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Eigensolutions and Thermodynamic Properties of Kratzer Plus Generalized Morse Potential

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In this study, we apply the parametric Nikiforov-Uvarov method to obtain the bound state solution of Schrödinger wave equation in the presence of Kratzer plus generalized Morse potential (KPGM). The energy eigen equation and the corresponding normalised wave function were obtained in closed form. The resulting energy eigen equation was used to study partition function and other thermodynamic properties such as vibrational mean energy, vibrational specific heat capacity, vibrational mean free energy and vibrational entropy for the proposed potential as applied to lithium hydride diatomic molecule. The thermodynamic plots obtained were in excellent agreement to work of existing literatures. The wave function and probability density plots for the diatomic molecules were obtained through a well designed and implemented maple programme.

Keywords: nikiforov-uvarov method, kratzer plus generalised morse potential, thermodynamic properties, schrodinger wave equation, diatomic molecules

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1 INTRODUCTION

The exact solutions of Schrödinger wave equation is one of the essential part in quantum mechanics, this is because Schrödinger wave equation is used to describe non-relativistic spinless particles and also has many applications in atomic, nuclear and high energy Physics [1–9]. This has prompted many researchers over the years to search for the solution of Schrödinger wave equation with different potentials [10–15]. However, different methods have been used to obtain approximate solution of Schrödinger wave equation, they include Nikiforov-Uvarov method (NU) [16–22], Supersymmetry quantum mechanics (SUSY) [23–28], Asymtotic Iteration method (AIM) [29, 30], Factorization method [31, 32], Exact and proper quantization method [33–36]. In solving the wave equation, the results obtained for various potential models are vastly applied [4, 31, 37, 38, 38, 39, 39–41]. A lot of researchers have studied bound state solutions of Schrödinger wave equation as applicable to different field of physical and chemical sciences including molecular spectroscopy and quauntum information. Ahmadov et al. [42] studied bound state solution to the Schrodinger equation at finite temperature with the sum of Cornell and Inversely quadratic potential with developed approximation to the centrifugal term using Nikiforov-Uvarov method. Their energy eigenvalues were applied to study charmonium and bottomium masses at finite and zero temperature in which their theoretical results were in total agreement with the experimental results. Ahmadov et al. [43] also studied finite temperature dependent Schrodinger equation with the sum of Cornell, Inversely quadratic and harmonic type potential. They obtained analytical expression for the energy eigenvalues and applied it to study heavy quarkonia and messon masses at different temperatures. Considering the application of bound state solutions of Schrödinger equation to quantum information; Shi et al. [44] evaluated Shannon information entropies in position and monentum spaces for an infinite spherical potential well where their result satisfies Beckner, Bialynicki-Birula and Mycieslki (BBM) inequality. Okon et al. [45] studied Fisher and Shannon information entropies for a noncentral Inversely quadratic plus exponential Mie-Type potential using parametric Nikiforov-Uvarov method where the evaluated Fisher and Shannon Information entropies for position and momemtum spaces.

The thermodynamic properties of a particular system is studied by finding the partition function which is a function of temperature. Other thermodynamic properties such as entropy, specific heat capacity, mean free energy and others are easily obtained using the partition function, which is widely applied in molecular physics and statistical physics [46–48].

In this research article, we solve the bound state solution of Schrödinger wave equation with Kratzer plus generalized Morse potential using the parametric Nikiforov-Uvarov method. We also extend our work to study the thermodynamic properties of the system as applied to lithium hydride (LIH) molecules. Hydride compound are most oftenly used as a portable sources of hydrogen gas [49]. Hydrides compound are used for advance fuel cells and battery applications. meanwhile, hydrogen can be stored as compressed hydrogen, liquid hydrogen as well as chemical storage [50]. Lithium hydride has high density hydrogen storage and serve as a precausor for building complex hydrides for industrial usage [51]. Lithium hydride is hetero diatomic molecule with applications in molecular spectroscopy. Evaluating the thermodynamic properties of this molecule will further reveals its statistical behaviour as well as its intrinsic properties. The Kratzer potential is a potential model that is used to described the internuclear vibration of diatomic molecules [52]. Kratzer potential is importance in the description of molecular structures and interraction existing between diatomic molecules and at the same time played a vital role in quantum chemistry [53] Kratzer potential is a limiting case of exponential type potentials [54]. Because of the Coulomb and the inverse square term present in Kratzer potential model, Kratzer potential can therefore be used to described molecules with short and long intermolecular distance. A lot of research work has been carried out using Kratzer potential within relativistic and nonrelativistic quantum mechanics. Such work can be find in Refs. [55–57]. Kratzer potential model is only characterised with dissociation energy D_e and equilibrium bond length r_e without the potential screening parameter α which characterises the strength of the potential. Morse potential has proved to be one of the most successful in explaining rotational and vibrational structure of diatomic molecules. As the internuclear distance gets larger, the potential vanishes to zero. Meanwhile, the combination of Kratzer and generalised Morse potential will provide a macroscopic description of the molecular interaction existing between diatomic molecules and incorporate all the experimental spectroscopic parameters needed for complete discription of molecular interaction. The Kratzer plus generalized Morse potential takes the form

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

where D_e is dissociation energy, r_e is the equilibrium bond length, r represent the interatomic distance, α is the screening parameter. This article is organised as follows: **Section 1** is the introduction of the article, The Parametric Nikiforov-Uvarov method and the non-relativistic solution is presented in **section 2**, Thermodynamic properties is expressed in **section 3**, while the numerical solution is shown in **section 4**. The article is concluded in **section 5**.

2 THE PARAMETRIC NIKIFOROV-UVAROV METHOD

In the parametric NU method, the second order linear differential equation is reduced to a generalised equation of hyper-geometric type which provides exact solutions interms of special orthogonal functions and the corresponding energy eigenvalues of the form. With the appropriate coordinate transformation $S = S(x)$ the equation can be written as [17, 58–63].

$$\psi''(s) + \frac{\tilde{\tau}(s)}{\sigma(s)}\psi'(s) + \frac{\tilde{\sigma}(s)}{\sigma^2(s)}\psi(s) = 0 \tag{2}$$

where $\tilde{\tau}(s)$ is the polynomial of degree one, $\sigma(s)$ and $\tilde{\sigma}(s)$ are polynomials of at most degree two. Then the parametric NU differential equation is in the form [45].

$$\psi''(s) + \frac{(c_1 - c_2 s)}{s(1 - c_3 s)}\psi'(s) + \frac{1}{s^2(1 - c_3 s)^2}\left[-\Omega_1 s^2 + \Omega_2 s - \Omega_3\right]\psi(s) = 0 \tag{3}$$

The parametric constants are obtained as follows

$$\left.\begin{array}{l} c_1 = c_2 = c_3 = 1;\ c_4 = \frac{1}{2}(1 - c_1);\ \ c_5 = \frac{1}{2}(c_2 - c_3);\ \ c_6 = c_5^2 + \epsilon_1 \\ c_7 = 2c_4c_5 - \Omega_2;\ c_8 = c_4^2 + \Omega_3;\ \ c_9 = c_3c_7 + c_3^2c_8 + c_6 \\ c_{10} = c_1 + 2c_4 + 2\sqrt{c_8}\,;\ \ c_{11} = c_2 - 2c_5 + 2\left(\sqrt{c_9} + c_3\sqrt{c_8}\right) \\ c_{12} = c_4 + \sqrt{c_8}\,;\ c_{13} = c_5 - \left(\sqrt{c_9} + c_3\sqrt{c_8}\right) \end{array}\right\}. \tag{4}$$

The eigen energy equation is given as

$$c_2 n - (2n + 1)c_5(2n + 1)\left(\sqrt{c_9} + c_3\sqrt{c_8}\right) + n(n - 1)c_3 + c_7 2c_3c_8 + 2\sqrt{c_8c_9} = 0 \tag{5}$$

The corresponding total wave function is then given as

$$\Psi(s) = N_{nl}s^{c_{12}}(1 - c_3 s)^{-c_{12} - \frac{c_{11}}{c_3}} P_n^{\left(c_{10}-1,\ \frac{c_{11}}{c_3}-c_{10}-1\right)}(1 - 2c_3 s) \tag{6}$$

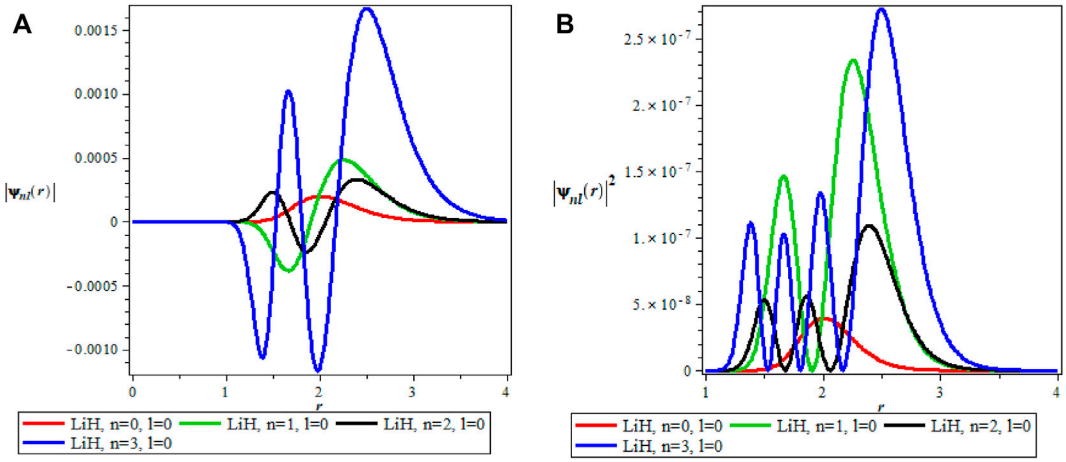

FIGURE 1 | (A) Wavefunction plot for fixed *l* = 0 for LiH molecule. **(B)** Probabilty density plot for fixed *l* = 0 for LiH molecule.

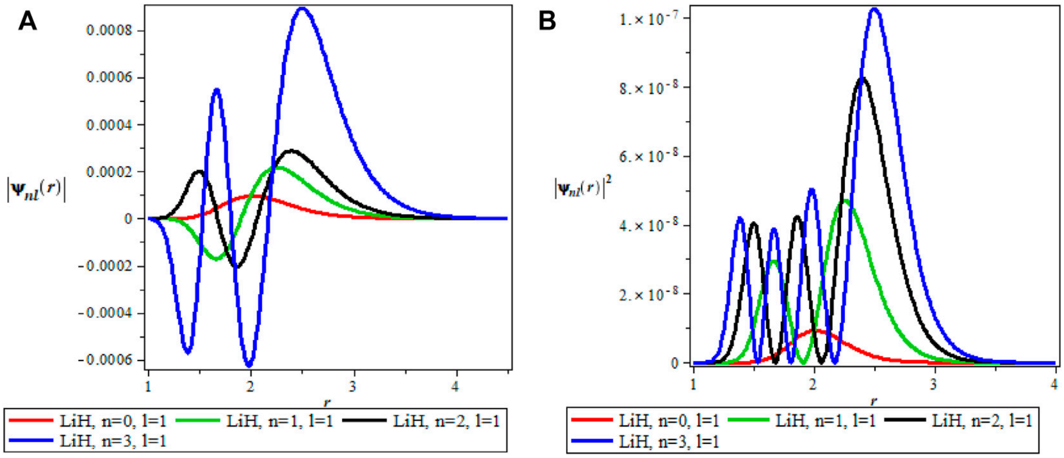

FIGURE 2 | (A) Wavefunction plot for fixed *l* = 1 for LiH molecule. **(B)** Probabilty density plot for fixed *l* = 1 for LiH molecule.

2.1 Non-Relativistic Solution With KPGMP

The Schrödinger wave equation for an arbitrary external potential $V(r)$ in spherical coordinate is written as [4].

$$\frac{d^2\psi_{n\ell}(r)}{dr^2}+\frac{2\mu}{\hbar^2}\left[E-V(r)-\frac{\hbar^2\ell(\ell+1)}{2\hbar r^2}\right]\psi_{n\ell}=0 \tag{7}$$

where E is the exact bound state energy eigenvalues, $R_{n\ell}(r)$ is the eigenfunction, $\mu=\frac{m_1m_2}{m_1+m_2}$ being the reduced mass, ($\hbar=\mu=1$). n denotes the principal quantum number (n and ℓ are known as the vibration-rotation quantum numbers), r is the internuclear separation.

Also, on substituting **Eq. 1** into **Eq. 6**, the radial part of the Schrödinger equation for the KPGM is given as

$$\frac{d^2\psi_{n\ell}(r)}{dr^2}+\frac{2\mu}{\hbar^2}\left[E+\left(-2D_e\left(\frac{r_e}{r}-\frac{r_e^2}{2r^2}\right)+D\left(1-\frac{be^{\alpha r}}{1-e^{\alpha r}}\right)^2\right)-\frac{\hbar^2\ell(\ell+1)}{2\mu r^2}\right]\psi_{n\ell}(r)=0. \tag{8}$$

The Green-Aldrich approximation is given as [64].

$$\frac{1}{r^2}=\frac{4\alpha^2e^{-2\alpha r}}{(1-e^{-\alpha r})^2},\quad \frac{1}{r}=\frac{2\alpha e^{-\alpha r}}{1-e^{-\alpha r}}. \tag{9}$$

On Substituting the transformation $s=e^{\alpha r}$ and applying the Green-Aldrich approximation into **Eq. 7** yields

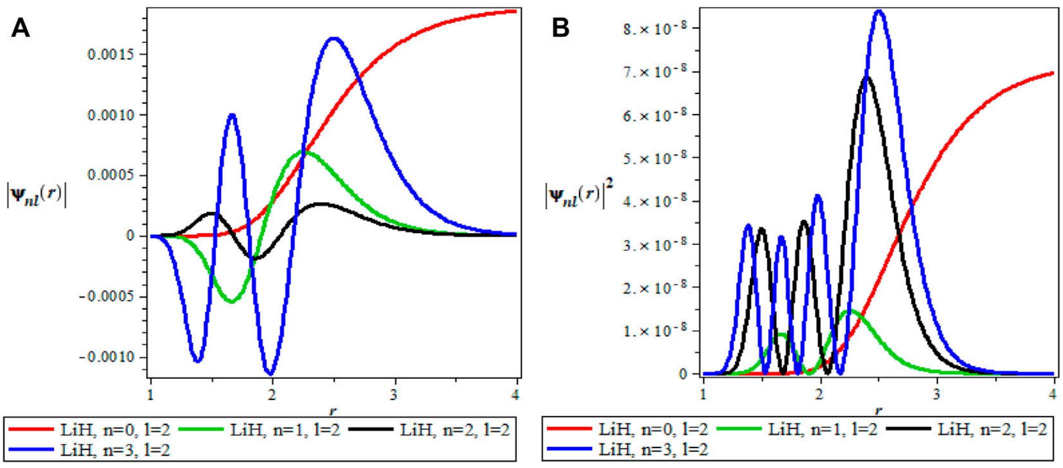

FIGURE 3 | (A) Wavefunction plot for fixed l = 2 for LiH molecule. **(B)** Probabilty density plot for fixed l = 2 for LiH molecule.

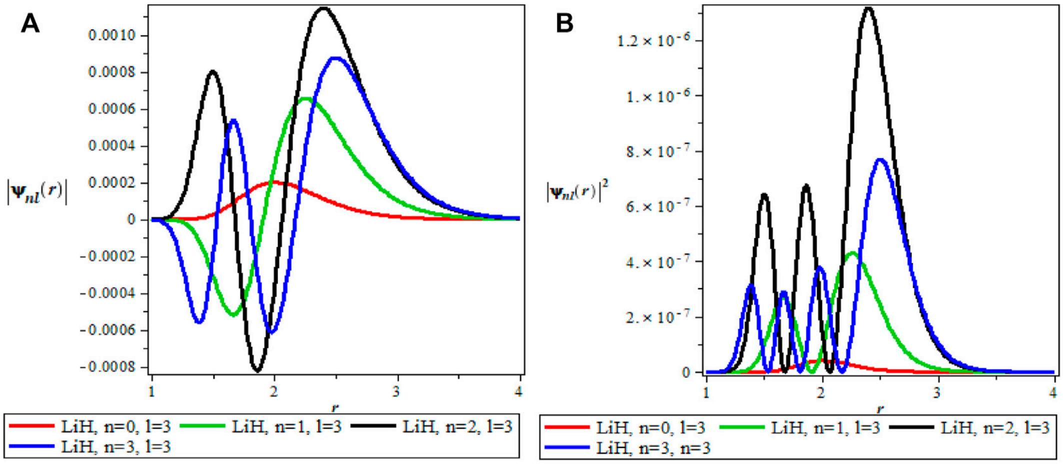

FIGURE 4 | (A) Wavefunction plot for fixed l = 3 for LiH molecule. **(B)** Probabilty density plot for fixed l = 3 for LiH molecule.

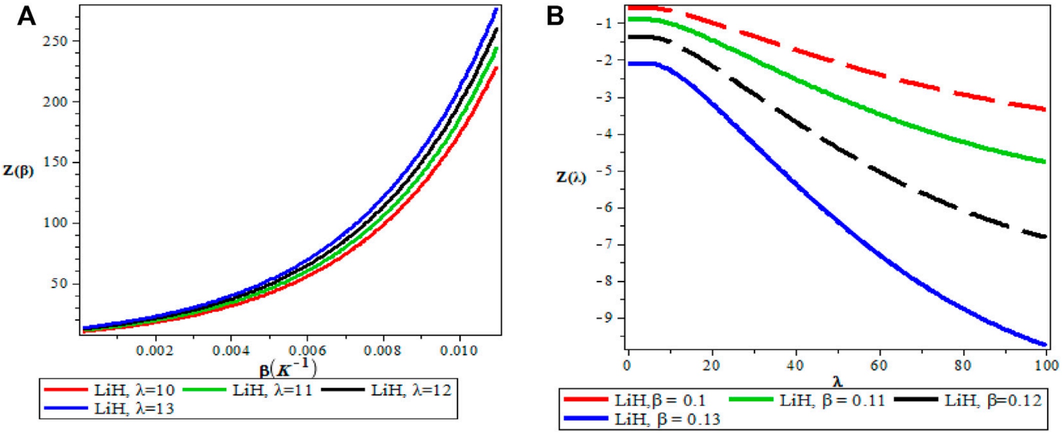

FIGURE 5 | (A) Variation of Partition Function With Respect to β **(B)** Variation of Partition Function With Respect to λ.

$$\frac{d^2\psi(s)}{dr^2}+\frac{(1-s)}{s(1-s)}\frac{d\psi(s)}{dr}+\frac{1}{s^2(1-2)^2}\begin{bmatrix}-\left(\xi^2-A-B-C-F-G-4\lambda\right)s^2\\ +\left(2\xi^2+A+2C+F\right)s-\left(-\xi^2-C\right)\end{bmatrix}\psi(s)=0 \tag{10}$$

where

$$-\xi^2=\frac{2\mu E}{\alpha^2\hbar^2},A=\frac{8\,\mu D_e r_e}{\alpha\hbar^2},B=\frac{8\,\mu D_e r_e^2}{\alpha^2\hbar^2},\quad C=\frac{2\mu D}{\alpha^2\hbar^2},F\frac{4\mu Db}{\alpha^2\hbar^2},G=\frac{2\mu Db^2}{\alpha^2\hbar^2}. \tag{11}$$

Comparing **Eq. 9** with the standard parametric NU differential equation of **(2)**, the parameters are obtained as follows:

$$\left.\begin{aligned}\Omega_1 &= \xi^2-A-B-C-F-G-4\lambda,\Omega_2=2\xi^2+A+2C+F,\quad \Omega_3=\xi^2-C\\ c_1 &= c_2=c_3=1,\ c_4=0,\ c_5=-\frac{1}{2},\ c_6=\frac{1}{4}+\xi+A+B+C+F+G+4\lambda,\\ c_7 &= -2\xi^2-A-2C-F,\ c_8=\xi^2,\ c_9=\frac{1}{4}+B+G+4\lambda,\ c_10=1+2\sqrt{\xi^2+C}\\ c_{11} &= 2+2\left(\sqrt{\frac{1}{4}+B+G+C+4\lambda+\xi^2}\right),\ c_{12}=\sqrt{\xi^2+C}\ ,\\ c_{13} &= -\frac{1}{2}-\left(\sqrt{\frac{1}{4}+B+G+C+4\lambda+\xi^2}\right)\end{aligned}\right\}. \tag{12}$$

By substituting the appropriate parameters of **Eq. 11** into equations (?) and equation (?), then simplify gives the respective wave function and energy eigenvalue equation for the KPGMP as

$$\psi_{n\ell}=N_{n\ell}s^{\gamma}(1-s)^{\delta}P_n^{[2\gamma,2\delta-1]}(1-2s),\quad s=e^{\alpha r} \tag{13}$$

and

$$E_{n\ell}=-\frac{\alpha^2\hbar^2}{2\mu}\left[\frac{\left(n^2+n+\frac{1}{2}\right)+(2n+1)\eta-\frac{8\mu D_e r_e}{\alpha\hbar^2}-\frac{8\mu Db}{\alpha^2\hbar^2}}{(2n+1)+2\eta}\right]^2-\frac{2\mu Db^2}{\alpha^2\hbar^2} \tag{14}$$

where

$$\gamma=\sqrt{\frac{2\mu D}{\alpha^2\hbar^2}-\frac{2\mu E}{\alpha^2\hbar^2}},\quad \delta=\frac{1}{2}+\sqrt{\frac{1}{4}+\frac{8\mu D_e r_e^2}{\alpha^2\hbar^2}+\frac{2\mu Db^2}{\alpha^2\hbar^2}+4\ell(\ell+1)},\quad \eta=\sqrt{\frac{1}{4}+\frac{8\mu D_e r_e^2}{\alpha^2\hbar^2}+\frac{2\mu Db^2}{\alpha^2\hbar^2}+4\ell(\ell+1)} \tag{15}$$

The normalization constant in **Eq. 12** can be obtain using the normalization condition [1, 4].

$$\int_0^\infty|\psi_{n\ell}|^2dr=\int_0^\infty|N_{n\ell}s^{\gamma}(1-s)^{\delta}P_n^{[2\gamma,2\delta-1]}(1-2s)|^2ds=1, \tag{16}$$

the wavefunction is assumed to be in the bound at $r\ \varepsilon\ (0,\infty)$ and $s=e^{\alpha r}\ \varepsilon\ (1,0)$ **Eq. 15** becomes

$$-\frac{N_{n\ell}^2}{\alpha}\int_0^1 s^{2\gamma}(1-s)^{2\delta}P_n^{[2\gamma,2\delta-1]}(1-2s)|^2\frac{ds}{s}=1. \tag{17}$$

Let $z=1-2s$ thus, the limit of integration of **Eq. 16** changes from $s\ \varepsilon(1,0)$ to $z\ \varepsilon(-1,1)$. Then **Eq. 16** reduces to

$$\frac{N_{n\ell}^2}{2\alpha}\int_{-1}^1\left(\frac{1-z}{2}\right)^{2\gamma-1}\left(\frac{1+z}{2}\right)^{2\delta}\left[P_n^{[2\gamma,2\delta-1]}(z)\right]^2dz=1. \tag{18}$$

Applying the standard integral [1, 4].

$$\int_{-1}^1\left(\frac{1-w}{2}\right)^x\left(\frac{1+w}{2}\right)^y\left[P_n^{(x,y-1)}(w)\right]^2dw=\frac{2^{x+y+1}\Gamma(x+n+1)\Gamma(y+n+1)}{n!\Gamma(x+y+n+1)\Gamma(x+y+2n+1)}. \tag{19}$$

Also, let $z=w$, $x=2\gamma-1$, $y=2\delta$. Then the normalization constant can be obtained as

$$N_{n\ell}=\sqrt{\frac{2\alpha(n!)\Gamma(2\gamma+2\delta+n)\Gamma(2\gamma+2\delta+2n)}{2^{(2\gamma+2\delta)}\Gamma(2\gamma+n)\Gamma(2\delta+n+1)}}, \tag{20}$$

therefore, the total normalized wave function is given as

$$\psi(s)=\sqrt{\frac{2\alpha(n!)\Gamma(2\gamma+2\delta+n)\Gamma(2\gamma+2\delta+2n)}{2^{(2\gamma+2\delta)}\Gamma(2\gamma+n)\Gamma(2\delta+n+1)}}\ s^{\gamma}(1-s)^{\delta}P_n^{[2\gamma,2\delta-1]}(1-2s). \tag{21}$$

3 THERMODYNAMIC PROPERTIES FOR THE POTENTIAL MODEL

The thermodynamic properties for KPGM will be studied by first obtaining the vibrational partition function defined as

$$Z(\beta)=\sum_{n=0}^{\lambda}e^{-\beta E_n} \tag{22}$$

where λ is an upper bound of the vibrational quantum number obtain from the numerical solution of $\frac{dE_n}{dn}=0$, $\beta=\frac{1}{kT}$ where K and T are Boltzmann constant and absolute temperature respectively. In the classical limit, the summation in 21 can be replaced with the integral:

$$Z(\beta)=\int_0^{\lambda}e^{-\beta E_n}dn \tag{23}$$

The energy equation of **Eq. 13** can be simplified to

$$E_{nl}=Q_1-Q_2\left[(n+\Delta)+\frac{Q_3}{(n+\Delta)}\right]^2 \tag{24}$$

where

$$Q_1=\frac{-2\mu Db^2}{\alpha^2\hbar^2},Q_2=\frac{\alpha^2\hbar^2}{8\mu},Q_3=-\frac{\mu D_e r_e^2}{2\alpha^2\hbar^2}-\frac{\mu Db^2}{8\alpha^2\hbar^2}-\frac{\ell(\ell+1)}{4}-\frac{4\mu D_e}{\alpha^2\hbar^2},\quad \Delta=\frac{1}{2}+\frac{1}{2}\sqrt{1+\frac{2\mu D_e r_e^2}{\alpha^2\hbar^2}+\frac{\mu Db^2}{2\alpha^2\hbar^2}+\ell(\ell+1)} \tag{25}$$

The energy **Eq. 23** can then be express in the form

$$E_{nl}=-\left[Q_2\rho^2+\frac{Q_2Q_3^2}{\rho^2}\right]-[2Q_2Q_3-Q_1],\ \rho=n+\Delta \tag{26}$$

Hence, the partition function **Eq. 22** can be express in the classical limit as

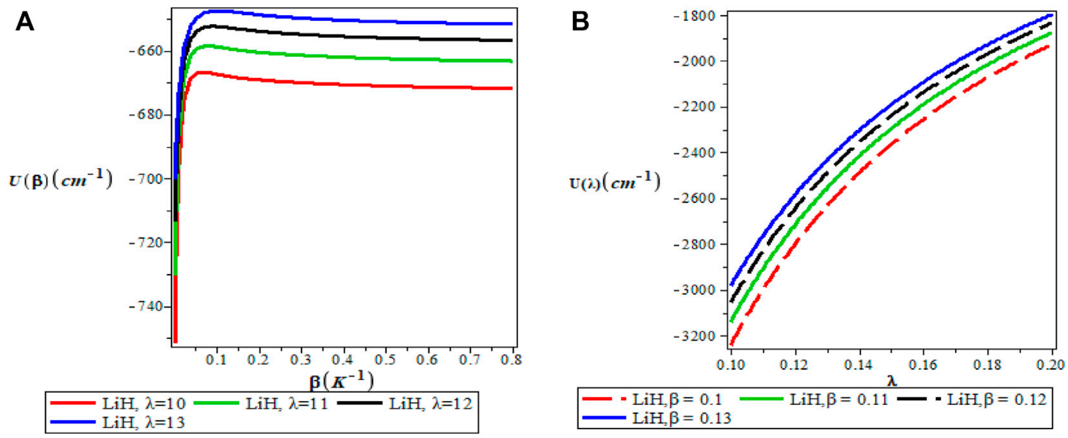

FIGURE 6 | (A) Variation of Vibrational Mean Energy With Respect to β **(B)** Variation of Vibrational Mean Energy With Respect to λ.

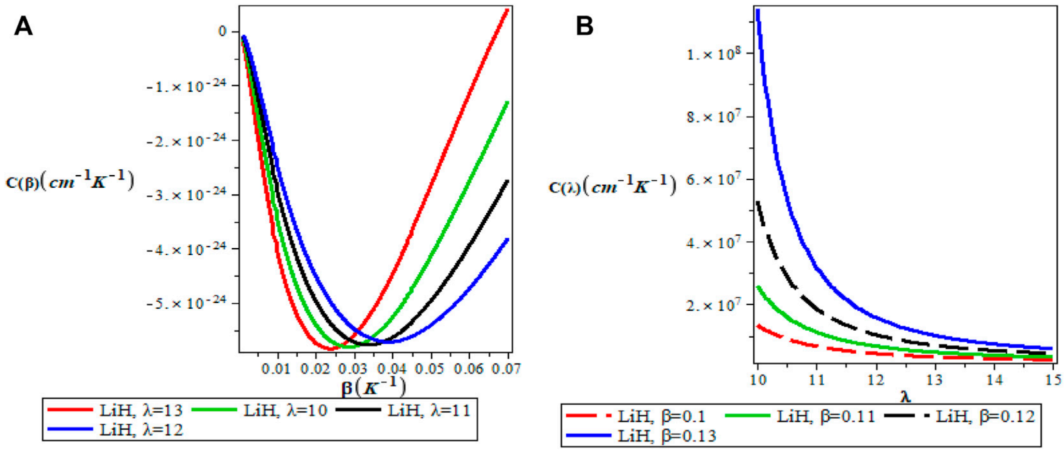

FIGURE 7 | (A) Variation of Specific Heat Capacity With Respect to β **(B)** Variation of Specific Heat Capacity With Respect to λ.

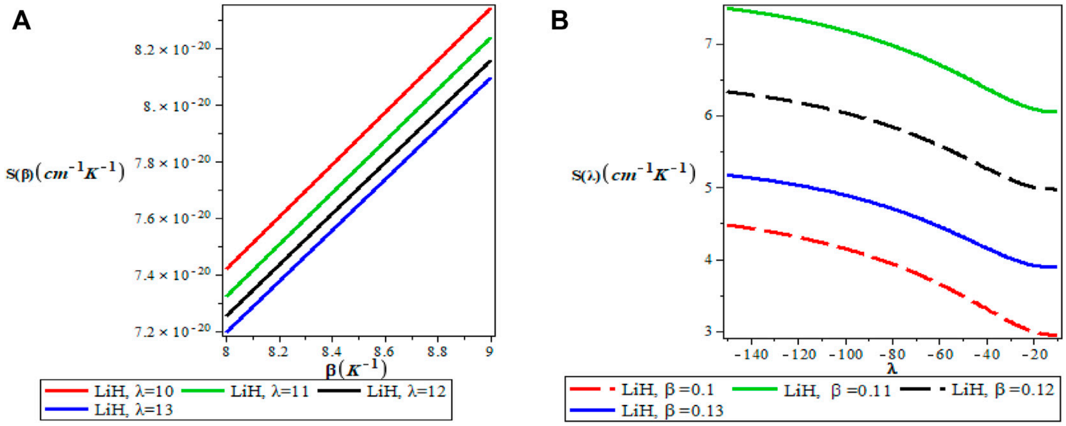

FIGURE 8 | (A) Variation of Vibrational Entropy With Respect to β **(B)** Variation of Vibrational Entropy With Respect to λ.

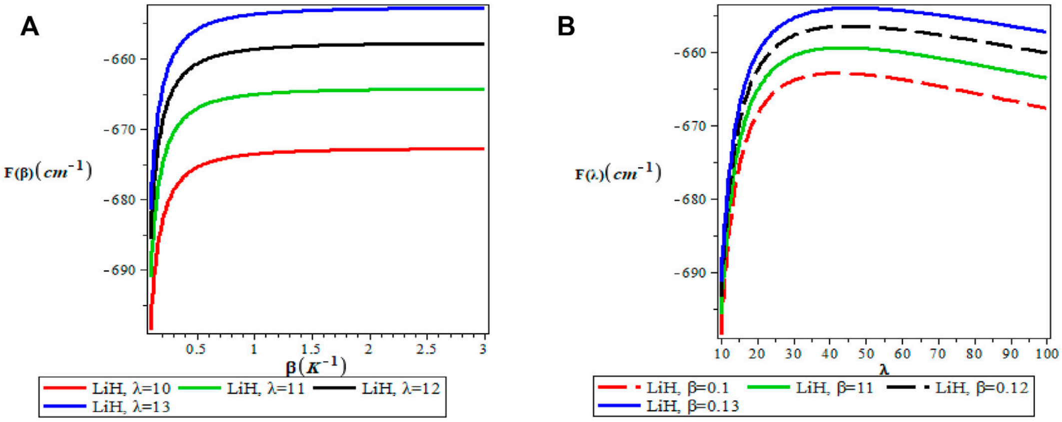

FIGURE 9 | (A) Variation of Vibrational Free Energy With Respect to β **(B)** Variation of Vibrational Free Energy With Respect to λ.

$$Z(\beta) = e^{\beta(2Q_2Q_3 - Q_1)} \int_0^{\lambda} e^{\left(Q_2\rho^2 + \frac{Q_2Q_3^2}{\rho^2}\right)} d\rho \tag{27}$$

Eq. 22 is integrated using MAPLE package. Hence, the integral **Eq. 22** which is the partition function is given as

$$Z(\beta) = \frac{\zeta_1}{4\sqrt{-\beta Q_2}} \left[\begin{array}{l} 1 + \operatorname{erf}\left(\lambda\sqrt{-\beta Q_2} - \frac{\sqrt{-\beta Q_2 Q_3^2}}{\lambda}\right) - e^{4\sqrt{-\beta Q_2}\sqrt{-\beta Q_2 Q_3^2}} \\ \operatorname{erfc}\left(\lambda\sqrt{-\beta Q_2} + \frac{\sqrt{-\beta Q_2 Q_3^2}}{\lambda}\right) \end{array} \right] \tag{28}$$

where

$$\zeta_1 = \sqrt{\pi}\exp\left(-\beta Q_1 + 2\beta Q_2 Q_3 - 2\sqrt{-\beta Q_2}\sqrt{-\beta Q_2 Q_3^2}\right) \tag{29}$$

Using the partition function 27, other thermodynamic properties are obtain as follows.

a) Vibrational mean energy:

$$U(\beta) = -\frac{\partial \ln Z(\beta)}{\partial \beta} = \left[\frac{\begin{array}{c} \sqrt{-\beta Q_2 Q_3^2}\left(\sqrt{\pi}\,\zeta_2(2\beta Q_1 + 1) + \zeta_4\right) \\ +\zeta_2\sqrt{-\beta Q_2 Q_3^2} - 4\sqrt{\pi}\,\beta\zeta_3 Q_2 Q_3^2\sqrt{-\beta Q_2} \end{array}}{2\sqrt{\pi}\,\beta\zeta_2\sqrt{-\beta Q_2 Q_3^2}} \right] \tag{30}$$

where

$$\left.\begin{array}{l} \zeta_2 = \operatorname{erfc}\left(\lambda\sqrt{-\beta Q_2} - \frac{\sqrt{-\beta Q_2 Q_3^2}}{\lambda}\right) + e^{4\sqrt{-\beta Q_2}\sqrt{-\beta Q_2 Q_3^2}} \operatorname{erfc}\left(\lambda\sqrt{-\beta Q_2} + \frac{\sqrt{-\beta Q_2 Q_3^2}}{\lambda}\right) - 2 \\ \zeta_3 = \operatorname{erfc}\left(\lambda\sqrt{-\beta Q_2} - \frac{\sqrt{-\beta Q_2 Q_3^2}}{\lambda}\right) - e^{4\sqrt{-\beta Q_2}\sqrt{-\beta Q_2 Q_3^2}} \operatorname{erfc}\left(\lambda\sqrt{-\beta Q_2} + \frac{\sqrt{-\beta Q_2 Q_3^2}}{\lambda}\right) - 2 \\ \zeta_4 = 4\lambda\sqrt{-\beta Q_2}\exp\left(\frac{\beta Q_2(\lambda^4 + Q_3^2)}{\lambda^2} + 2\sqrt{-\beta Q_2}\sqrt{-\beta Q_2 Q_3^2}\right) \end{array}\right\}. \tag{31}$$

b) Vibrational specific heat capacity:

$$\begin{aligned} C(\beta) &= k\beta^2\left(\frac{\partial^2 \ln Z(\beta)}{\partial \beta^2}\right) \\ &= \frac{k\beta^2\left(-\pi\lambda\zeta_2^2\sqrt{-\beta Q_2}\sqrt{-\beta Q_2 Q_3^2} + \zeta_8 - \zeta_9\right)}{2\pi\beta^2\lambda\zeta_2^2\sqrt{-\beta Q_2}\sqrt{-\beta Q_2 Q_3^2}} \end{aligned} \tag{32}$$

where

$$\left.\begin{array}{lcl} \zeta_5 & = & e^{\frac{\beta Q_2(\lambda^4 + Q_3^2)}{\lambda^2}}\left(4\lambda^2\sqrt{-\beta Q_2} + \sqrt{-\beta Q_2 Q_3^2}\right) - 8\sqrt{\pi}\,\lambda e^{2\sqrt{-\beta Q_2}\sqrt{-\beta Q_2 Q_3^2}} \\ & & \sqrt{-\beta Q_2}\sqrt{-\beta Q_2 Q_3^2}\operatorname{erfc}\left(\lambda\sqrt{-\beta Q_2} + \frac{\sqrt{-\beta Q_2 Q_3^2}}{\lambda}\right) \\ \zeta_6 & = & \left(\sqrt{-\beta Q_2 Q_3^2} - 4\lambda^2\sqrt{-\beta Q_2}\right)\exp\left(\frac{\beta Q_2(\lambda^4 + Q_3^2)}{\lambda^2} + 2\sqrt{-\beta Q_2}\sqrt{-\beta Q_2 Q_3^2}\right) \\ & & +16\sqrt{\pi}\,\lambda\sqrt{-\beta Q_2}\sqrt{-\beta Q_2 Q_3^2} \\ \zeta_7 & = & \zeta_5\operatorname{erfc}\left(\lambda\sqrt{-\beta Q_2} - \frac{\sqrt{-\beta Q_2 Q_3^2}}{\lambda}\right) + \zeta_6 e^{2\sqrt{-\beta Q_2}\sqrt{-\beta Q_2 Q_3^2}} \\ & & \operatorname{erfc}\left(\lambda\sqrt{-\beta Q_2} + \frac{\sqrt{-\beta Q_2 Q_3^2}}{\lambda}\right) - 2e^{\frac{\beta Q_2(\lambda^4 + Q_3^2)}{\lambda^2}}\left(4\lambda^2\sqrt{-\beta Q_2} + \sqrt{-\beta Q_2 Q_3^2}\right) \\ \zeta_8 & = & 4\sqrt{\pi}\,\beta^2 Q_2^2 e^{2\sqrt{-\beta Q_2}\sqrt{-\beta Q_2 Q_3^2}}\left(\zeta_7 Q_3^2 - \lambda^4\zeta_2\sqrt{-\beta Q_2 Q_3^2}\,e^{\frac{\beta Q_2(\lambda^4 + Q_3^2)}{\lambda^2}}\right) \\ \zeta_9 & = & 2\beta\lambda^2 Q_2\sqrt{-\beta Q_2 Q_3^2}\exp\left(\frac{\beta Q_2(\lambda^4 + Q_3^2)}{\lambda^2} + 2\sqrt{-\beta Q_2}\sqrt{-\beta Q_2 Q_3^2}\right) \\ & & \left(4\lambda\sqrt{-\beta Q_2}\exp\left(\frac{\beta Q_2(\lambda^4 + Q_3^2)}{\lambda^2} + 2\sqrt{-\beta Q_2}\sqrt{-\beta Q_2 Q_3^2}\right) - \sqrt{\pi}\,\zeta_2\right) \end{array}\right\}. \tag{33}$$

(c) Vibrational entropy

$$\begin{aligned} S(\beta) &= k\ln Z(\beta) - k\beta\frac{\partial \ln Z(\beta)}{\partial \beta} \\ &= \mathrm{kLog}\left(-\frac{\sqrt{\pi}\,\zeta_2\exp\left(-\beta Q_1 + 2\beta Q_2 Q_3 - 2\sqrt{-\beta Q_2}\sqrt{-\beta Q_2 Q_3^2}\right)}{4\sqrt{-\beta Q_2}}\right) \\ &\quad + \frac{k\left(\zeta_{10} - \zeta_{11} + \sqrt{\pi}\,\zeta_2(2\beta Q_1 - 4\beta Q_2 Q_3 + 1)\right)}{2\sqrt{\pi}\zeta_3} \end{aligned} \tag{34}$$

where

$$\left.\begin{aligned}\zeta_{10} &= 4\sqrt{\pi}\sqrt{-\beta Q_2}\sqrt{-\beta Q_2 Q_3^2}\,\mathrm{erfc}\left(\lambda\sqrt{-\beta Q_2}-\frac{\sqrt{-\beta Q_2 Q_3^2}}{\lambda}\right)+4\lambda\sqrt{-\beta Q_2}\\ &\quad \exp\left(\frac{\beta Q_2\left(\lambda^4+Q_3^2\right)}{\lambda^2}+2\sqrt{-\beta Q_2}\sqrt{-\beta Q_2 Q_3^2}\right)-8\sqrt{\pi}\sqrt{-\beta Q_2}\sqrt{-\beta Q_2 Q_3^2}\\ \zeta_{11} &= 4\sqrt{\pi}\,e^{4\sqrt{-\beta Q_2}\sqrt{-\beta Q_2 Q_3^2}}\sqrt{-\beta Q_2}\sqrt{-\beta Q_2 Q_3^2}\,\mathrm{erfc}\left(\lambda\sqrt{-\beta Q_2}+\frac{\sqrt{-\beta Q_2 Q_3^2}}{\lambda}\right)\end{aligned}\right\}. \tag{35}$$

(c) Vibrational free energy

$$\begin{aligned}F(\beta) &= -kT\ln Z(\beta)\\ &= \frac{\sqrt{\pi}\zeta_2\ln\exp\left(-\beta Q_1+2\beta Q_2 Q_3-2\sqrt{-\beta Q_2}\sqrt{-\beta Q_2 Q_3^2}\right)}{4\beta\sqrt{-\beta Q_2}}\end{aligned} \tag{36}$$

4 RESULTS AND DISCUSSION

The thermodynamics properties of KPGM was studied, the plots of the wavefunction and thermodynamics properties as a function of the inverse temperature parameter β and λ for Lithium hydride (LiH) diatomic molecule are shown in **Figures 1–4** and **Figures 5–9** respectively. The spectroscopic parameter for Lithium hydride is adopted from Ref. [54]. **Figure 1A** is the wave function plot for fixed l = 0 which begins with a commom origin and proceed to a continous sinusoidal curve with various maximum and minimum turning points for Lithium hydride molecule. From the graph, it can be observed that the peaks of the turning points increases with increase in the principal quantum number (n), as such n = 0 has the lowest peak. The probability density curve for fixed l = 0 is displayed in **Figure 1B**. This plot follows normal distribution with several maximum points which also increases with an increase in the principal quantum number. The probability density curve completely describe the localization of electrons of LiH molecule, hence electron is more localized at n = 3 which has the highest maximum point. The same description of **Figure 1A** is applicable to **Figures 2A**, **4A** while **Figures 2B**, **4B** also have the same description as **Figure 1B**. The wavefunction graph in **Figure 3A** has maximum and minimum turning points at higher quantum states except at the ground state (n = 0) where there is a divergence in the curve. In **Figure 3B**, the probability density plot is sinusoidal in nature which shows the localization of electrons for higher quantum state while diverges at the ground state.

Figures 5A,B show the variation of the vibrational partition function. It is observed in **Figure 5A** that the partition function $Z(\beta)$ increases exponentially from the origin with increase in the inverse temperature parameter (β) but the partition function $Z(\lambda)$ decreases with increase in λ as presented in **Figure 5B** for LiH diatomic molecule. The mean vibrational energy $U(\beta)$ as displayed in **Figure 6A** increases monotonically with increase in the values of β with slight maximum turning points. The plot of $U(\lambda)$ against λ has a hyperbolic nature. From **Figure 7A**, The vibrational specific heat capacity $C(\beta)$ first decreases with an increase in inverse temperature parameter to a minimum value and then increase monotonically. However, the graph of vibrational specific heat capacity ($C(\beta)$) as a function of β has various minimum turn points that touch the horizontal axis. $C(\lambda)$ decreases exponentially with λ in **Figure 7B**. Plots of the vibrational entropy with different values of β and λ is shown in **Figures 8A,B** respectively. As seen in **Figure 8A**, the vibrational entropy $C(\beta)$ increases linearly with increasing values of β while $S(\lambda)$ decreases with increasing values of λ. Plots of the mean free energy $F(\beta)$ as a function of β increases monotonically with an increase in β for various values of λ as presented in **Figure 9A**. In **Figure 9B**, the vibrational free energy exhibited an hyperborlic nature which increases with an increase in λ. In order to prove the accuracy of work, the thermodynamic plots for this present work as applied to lithium hydride molecule are in excellent agreement to work of Okorie et al. [65] using improved deformed exponential type potential.

5 CONCLUSION

In this work, we have solved the Schrödinger wave equation in the presence of Kratzer plus generalized Morse potential (KPGM) using Parametric Nikiforov-Uvarov method. The energy eigenvalues and the corresponding normalised wave function were obtained and presented in a closed and compact form. However, we studied the thermodynamics properties of KPGM which are: vibrational partition (Z), vibrational mean energy(U), specific heat capacity(C), vibrational entropy (s), and mean free energy (F). Also, we have plotted the variation of these thermodynamic functions as a function of inverse temperature parameter(β) and upper bound vibrational quantum number (λ) for Lithium hydride diatomic molecule. We analytically obtained the normalised wave function expressed in terms of hypergeometric function of Jacobi polynomial. The normalised wave function and probability density plots for the Lithium hydride molecule were obtained through a well designed Maple programming. This research work has application in molecular spectroscopy. Lithium hydride is heteronuclear diatomic molecule which has high density hydrogen storage and serve as a precausor for building complex hydrides. The thermodynamic plots obtained are in excellent agreement to work of an existing literature. Further research work can be carried out with Kratzer plus generalised Morse potential using other methods like the supersymmetric quantum mechanics approach to investigate other properties like expectation values as well as superstatistic formulation.

DATA AVAILABILITY STATEMENT

The raw data supporting the conclusion of this article will be made available by the authors, without undue reservation.

AUTHOR CONTRIBUTIONS

CI, IO, AA, and KO, conceived the original idea and wrote the first draft. EO, CO, and RJ carried out the thermodynamic plots. MU, EI, and JA carried out literature searches and editing of the final manuscript. All authors contributed to the manuscript.

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