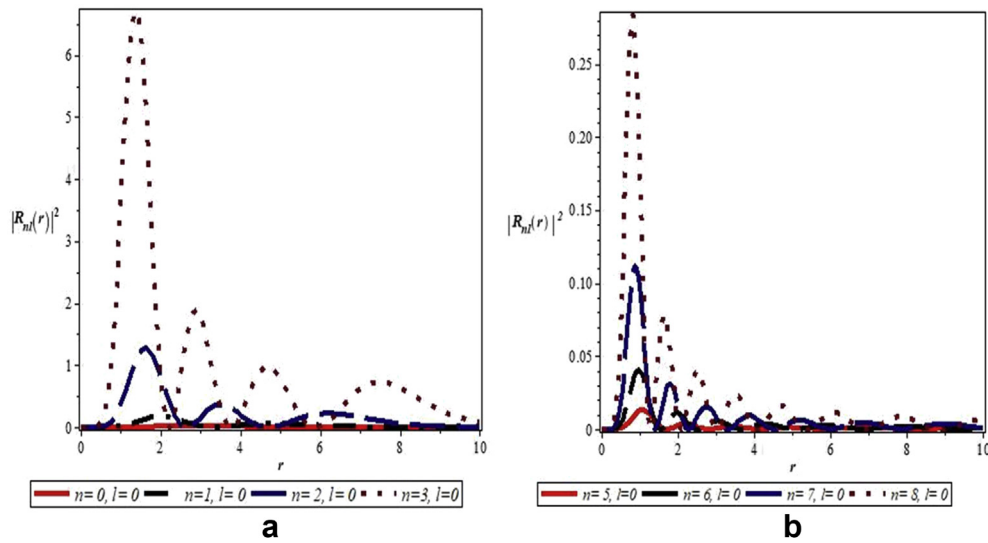
4. Discussion of results

In Figure 1, the shape of the IQHKP is plotted against the internuclear distance, r, alongside the Hellmann and Kratzer potentials. The shape of the IQHKP is more similar to the Kratzer potential than the Hellmann potential. Thus, a particle confined in the IQHKP feels more of the effect of the Kratzer than the Hellmann potential. In Figure 2a,b, the probability densities of the low and high lying states are shown respectively against the radial distance, r, with $l= 0$. It is observed that the high lying states are more concentrated and show higher localization than the low lying states. The radial probability density plot peaks in both cases are observed to decrease as the radial distance, r, increases. Also, in both cases, the radial probability density peaks shift to lower values as r increases, while the probability density approaches zero. The plots were made using the parameters $\alpha = 0.01, D_e = 6, A = 1, B = 1, r_e = 1.5$.

In Figure 3, the variation of the energy of the IQHKP with the adjustable screening parameter, α, is shown for values of quantum numbers n and $\ell = 0$. The energy is seen to increase as α increase. In Figure 4, the energy is observed to decrease linearly with an increase in the potential parameter, A. The reverse trend is observed in Figure 5, as energy increases with parameter, B. Figure 6 shows the variation of energy with the dissociation energy, D_e. It can be observed that the energy decreases with an increase in dissociation energy, D_e. The plots were made with $l = 0, D_e = 6, A = 1, B = 1, r_e = 1.5$.

Figure 7 is a plot of the vibrational partition function, Z, versus temperature, T, for some values of the upper bound quantum number, η. It is observed that in all cases, the partition function decreases first, then tends to a constant value as temperature increases. This implies that the probability of the system occupying a given microstate increases first then remains constant as the temperature, T, increases. This is in line with the predictions of classical thermodynamics since an increase in temperature causes an increase in the energy of the system and consequently an increase in accessible microstates. In Figure 8, the free energy, F, and temperature show an inversely proportional relationship, since, F decreases monotonically as T increase. In Figure 9, the vibrational entropy, S, shows a reverse trend to that shown by the partition function in Figure 7. In Figure 10, the internal energy, U, also shows the same trend as the entropy, S as it is observed to increase sharply first, then, tends to a constant value for all η values. In Figure 11, the vibrational specific heat decreases sharply as temperature increases up to 10 K, then tends to a constant value afterward (C(T) → 0). This implies that as the temperature increases beyond 10 K, the system behavior transcends towards that of a perfect adiabatic system with perfect insulation from the surrounding. This is verified by the results of the entropy, since for an adiabatic system the entropy cannot decrease, it either increases or remains constant (see Figure 9). The plots were made with $\alpha = 0.01, D_e = 6, A = 1, B = 1, r_e = 1.5$.

Table 1 shows numerical results of the IQHKP for some values of screening parameter, α. In all the cases, the energy is observed to increase with the quantum numbers n and l. Table 2 presents the energy eigenvalues of IQHKP. The energy is observed to increase with quantum numbers n and l for all values of α. Table 3 presents the results of energy of the inversely quadratic Yukawa potential for arbitrary quantum numbers n and l for $\alpha = 0.01, 0.05,$ and 0.1. The energy is also observed to increase as n and l increase.

4.1. Important cases of IQHKP

After studying the nonrelativistic solutions of IQHKP, we examine some important cases:

Case 1. The first case corresponds to the Kratzer potential (A = B = 0):

$$V(r) = -2D_e\left(\frac{r_e}{r} - \frac{1}{2}\frac{r_e^2}{r^2}\right). \tag{27}$$

Figure 2. Plot of radial probability density against the radial distance for (a) low lying states, (b) high lying states.
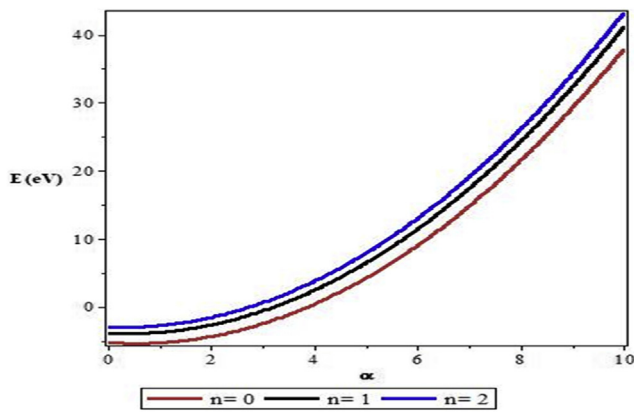

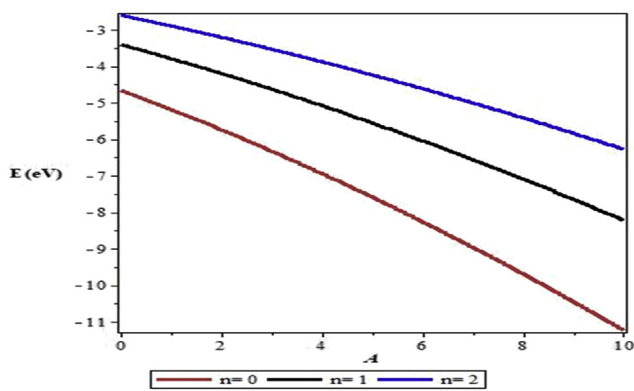**Figure 3.** Variation of the energy of the IQHK potential with the screening parameter, α.

Figure 4. Variation of the energy of the IQHK potential with the potential parameter, A.

The energy Eq. (13) reduces to the corresponding values for Kratzer potential. Thus we have

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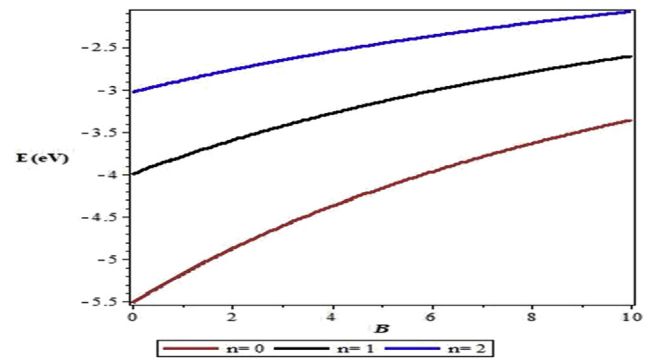

Figure 5. Variation of the energy of the IQHK potential with the potential parameter, B.

Eq. (28) is identical to Eq. (18) in ref. [13], and Eq. (115) in ref. [21] when $l = L$. If we set $r_e = A$, $B = r_e^2$ and $\sigma = \frac{1}{2}\left(1 + \sqrt{(1+2l)^2 + \frac{8\mu}{\hbar^2}D_e B} \right)$, then Eq. (28) will be the same as Eq. (46) in ref. [20].

Case 2. Case two corresponds to the Inversely quadratic Hellman potential ($D_e = 0$):
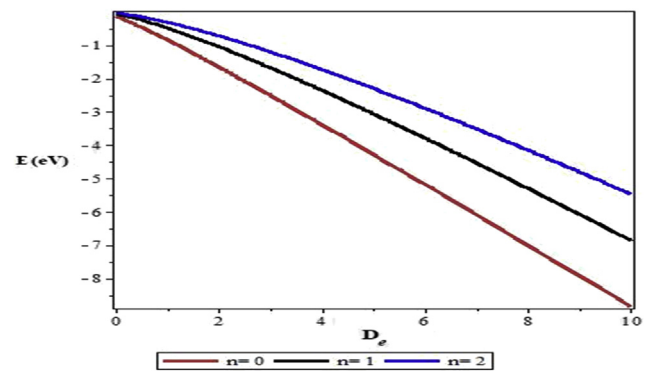

Figure 6. Variation of the energy of the IQHK potential with the dissociation energy, D_e.
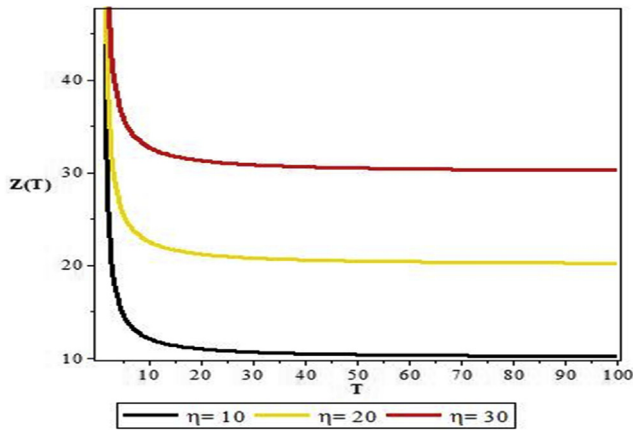
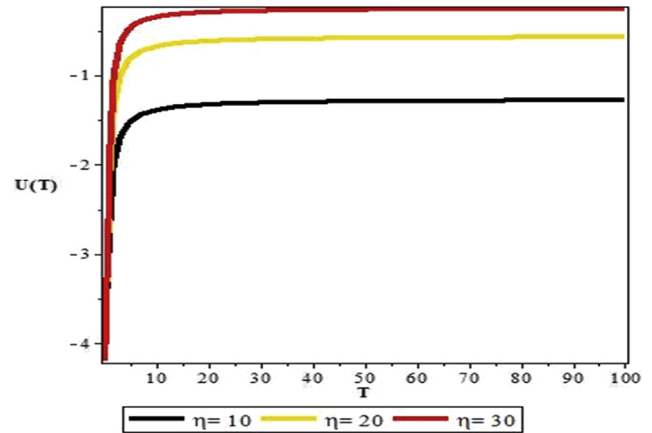**Figure 7.** Variation of the vibrational partition function of the IQHK potential with temperature, T.

Figure 10. Variation of the vibrational internal energy of the IQHK potential with temperature, T.
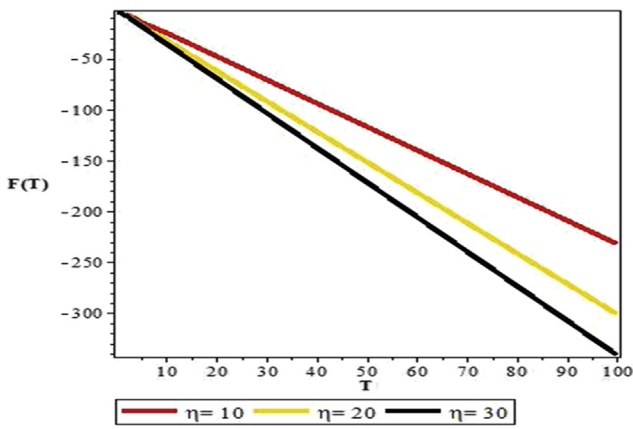

Figure 8. Variation of the vibrational free energy of the IQHK potential with temperature, T.

$$V(r) = -\frac{A}{r} + \frac{Be^{-\alpha r}}{r^2}. \tag{29}$$

Here, we obtain the energy spectrum as:

$$E_{nl} = \frac{\alpha^2 B}{2} - \frac{\hbar^2}{2\mu}\left(\frac{\frac{\mu}{\hbar^2}(A + \alpha B)}{\frac{1}{2} + n + \sqrt{\left(l + \frac{1}{2}\right)^2 + \frac{2\mu B}{\hbar^2}}}\right)^2. \tag{30}$$
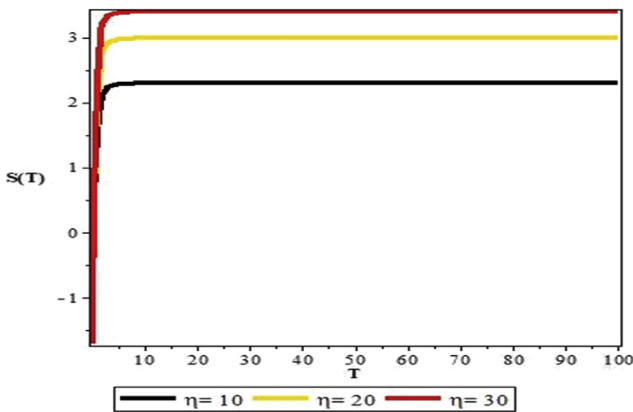

Figure 9. Variation of the vibrational entropy of the IQHK potential with temperature, T.
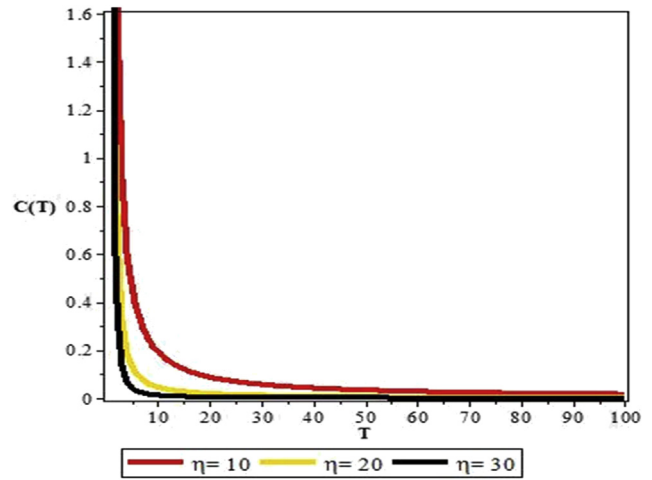

Figure 11. Variation of the vibrational specific heat of the IQHK potential with temperature, T.

Eq. (30) is the same as Eq. (16) in ref. [11]. Eq. (30) is also similar to Eq. (34) in Ref. [7] under the condition $\frac{\alpha^2}{2} = \delta^2, B = b, A = a$.

Case 3. The third case gives Inversely quadratic Yukawa potential (A = 0, D_e = 0):

Table 1. Energy eigenvalues of the inversely quadratic Hellman-Kratzer (IQHK) potential with D_e =6; r_e =1.5; A = 1, B = 2; $\mu = \hbar = 1$.

n	L	α = 0.01	α = 0.05	α = 0.1
0	0	-4.876669242	-4.915379866	-4.959510796
1	0	-3.598037370	-3.625969268	-3.656563172
2	0	-2.763503540	-2.784400411	-2.806159008
	1	-2.647001960	-2.666916735	-2.687441916
3	0	-2.188906365	-2.204959446	-2.220634714
	1	-2.106490249	-2.121848571	-2.136651290
	2	-1.961236202	-1.975370048	-1.988634946
4	0	-1.776518042	-1.789094734	-1.800404000
	1	-1.716087403	-1.728154672	-1.738824150
	2	-1.608732197	-1.619894474	-1.629427370
	3	-1.474207334	-1.484235581	-1.492344246
5	0	-1.470567948	-1.480565515	-1.488635650
	1	-1.424949166	-1.434562172	-1.442149336
	2	-1.343375184	-1.352300531	-1.359024061
	3	-1.240154422	-1.248209630	-1.253840350
	4	-1.128651574	-1.135766824	-1.140217050

Table 2. Energy eigenvalues of the inversely quadratic Hellman (IQH) potential with; $A = -1$, $B = 1$, $\mu = \hbar = 1$.

n	l	$\alpha = 0.01$	$\alpha = 0.05$	$\alpha = 0.1$
0	0	-0.12246250000	-0.1115625000	-0.09625000000
1	0	-0.05440000000	-0.04888888890	-0.04000000000
2	0	-0.03057812500	-0.02695312500	-0.02031250000
	1	-0.02350130510	-0.02043661652	-0.01446388851
3	0	-0.01955200000	-0.01680000000	-0.01120000000
	1	-0.01579339544	-0.01333898520	-0.008093715240
	2	-0.01201842267	-0.009862898140	-0.004973903035
4	0	-0.01356250000	-0.01128472222	-0.006250000000
	1	-0.01133222420	-0.009231029840	-0.004406796865
	2	-0.008966471095	-0.007052586640	-0.002451629005
	3	-0.007106704375	-0.005340068050	-0.000914631715
5	0	-0.009951020410	-0.007959183675	-0.003265306120
	1	-0.008520741840	-0.006642148265	-0.002083257720
	2	-0.006941216765	-0.005187683020	-0.000777865095
	3	-0.005646660125	-0.003995623675	0.000292016424
	4	-0.004644554752	-0.003072860589	0.001120202685

Table 3. Energy eigenvalues of the Inversely quadratic Yukawa (IQY) potential with $B = 0.5$; $\mu = \hbar = 1$.

n	l	$\alpha = 0.01$	$\alpha = 0.05$	$\alpha = 0.1$
0	0	0.00002022542486	0.0005056356216	0.002022542486
1	0	0.00002317627458	0.0005794068645	0.002317627458
2	0	0.00002404508497	0.0006011271243	0.002404508497
	1	0.00002432483082	0.0006081207704	0.002432483082
3	0	0.00002441386755	0.0006103466888	0.002441386755
	1	0.00002455546751	0.0006138866878	0.002455546751
	2	0.00002467403841	0.0006168509603	0.002467403841
4	0	0.00002460395796	0.0006150989490	0.002460395796
	1	0.00002468533654	0.0006171334134	0.002468533654
	2	0.00002475837586	0.0006189593965	0.002475837586
	3	0.00002481135064	0.0006202837660	0.002481135064
5	0	0.00002471460128	0.0006178650319	0.002471460128
	1	0.00002476561269	0.0006191403172	0.002476561269
	2	0.00002481376197	0.0006203440492	0.002481376197
	3	0.00002485037216	0.0006212593041	0.002485037216
	4	0.00002487769977	0.0006219424943	0.002487769977

$$V(r) = \frac{Be^{-\alpha r}}{r^2}. \tag{31}$$

The corresponding energy equation is given as

$$E_{nl} = \frac{\alpha^2 B}{2} - \frac{\hbar^2}{2\mu}\left(\frac{\frac{\mu\alpha B}{\hbar^2}}{\frac{1}{2} + n + \sqrt{\left(l + \frac{1}{2}\right)^2 + \frac{2\mu B}{\hbar^2}}}\right)^2. \tag{32}$$

Eq. (32) is consistent with Eq. (33) in ref. [7] with the condition $\frac{\alpha^2}{2} = \delta^2$, $B = -2V_0$.

Case 4. The fourth case is the coulomb potential ($D_e = B = 0$):

$$V(r) = -\frac{A}{r}. \tag{33}$$

The energy spectrum here is obtained as

$$E_{nl} = -\frac{\mu A^2}{2\hbar^2(n + l + 1)^2}. \tag{34}$$

Eq. (34) is in agreement with Eqs. (36), (50), (161) and (61) in refs. [5, 20, 21, 22], respectively. Eq. (34) will be seen to be consistent with Eq. (50) in ref. [45] if $D = 3$. If $(n + l + 1)$ is set to n_p and A is set to Ze^2, Eq. (34) will be similar to Eq. (48) of ref. [23]. In refs. [6, 46], the authors did not set $\alpha = 0$ in Eqs. (31) and (33) respectively, those equations will be identical to Eq. (34) above.

5. Conclusion

In this paper, we obtain the solutions of the Schrödinger equation for IQHKP using the formula method. The obtained solutions are applied to the study of thermodynamic properties. The numerical results are also presented. To demonstrate the accuracy of our method, we considered 4 special cases derived from IQHKP and confirmed that our results were in agreement with previous findings in the literature. Finally, our approach presents a novel and accurate way of obtaining bound state solutions with different potentials quickly and easily and will be useful to the theorist. Considering the validity of the results obtained in this work, we can conclude that IQHKP is one of the important realistic models that could have potential applications in atomic, molecular, and nuclear physics.

Declarations

Author contribution statement

C.P. Onyenegecha, K. El Anouz: Conceived and designed the experiments; Wrote the paper.

A.I. Opara: Performed the experiments; Wrote the paper.

I.J. Njoku, A. El Allati: Analyzed and interpreted the data; Wrote the paper.

C.J. Okereke: Contributed reagents, materials, analysis tools or data; Wrote the paper.

Data availability statement

Data will be made available on request.

Declaration of interests statement

The authors declare no conflict of interest.

Additional information

No additional information is available for this paper.

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