

Solutions of the Schrodinger Equation for the Hulthen-Type Potential Plus Modified Kratzer Potential: Application to Ionic Crystals

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ABSTRACT

The approximate analytical solution of the radial Schrodinger equation has been extended to ionic crystal using the Hulthen-type plus modified Kratzer potential model, within the framework of Nikiforov-Uvarov method using Greene-Aldrich approximation. The aim of combining these potentials is to have a wide application. The energy eigenvalues for NaCl, NaF, NaBr and NaI ionic crystals were computed for various vibrational and rotational quantum numbers. Special cases were considered when the potential parameters were altered, resulting into Hulthen-Type Potential and Modified Kratzer Potential. Their energy eigenvalues expressions and numerical computations agreed with the already existing literatures. Also, spectroscopic parameter for ionic crystals were used in plotting graphical variation of the bound state energy eigenvalues for the ionic crystals with different potential parameters and quantum numbers were discussed. Our results are in agreement with the reports of other researchers.

Keywords:

Hulthen-Type Potential, Modified Kratzer Potential, Nikiforov-Uvarov method, Schrödinger equation.

INTRODUCTION

An Ionic crystal is a crystalline form of an ionic compound. They are solid consisting of ions bound together by their electrostatic attraction into regular lattice held together by the electrostatic force of attraction (Sherman, 1932). They are good conductors of electricity when molten, but very poor in the solid state. The exact arrangement of ions in an ionic lattice varies according to the size of the ions in the solid (Pearson, 1963).

The exact or approximate solutions of Schrödinger equation play an important role in many branches of modern physics and chemistry (Chung et al., 1999). The solution of this equation is used in the description of particle dynamics in non-relativistic regime. (Ikhdair, 2011; Maghsoodi et al., 2012). Non-relativistic wave equations in quantum mechanics cannot be over emphasized. as such, non-relativistic spineless particles can be described using Schrödinger wave equation (Yahya & Oyewumi, 2015), and while in relativistic quantum mechanics the Dirac and Klein-Gordon equations are frequently used as wave equation. The Dirac equation can describe the dynamics of a particle with half-integral spin such as fermions. Also, Klein-Gordon equation is suitable for the description of spin-zero particle dynamics such as bosons. In most cases, Schrödinger and Klein-Gordon equations cannot be

solved analytically except by the using an approximation for the centrifugal term. The exact solution of the Schrodinger equation with a chosen potential model is fundamental for understanding the energy spectrum of a particle (Chun-Feng et al., 1991; Ikhdair & Falaye, 2013) The exact solution of Schrodinger wave equation is only possible for a few potential such as harmonic oscillator potential, coulomb potential, kratzer potential, etc. (Ikot et al., 2011), while others can only be solved approximately (Egrifes et al., 2000; Chen & Sun, 2008; Hamzavi et al., 2013), with the use of different approximation schemes (Pekeris, 1934).

Some of the potential investigated includes: coulomb potential (Ma et al., 2014), Eckat potential (Akpan et al., 2012), Kratzer potential (Berkdemir et al., 2006; Hassannabadi et al., 2011), Ring-Shaped potential (Dong & Lozada-Cassou, 2006), Hulthen potential (Saad, 2007; Ikhdair, 2009), Yukawa potential (Ahmadov et al., 2019; Anita et al., 2015 and Ikot et al., 2013), Rosen-Morse potential (Gu et al., 2008; Qiang & Dong, 2007), Woods-Saxon's potential (Arda, 2009; Badalov et al., 2010; Ikhdair & Sever, 2007), and several other potentials as well (Nugraha et al., 2017)

To obtain the approximate or exact solution of quantum mechanics equation, different methods have been developed like factorization method (Dong, 2007),

Laplace transform approach (Arda & Sever, 2012; Das & Arda, 2017), the path integration method (Liu et al., 2018), the exact quantization method (Gu et al., 2008), the Nikiforov-Uvarov method (Anita et al., 2015; Ikhdaïr & Sever, 2007; Nikiforov-Uvarov, 1988; Edet et al., 2020), the flite-difference version of the relativistic quantum mechanics (Nagiyeu & Ahmadov, 2019), and singular Manifold method (Saleh et al., 2019), Nikiforov-Uvarov (NU) method (Onate & Idiodi, 2015), Supersymmetry quantum mechanics (SUSYQM) (Onate & Ojonubah, 2013; Onate et al., 2017), Asymptotic iteration method (AIM) (Ciftci et al., 2003; Nugraha et al., 2017), Proper and exact quantization rule (Qiang & Dong, 2007; Ikhdaïr & Sever, 2009), Factorization method (Dong, 2007), Functional Analysis Approach, FAA (also known as Modified factorization method) (Jia & Jia, 2017),

In the last few decades, a great deal of interest has been raised in many branches of physics in order to calculate the energy eigenvalues and Eigen functions of diatomic molecules. Recently, Ahmadov et al. (2019) solved the Klein Gordon (KG) equation with the linear combination of Hulthen and Yukawa potential using Nikiforov-Uvarov method (Heseyin and sever, 2012). However, no study has been reported on the Eigen value and Eigen function of ionic crystals with Hulthen-Type Potential plus modified kratzer potential with ionic crystal dissociation (D_e) energy Madelung constant(α) and equilibrium bond length parameters (r_e) using Nikiforov-Uvarov method. With the above mentioned studies on these different potentials and their importance, we seek to investigate the solutions of Schrodinger equation with the linear combination of Hulthen-type potential plus modified kratzer potential for ionic crystal such as NaCl, NaF, NaBr and NaI. The potential takes the form

$$V(r) = -\frac{Ae^{-2\alpha r}}{1-e^{-2\alpha r}} + D_e \left(\frac{r-r_e}{r}\right)^2 \quad (1)$$

Where D_e the dissociation energy, r_e is the equilibrium internuclear separation, r is the interatomic distance A is the depth of the potential, and α is madelung constant of the ionic crystal. It can be deduced that when $D_e = 0$, the above combined potential reduces to the Hulthen-Type Potential. Also, when $A = 0$, equation (1) reduces to the modified kratzer potential.

The Hulthen potential is a short range potential which behave like a coulomb potential for small values of r and decreases exponentially for large values of r . The Hulthen potential has been used in many branches of physics, such as nuclear physics (Hulthen et al., 1957), atomic physics (Tietz, 1961; Lam & Varshni, 1971), Solid state physics (Berezin, 1972), and chemical physics (Pyykko & Jokisaari, 1975). The model of the three-dimensional delta-function could well be considered as Hulthen potential with the radius of the force going down to zero (Berezin, 1986). The

Schrödinger equation for this potential can be solved in a closed form for s-waves. For $\ell \neq 0$, a number of method have been employed to find approximate solution for the Schrödinger equation with the Hulthen potential (Lai, 1980; Patil, 1984; Popov & Wienberg, 1985; Roy & Roychoudhury, 1987). The Hulthen-Type potential which is a modified Hulthen potential is used in the work

The Modified kratzer potential (Kratzer, 1920) is mostly applied in atomic physics, physics and quantum chemistry (Sadeghi, 2007), and it is used to describe the interactions of molecules in quantum mechanics. The potential is made up of a long-range attraction and a repulsive part. The integration of these parts makes this potential reliable in terms of its vibrational and rotational energy eigenvalues (Roy & Bernstein 1970; Bayrak, 2017). The potential is known to approach infinity when the internuclear distance approaches zero, due to the repulsion that exist between the molecules of the potential. As the internuclear molecular distance approaches infinity, the potential decomposes to zero (Saad et al., 2008; Hassanabadi et al., 2011).

MATERIALS AND METHODS

Overview of Nikiforov-Uvarov Method

The Nikiforov-Uvarov (NU) method is based on solving the hypergeometric-type second order differential equations by means of the special orthogonal functions (Szego, 1939), using coordinate transformation appropriately. The basic equation of NU method is given in the form: (Karayer et al., 2015; Pahlavani, 2012; Nikiforov & Uvarov, 1988):

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

where $\tilde{\tau}(s)$ is a polynomial of at most first-degree, while $\sigma(s)$ and $\tilde{\sigma}(s)$ are polynomials of at most second-degree $\psi(s)$ is a function of hypergeometric-type.

$$\psi(s) = \phi(s)y(s) \quad (3)$$

then Equation (2) reduces to hypergeometric-type:

$$\sigma(s)y'' + \tau(s)y' + \lambda y = 0 \quad (4)$$

where

$$\lambda = \lambda_n = -n\tau' - \frac{n(n-1)}{2}\sigma'', \quad n = 0,1,2,\dots \quad (5)$$

and $\tau(s)$ is defined as:

$$\tau(s) = \tilde{\tau}(s) + 2\pi(s) \quad (6)$$

which must have a negative derivative. Equation (7) has polynomial solutions $y_n(s)$ that are given by the Rodrigues relation

$$y_n(s) = \frac{B_n}{\rho(s)} \frac{d^n}{ds^n} [\sigma^n(s)\rho(s)] \quad (7)$$

where B_n is the normalization constant and $\rho(s)$ is called the density or weight function and must satisfy the condition

$$(\sigma\rho)' = \tau\rho \quad (8)$$

The function $\phi(s)$ satisfies

$$\frac{\phi'}{\phi} = \frac{\pi}{\sigma} \quad (9)$$

where $\pi(s)$ and the parameter λ are defined as

$$\pi(s) = \frac{\sigma'(s) - \tilde{\tau}(s)}{2} \pm \sqrt{\left(\frac{\sigma'(s) - \tilde{\tau}(s)}{2}\right)^2 - \tilde{\sigma}(s) + k(s)\sigma(s)} \quad (10)$$

and

$$\lambda = k + \pi' \quad (11)$$

The function $\pi(s)$ is a polynomial of first degree at most and thus the expression under the square root in Equation (10) must be a square of a polynomial of first degree. The determination of k is thus important in the calculation of $\pi(s)$.

Approximate analytical solutions of the Hulthen-Type Potential Plus Modified Kratzer potential

The Schrödinger equation for motion of a particle with the reduced mass μ in the spherical symmetric potential described by the spherical coordinates is given by

$$\frac{-\hbar^2}{2\mu} \left[\frac{\partial^2}{\partial r^2} + \frac{2}{r} \frac{\partial}{\partial r} + \frac{1}{r^2} \left(\frac{1}{\sin\theta} \frac{\partial}{\partial \theta} \left(\sin\theta \frac{\partial}{\partial \theta} \right) + \frac{1}{\sin^2\theta} \frac{\partial^2}{\partial \phi^2} \right) + V(r) \right] \psi_{nlm}(r, \theta, \phi) = E_{nl} \psi_{nlm}(r, \theta, \phi) \quad (12)$$

In order to obtain the bound state solution of $\ell \neq 0$, we insert the potential in equation (1) into equation (13) then the equation becomes:

$$\frac{d^2 R_{nl}(r)}{dr^2} + \frac{2\mu}{\hbar^2} \left[E_{nl} - V(r) - \frac{\ell(\ell+1)\hbar^2}{2\mu r^2} \right] R_{nl}(r) = 0 \quad (13)$$

Where μ is the reduced mass, E_{nl} is the rotational vibrational energy spectra of the ionic molecule, \hbar is the reduced plank's constant, and n and ℓ are the radial and orbit angular momentum quantum numbers respectively

$$\frac{d^2 R_{nl}(r)}{dr^2} + \frac{2\mu}{\hbar^2} \left[E_{nl} + \frac{Ae^{-2\alpha r}}{1-e^{-2\alpha r}} - D_e \left(\frac{r-r_e}{r} \right)^2 - \frac{\ell(\ell+1)\hbar^2}{2\mu r^2} \right] R_{nl}(r) = 0 \quad (14)$$

$$\frac{d^2 R_{nl}(r)}{dr^2} + \frac{2\mu}{\hbar^2} \left[E_{nl} + \frac{Ae^{-2\alpha r}}{1-e^{-2\alpha r}} - D_e + \frac{2D_e r_e}{r} - \frac{D_e r_e^2}{r^2} + \frac{Ae^{-2\alpha r}}{r} - \frac{\ell(\ell+1)\hbar^2}{2\mu r^2} \right] R_{nl}(r) = 0 \quad (15)$$

$$\frac{d^2 R_{nl}(r)}{dr^2} + \left[\frac{2\mu}{\hbar^2} E_{nl} + \frac{2\mu}{\hbar^2} \frac{Ae^{-2\alpha r}}{1-e^{-2\alpha r}} - \frac{2\mu}{\hbar^2} D_e + \frac{4\mu D_e r_e}{\hbar^2 r} - \frac{2\mu D_e r_e^2}{\hbar^2 r^2} - \frac{\ell(\ell+1)}{r^2} \right] R_{nl}(r) = 0 \quad (16)$$

We employ the Pekeris approximation scheme (Pekeris, 1934) to get rid of the centrifugal barrier

$$\frac{1}{r^2} \approx \frac{4\alpha^2 e^{-2\alpha r}}{(1-e^{-2\alpha r})^2} \quad (17)$$

$$\frac{1}{r} \approx \frac{2\alpha e^{-2\alpha r}}{(1-e^{-2\alpha r})} \quad (18)$$

$$\frac{d^2 R_{nl}(r)}{dr^2} + \left[\frac{2\mu}{\hbar^2} (E_{nl} - D_e) + \frac{2\mu A e^{-2\alpha r}}{\hbar^2 (1-e^{-2\alpha r})} + \frac{4\mu D_e r_e}{\hbar^2} \frac{2\alpha e^{-2\alpha r}}{(1-e^{-2\alpha r})} - \frac{2\mu D_e r_e^2}{\hbar^2} \frac{4\alpha^2 e^{-2\alpha r}}{(1-e^{-2\alpha r})^2} + \frac{\ell(\ell+1)4\alpha^2 e^{-2\alpha r}}{(1-e^{-2\alpha r})^2} \right] R_{nl}(r) = 0 \quad (19)$$

by using the coordinate transformation

$$s = e^{-2\alpha r} \quad (20)$$

we obtain the differential equation of the form

$$\frac{d^2 R_{nl}(s)}{ds^2} + \left[\frac{2\mu}{\hbar^2} (E_{nl} - D_e) + \frac{2\mu A s}{\hbar^2 (1-s)} + \frac{8\mu D_e r_e}{\hbar^2} \frac{\alpha s}{(1-s)} - \frac{8\mu D_e r_e^2}{\hbar^2} \frac{\alpha^2 s}{(1-s)^2} - \frac{4\ell(\ell+1)\alpha^2 s}{(1-s)^2} \right] R_{nl}(s) = 0 \quad (21)$$

Equation (21) can be simplified into the form

$$\frac{d^2 R_{nl}(s)}{ds^2} + \frac{(1-s)}{s(1-s)} \frac{dR}{ds} + \frac{1}{s^2(1-s)^2} [-\mathcal{E}_n(1-s)^2 + \beta s(1-s) + \gamma s(1-s) - \delta s - \omega s] R_{nl}(s) = 0 \quad (22)$$

$$\mathcal{E}_n = -\frac{\mu}{2\alpha^2 \hbar^2} (E_{nl} - D_e)$$

$$\beta = \frac{\mu A}{2\alpha \hbar^2}$$

$$\gamma = \frac{2\mu D_e r_e}{\alpha \hbar^2}$$

$$\delta = \frac{2\mu D_e r_e^2}{\hbar^2}$$

$$\omega = \ell(\ell+1) \quad (23)$$

$$\frac{d^2 R_{nl}(s)}{ds^2} + \frac{(1-s)}{s(1-s)} \frac{dR}{ds} + \frac{1}{s^2(1-s)^2} [-(\mathcal{E}_n + \beta + \gamma)s^2 + (2\mathcal{E}_n + \beta + \gamma - \delta - \omega)s - (\mathcal{E}_n)] R_{nl}(s) = 0 \quad (24)$$

Comparing equation (2) and (24) we have the following parameters

$$\tilde{\tau} = 1 - s$$

$$\sigma = s(1-s)$$

$$\tilde{\sigma}(s) = -(\mathcal{E}_n + \beta + \gamma)s^2 + (2\mathcal{E}_n + \beta + \gamma - \delta - \omega)s - (\mathcal{E}_n) \quad (25)$$

Substituting these polynomials into equation (10) we obtained

$$\pi(s) = -\frac{s}{2} \pm \sqrt{(a-k)s^2 + (k+b)s + c} \quad (26)$$

where

$$\begin{aligned} a &= \frac{1}{4} + \mathcal{E}_n + \beta + \gamma \\ b &= -2\mathcal{E}_n - \beta - \gamma + \delta + \omega \\ c &= \mathcal{E}_n \end{aligned} \quad (27)$$

To find the constant k, the discriminant of the expression under the square root of equation (26) must be zero. As such we have

$$\pi(s) = -\frac{s}{2} \pm \left(\sqrt{\frac{1}{4} + \delta + \omega + \sqrt{\mathcal{E}_n}} s - \sqrt{\mathcal{E}_n} \right) \quad (28)$$

$$\text{for } k_{\pm} = -(-\beta - \gamma + \delta + \omega) + 2\sqrt{\mathcal{E}_n} \sqrt{\frac{1}{4} + \delta + \omega} \quad (29)$$

From the knowledge of NU method, we choose the expression $\pi(s)_-$ in which the function $\pi(s)$ has negative derivative. This is given by

$$\pi(s)_- = -\frac{s}{2} - \left(\sqrt{\frac{1}{4} + \delta + \omega + \sqrt{\mathcal{E}_n}} s - \sqrt{\mathcal{E}_n} \right) \quad (30)$$

Where $\tau(s)$ being obtained as

$$\tau(s) = 1 - 2s - 2 \left(\sqrt{\frac{1}{4} + \delta + \omega + \sqrt{\mathcal{E}_n}} s + 2\sqrt{\mathcal{E}_n} \right) \quad (31)$$

Referring to equation (11), we define the constant λ as

$$\lambda = -(-\beta - \gamma + \delta + \omega) + 2\sqrt{\mathcal{E}_n} \sqrt{\frac{1}{4} + \delta + \omega} - \frac{1}{2} - \left(\sqrt{\frac{1}{4} + \delta + \omega + \sqrt{\mathcal{E}_n}} \right) \quad (32)$$

Substituting equation (30) into equation (5) and carrying out simple algebra, where

$$\tau'(s) = -2 - 2 \left(\sqrt{\frac{1}{4} + \delta + \omega + \sqrt{\mathcal{E}_n}} \right) \quad (32)$$

And

$$\sigma''(s) = 2 \quad (34)$$

We have

$$\mathcal{E}_n = \frac{1}{4} \left[\frac{\left(n + \frac{1}{2} + \sqrt{\frac{1}{4} + \delta + \omega} \right)^2 - \beta - \gamma}{\left(n + \frac{1}{2} + \sqrt{\frac{1}{4} + \delta + \omega} \right)} \right]^2 \quad (35)$$

$$\mathcal{E}_n = \frac{1}{4} \left[\frac{(n+\xi)^2 - \beta - \gamma}{(n+\xi)} \right]^2 \quad (36)$$

Where

$$\xi = \frac{1}{2} \left(1 + 2 \sqrt{\frac{1}{4} + \delta + \omega} \right) \quad (37)$$

Substituting equation (22) and (37) into (36) yields the energy eigen equation of the Hulthen-type potential plus modified krater potential in the form

$$E_{nl} = D_e - \frac{\alpha^2 \hbar^2}{2\mu} \left[\frac{\left(n + \frac{1}{2} + \sqrt{\frac{1}{4} + \frac{2\mu D_e r_e^2}{\hbar^2} + \ell(\ell+1)} \right)^2 - \frac{\mu A}{2\alpha \hbar^2} - \frac{2\mu D_e r_e}{\alpha \hbar^2}}{\left(n + \frac{1}{2} + \sqrt{\frac{1}{4} + \frac{2\mu D_e r_e^2}{\hbar^2} + \ell(\ell+1)} \right)} \right]^2 \quad (38)$$

The Corresponding wave function can be evaluated by substituting $\pi(s)_-$ and $\sigma(s)$ from equation (30) and (25) respectively into equation (9) and solving the first-order differential equation. This gives

$$\phi(s) = s \sqrt{\mathcal{E}_n} (1-s)^{\frac{1}{2} + \sqrt{\frac{1}{4} + \delta + \omega}} \quad (39)$$

The weight function $\rho(s)$ from eq (8) can be obtained as

$$\rho(s) = s^{2\sqrt{\mathcal{E}_n}} (1-s)^{2\sqrt{\frac{1}{4} + \delta + \omega}} \quad (40)$$

From Rodrigues relation of eq (7), we obtain

$$y_n(s) = B_n s^{-2\sqrt{\mathcal{E}_n}} (1-s)^{2\sqrt{\frac{1}{4} + \delta + \omega}} \left[s^{n+2\sqrt{\mathcal{E}_n}} (1-s)^{n+2\sqrt{\frac{1}{4} + \delta + \omega}} \right] \quad (41)$$

$$y_n(s) = B_n P_n \left(2 \sqrt{\varepsilon_n} \sqrt{\frac{1}{4} + \delta + \omega} \right) (1 - 2s) \quad (42)$$

Where $P_n^{(\theta, \vartheta)}$ is the Jacobi polynomial.

Substituting $\phi(s)$ and $y_n(s)$ from equation (39) and (41) respectively, into equation (3) we obtain

$$\psi(s) = B_n s^{\sqrt{\varepsilon_n}} (1-s)^G P_n^{(2\sqrt{\varepsilon_n}, 2G-1)}(1-2s) \quad (43)$$

Where

$$G = \frac{1}{2} + \sqrt{\frac{1}{4} + \delta + \omega} \quad (44)$$

From the definition of Jacobi polynomials (Abramowitz & Stegun, 1964)

$$P_n^{(\theta, \vartheta)}(\omega) = \frac{\Gamma(n+\theta+1)}{n! \Gamma(\theta+1)} {}_2F_1 \left(-n, \theta + \vartheta + n + 1; \frac{1-\omega}{2} \right) \quad (45)$$

In terms of hypergeometric polynomials, equation (43) can be written as

$$\psi(s) = B_n s^{\sqrt{\varepsilon_n}} (1-s)^G \frac{\Gamma(n+2\sqrt{\varepsilon_n}+1)}{n! \Gamma(\sqrt{\varepsilon_n}+1)} {}_2F_1 \left(-n, 2\sqrt{\varepsilon_n} + 2G + n, 2\sqrt{\varepsilon_n} + 1; s \right) \quad (46)$$

Special Cases

In this section, we make some adjustments of constant in equation (3) to have the following cases

Hulthen-type potential

If $D_e = 0$ in equation (1), we can obtain the Hulthen-type potential as

$$V(r) = - \frac{Ae^{-2\alpha r}}{1-e^{-2\alpha r}} \quad (47)$$

From equ (38), the energy eigenvalue equation for the Hulthen-type potential reduces to

$$E_{nl} = - \frac{\alpha^2 \hbar^2}{2\mu} \left[\frac{\left(n + \frac{1}{2} + \sqrt{\frac{1}{4} + \ell(\ell+1)} \right)^2 - \frac{\mu A}{2\alpha \hbar^2}}{\left(n + \frac{1}{2} + \sqrt{\frac{1}{4} + \ell(\ell+1)} \right)} \right]^2 \quad (48)$$

The result in equation (48) is very consistent with the result obtained in equation (18) of Ramantswana et al. (2023)

Modified Kratzer Potential

When the parameter A is set to zero equation (1) reduces the potential to the modified Kratzer potential as

$$V(r) = D_e \left(\frac{r-r_e}{r} \right)^2 \quad (49)$$

And its energy eigenvalue equation can also be deduced from equation (38) as

$$E_{nl} = D_e - \frac{\alpha^2 \hbar^2}{2\mu} \left[\frac{\left(n + \frac{1}{2} + \sqrt{\frac{1}{4} + \frac{2\mu D_e r_e^2}{\hbar^2} + \ell(\ell+1)} \right)^2 - \frac{2\mu D_e r_e}{\alpha \hbar^2}}{\left(n + \frac{1}{2} + \sqrt{\frac{1}{4} + \frac{2\mu D_e r_e^2}{\hbar^2} + \ell(\ell+1)} \right)} \right]^2 \quad (50)$$

As $\alpha \rightarrow 0$ we obtain the energy eigenvalue for modified Kratzer potential to be

$$E_{nl} = D_e - \frac{\hbar^2}{2\mu} \left[\frac{\frac{2\mu D_e r_e}{\hbar^2}}{\left(n + \frac{1}{2} + \sqrt{\frac{1}{4} + \frac{2\mu D_e r_e^2}{\hbar^2} + \ell(\ell+1)} \right)} \right]^2 \quad (51)$$

The result in equation (51) is very consistent with result of equation (14) Berkdemir et al. (2006)

RESULTS AND DISCUSSION

In our study, the energy eigenvalues (in eV) of the Hulthen-type potential and the modified Kratzer potential were computed for NaCl, NaBr, NaF and NaI ionic crystals using eq (38), with the aid of the ionic spectroscopic parameters given in table 1. Our results are consistent with the results obtained by Bayrat et al. (2007). Also it is observed that in table 2, the energy eigen value become more bounded as the quantum state of these crystals increases. Special cases were considered when the potential parameters were altered,

resulting into Hulthen-Type Potential and Modified Kratzer Potential. We plotted the variation of the non-relativistic energy eigenvalues with the different potential parameters such as r_e , α , D_e , ℓ , μ , and n as shown in figure a-f respectively, for various values of n and ℓ quantum numbers. In this figures, there is an increase in energy eigenvalues as the various parameter increases. In fig a, b c and e, the increase in energy tends to spread out from zero position for different potential parameter such as r_e , α , D_e and μ respectively. We also observe a uniform increase in

energy as the parameter μ increases. Fig d shows a slide increase in the energy, with only NaF taking its source from the zero point. Also for Figure 1 (f), the increase in energy eigenvalue is uniform with only NaF again

taking its source from the origin. From graphs plotted, the vibrational quantum numbers show less effect on the energy eigenvalue than the rotational quantum numbers.

Table 1: Spectroscopic parameters for ionic crystals

Ionic Crystals	$r_e(\text{\AA})$	$D_e(\text{eV})$	α	$\mu(\text{a.m.u})$
NaCl	2.36	4.26	1.746941	13.94623
NaBr	2.50	3.80	1.746941	17.85312
NaF	1.93	4.99	1.746941	10.40219
NaI	2.71	3.10	1.746941	19.46370

Table 2: Energy eigenvalues in (eV) of Hulthen-type potential plus modified Kratzer potential for different values of n and ℓ for different ionic crystal

n	ℓ	NaCl	NaBr	NaF	NaI
0	0	-35.90594216	-36.59173994	-22.07152705	-38.42360954
1	0	-36.24700260	-38.07619532	-22.40993224	-38.71043558
	1	-36.24786114	-38.07687012	-22.41104750	-38.71105932
2	0	-36.58915599	-38.38055564	-22.74991379	-38.99801818
	1	-36.59001731	-38.38123231	-22.75103421	-38.99864360
	2	-36.59173994	-38.38258566	-22.75327504	-38.99989440
3	0	-36.93240068	-38.68575538	-23.09146714	-39.28635654
	1	-36.93326473	-38.68643392	-23.09259273	-39.28698357
	2	-36.93499280	-38.68779101	-23.09484386	-39.28823764
	3	-36.93758498	-38.68982666	-23.09822061	-39.29011877
4	0	-37.27673482	-38.99179346	-23.43458785	-39.57544970
	1	-37.27760158	-38.99247384	-23.43571858	-39.57607836
	2	-37.27933520	-38.99383466	-23.43798000	-39.57733574
	3	-37.28193550	-38.99587592	-23.44137218	-39.57922176
	4	-37.28540267	-38.99587592	-23.44589519	-39.58173645
5	0	-37.62215668	-39.29866882	-23.77927148	-39.86529684
	1	-37.62302622	-39.29935106	-23.78040734	-39.86592713
	2	-37.62476524	-39.30071559	-23.78267904	-39.86718776
	3	-37.62737376	-39.30276242	-23.78608661	-39.86907872
	4	-37.63085184	-39.30549144	-23.79063013	-39.87159996
	5	-37.63519944	-39.30890279	-23.79630964	-39.87475154

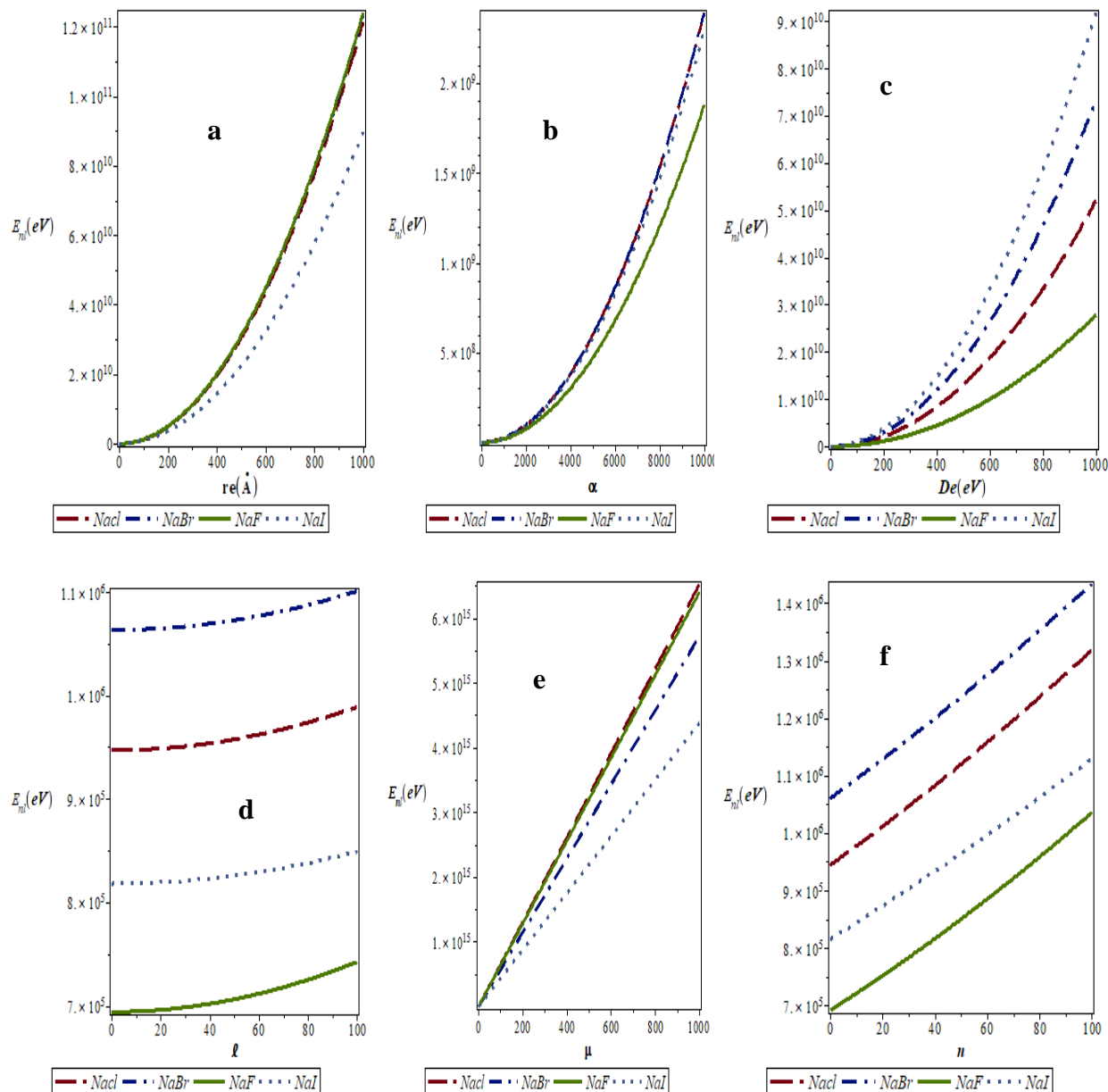


Figure 1: (a) Energy eigenvalues variation with equilibrium bond length for various Ionic crystal (b) Energy eigenvalues variation with for various Ionic crystal Madelung constant (c) Energy eigenvalues variation with dissociation energy for various Ionic crystal (d) Energy eigenvalues variation with angular momentum for various Ionic crystal (e) Energy eigenvalues variation with reduced mass for various Ionic crystal (f) Energy eigenvalues variation with principal quantum number for various Ionic crystal.

CONCLUSION

In this work, the approximate bound state solution of Schrodinger equation with Hulthen-type potential plus modified Kratzer potential were obtained, via the Nikifiriv-Uvarov method. The energy eigenvalues of the selected ionic crystals (NaCl, NaBr, NaF, and NaI) were computed, and a special case was considered. Our results are consistent with the results in the available literature. In addition, we presented the variations of the

energy eigenvalues with the potential parameters such as the equilibrium bond length, Madelung constant, dissociation energy, angular momentum, reduced mass and rotational quantum number and were discussed graphically and it was noted that the energy eigenvalues increase as the various potential parameters increases. Recently, there has been investigation into areas covering vibrational partition function and their thermochemical properties of diatomic molecules,

which can be extended to ionic crystals. Worth mentioning is the current research done on the prediction of enthalpy and entropy of gaseous dimer that can also be extended to ionic crystals. The result obtained in this study finds application in quantum chemistry, molecular physics amongst others. And can be extended to relativistic regime using other methods.

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CONFLICT OF INTEREST

The authors declare no competing of interests.

REFERENCES

Abramowitz, M. & Stegun, I. A., (1964) Handbook of Mathematical Functions with formulas, Grapgs and Mathematical tables. (New York: Dover).

Ahmadov, A. Aslanova, S. Orujova, M. S. Badalov, S. Dong, S. H. (2019) approximation bound state solution of Klein-Gordon equation with linear combination of Hulthen and Yukawa potentials, Phys. Lett. A 383 (24) 3010-3017.

Akpan, I. O., Antia, A. D., Ikot, A. N. (2012) Bound state solutions of Klein-Gordon equation with deformed equal scalar and vector eckart potential using newly improved approximation scheme, ISRN High Energy phys. 2012

Anita, A. D. Essien, I. Umoren, E. Eze, C. (2015) Approximate of the non-relativistic Schrödinger equation with inversely quadratic Yukawa potential plus Mobius square potential via parametric Nikiforov-Uvarov method. Adv. Phys. Theor. Appl. 44 (1) p.

Arda, A. Sever, R. (2009) Approximate i-state solution to the Klein-Gordon equation for modified woods-saxon potential with position dependent mass, Int. J. Mod. Phys. A 24 (20n21) 3985-3994.

Badalov, V. Ahmadov, H. Badalov, S. (2010) Any i-state solution to the Klein-Gordon equation for modified Woods-Saxon potential, Int. J. Mod. Phys. E 19 (07) 1463-1475.

Bayrak, O., kocak, G., Boztosun, I., (2006) J. Phys, A Math. Gen 39 6955.

Bayrak, O., Boztosun, I., Ciftci, H., (2007), Exact analytical solutions to the Kratzer potential by the asymptotic iteration method, international Journal of

Quantum chemistry 107 (3) 540-544. <https://doi.org/10.1002/qua.21141>.

Berezin, A. A. (1986) Phys.Rev. B, 33 pp. 2122

Berkdemir, C.,Berkdemir, A., Han,J., (2006) Bound state solutions of the Schrödinger equation for modified Kratzer's molecular potential, Chem. Phys. Lett. 417 (4-60) 326-328

Chen, C Y Lu, F L and Sun, D S., (2008) Cent Eur. J. Phys. 6 884

Cifteci, H., Hall, R. L., Saad, N.,(2003), Asymtotic iteration method for eigenvalue problems, Journal of Physics A: Mathematical and General 36 (47) 11807-11816 <https://doi.org/10.1088/03050083>.

Chun-Feng, H., Zhong-Xiang, Z. and Yan L. (1991) Bound state of the Klein-Gordon with vector and scalar Woods-Saxon potentials, Acta Physica Sinica 8 (8) 561-565. <https://doi.org/10.1088/1004-423X/8/8/001>.

Chun-Feng, H., Zhong-Xiang, Z., and Yan L.I (1991)Acta Physica Sinica 8, 561

Das, T. & Arda, A, (2017), Klein-Gordon equation for a charged particle in space varying electromagnrtic fields- a systematic study via Laplace transform, Chin. J. Phys.55 (2) 310-317

Dong,S.,Lozada-Cassou, M (2006) exact solutions of Klein-Gordon equation with scalar and vector ring-shaped potentials ,Phys. Scr. 74 (2) 285.

Dong S.H., Gu, X. Y. (2008) J. Phys. Conf. Ser. 96, 012109

Egrifes, H., Demirhan, D, and Buyukkilic, F., (2000) Phys. Lett. A.275 229

Gu, X- Y. Dong, S- H. Ma, Z- Q. (2008) Energy spectra for modified Rosen-Morse potential solved by the exact quantization rule, J. phys. A Math. Theor. 42 (3) 035303.

Hamzavi, M., Thlwe, K. E and Rajabi, A., (2013), Aproximate Bound states solution of the Hellmann potential Communication in Theoretical Physics, 60 1

Hassannabadi,H., Rahimov,H., Zarrinkamar, S., (2011) approximate solution of Klein-Gordon equation with Kratzer potential, Adv. High Energy phys. 2011 p.

Hulthen, L. Sugawara, M. Flugge(ed), S. (1957) Handbuckder physic, Springer

- Huseyin, R. & Sever, J. *J. math. chem.* 50 1938 (2012)
- Ikhdaïr, S. M. (2009) Bound state solution of the Klein-Gordon equation for vector and scalar general Hulthén-type potentials in D-dimension, *Int. J. Mod. Phys. C* 20 (01) 25-45.
- Ikhdaïr, S. M. Sever, R. (2007) Exact solution of the Klein-Gordon equation for the PT-symmetry Woods-Saxon potential by the Nikiforov-Uvarov Method, *Ann. Phys.* 16 (3) 218-232.
- Ikhdaïr, S. M. (2009) An improved approximation scheme for the centrifugal term and the Hulthén potential, *Eur. Phys. J. A* 39 (3) 307-314
- Ikhdaïr, S.M. and Falaye, B. J., (2013) *chem. Phys* 421 84
- Ikot, A. N. Maghsoodi E., Zarrinkamar, S. Hassanabadi, H. (2013) Relativistic spin and pseudospin symmetries of inverse quadratic Yukawa-plus Mobius square potentials including a Coulomb-like tensor interaction, *Few-Body syst.* 54 (11) 2027-2040.
- Ikot, A. N., Akpabio, L.E. and Umoren, E. B., (2011), Exact solution of Schrödinger equation with inverted Woods-Saxon potential and Manning-Rosen potential, *Journal Scientific. Research* 3(1) 25-33
- Jia, C. S., & Jia, Y. (2017), *Eur. J. D.* 71 3
- Karayer, H., Demirha, D., & Buyukkilic, F. (2015). Extension of Nikiforov-Uvarov Method for the Solution of Heun Equation. *Journal of Mathematical Physics*, 56, 063504, 1-14. <https://dx.doi.org/10.1063/1.4922601>
- Kratzer, A, (1920), Die ultraroten rotationsspektren der halogenwasserstoffe, *Z. Phys* 3 289 -307
- Lai, C.S. Lin, W. C. (1980) *phys. Let. A*, 78 pp. 335
- Liu, H-B. Yi, L-Z. Jia, C-S. (2018) solutions of the Klein-Gordon equation with the Tietz potential energy, *J. Math. Chem.* 56 (10) 2982-2994
- Ma, Z. Q. Dong, S. H. Gu, X. Y., Yu, J., Lozada-Cassou, M., (2014) The Klein-Gordon equation with a Coulomb plus scalar potential in D-dimensions, *Int. J. Mod. Phys. E* 13 (03) 597-610.
- Maghsoodi, E., Hassanabadi, H., Zarrinkamar, S., (2012), Spectrum of Dirac Equation under Deng-Fan scalar and vector potential and a coulomb Tensor interaction by SUSYQM, *Few-Body system* 53 (3-4) 525-538 <https://doi.org/10.1007/s00601-0314-5>
- Nagiyev, S. M. Ahmadov, A. (2019) exact solution of the relativistic finite-difference equation for Coulomb plus a ring-shaped-like potential. *Int. J. Mod. Phys. A* 34 (17) 1950089
- Nififorov, A. F, Uvarov, V. B., (1988), special functions of mathematical physics, 205 Springer
- Nugraha, D. A. Suparmi, A. Cari, C. Pratiwi, B. N. (2017) Asymptotic iteration method for analytical solution of Klein-Gordon equation for trigonometric Pöschl-Teller potential in D-dimensions, *journal of physics: conference series*, IOP Publishing,
- Oyewumi, K.J., Akinpelu, F.O., Agboola, A.D., (2008) *Int. J. Theor. Phys* 47, 1039
- Oñate, C., Onyeaju, M., Ikot, A., Ebomwonyi, O, (2017), Eigen solution and entropy system for Hellmann potential in the presence of the Schrödinger equation, *Eur. Phys. J. Plus* 132 (11) 462
- Oñate, C., Ojonubah, J., Adeoti, A., Eweh, J., Ugboja, M., (2014), Approximate eigen solutions of DKP and Klein-Gordon equation with Hellmann potential, *Afr. Rev. Phys. J.9* (006) 497-504.
- Payil, S. H (1984) *J. phys. A*, 17 pp. 575
- Pekeris C.I. (1934) *Phys. Rev.* 45 98
- Peng, X. L., Jiang, R., Jia, C. S., Zhang, L. H., and Zhao, Y. L, (2018), Gibbs free energy of gaseous phosphorus dimer, *Chem. Eng. Sci.* 190 122
- Popov, V.S. Wiengberg, V. M. (1985) *phys. Let. A*, 107 pp. 371
- Pyykko, P., Jokiasaari, (1975) *J. Chem. Phys.* 10 pp. 293
- Roy, B., Roychoudhury, R., (1987) *J. phys. A*, 20 pp. 3051
- Qiang, W. C. and Dong, S. H., (2007), Analytical approximations to the solutions of the Manning-Morse potential with Centrifugal term. *Phys. Lett. A* 368.13-17.
- Qiang, W.C. Dong, S.H. Analytical, (2007) approximation to the solution of the Manning-Rosen potential with centrifugal term, *Phys. Lett. A* 368 (1-2) 13-17
- Qiang, W.C. Dong, S.H. Analytical, (2007), Arbitrary i-state solution of the rotating Morse potential Rosen

potential through the exact quantization rule method, Phys. Lett. A 363 (3) 169-176

Pearson, R. G., (1963), Hard and Soft Acids and Bases. Journal of the American Chemical Society. 85 (22) 3533-3539

Ramantswana, M. Rampho, G. J. Edet, C. O Ikot, A.N Okorie, U. S. Qadir, K.W. Abdullah, H.Y. (2023) Determination of thermodynamic properties of CrH,NiC, and CuLi Diatomic Molecules with the linear combination of Hulthen-type potential plus Yukawa potential, physics open, doi: <https://doi.org/10.1016/j.physo.2022.100135>.

Saad, N.,(2007) the Klein-Gordon equation with a generalized Hulthen potential in D-dimensions, Phys. Scr. 76 (6) 623.

Saad, N.,(2008), The Klein-Gordon equation with Kratzer potential in D-dimensions, Central European Journal of Physics 6 (3) 717-729.

Sadeghi, J.,(2007), Factoeization method and solution of non-central modified Kratzer potential, Acta Physica Polonia A 112 (1) 23-28

Saleh, R., Kassem, M., Mabrouk, S., (2019) exact solution of nonlinear fractional order partial differential equations via singular manifold method, Chin. J. Phys. 61 290- 300

Szego, G. (1939), Orthogonal polynomials. American Mathematical society, New York.

Sherman, J. (1932), Crystal Energy of ionic compounds and thermochemical Applications, chemical Review. 11 (1) 93-170

Wei, G. F. Dong, S. H. (2010) Pseudospin symmetry in the relativistic Manning-Rosen potential including a Pekeris-type approximation to the pseudo-centrifugal term, Phys. Lett. B 686 (4-5) 288-292

Yahya, W. A. & Oyewumi, K. J, (2015) Journal of the Association of Arab Univ. for basic and Appl. Sci. 1815