EFEITO DE UMA BARREIRA NO AUTOVALOR ENERGÉTICO DA EQUAÇÃO DE SCHRÖDINGER NÃO RELATIVISTA E ALGUNS VALORES DE EXPECTATIVA DE POTENCIAIS COMBINADOS

EFFECT OF A BARRIER ON ENERGY EIGENVALUE OF THE NONRELATIVISTIC (SCHRÖDINGER EQUATION) AND SOME EXPECTATION VALUES OF COMBINED POTENTIALS

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RESUMO

A equação de Schrödinger foi proposta na física teórica para fornecer informações e o comportamento do sistema de partículas. A equação de Schrödinger foi recentemente resolvida para uma combinação de diferentes potenciais usando diferentes metodologias tradicionais. Os estudos não consideram o efeito de uma barreira entre os potenciais. Na realidade, a barreira entre os potenciais tem efeito sobre os autovalores de energia. No presente trabalho, um potencial do tipo Kratzer-Mie, que é uma combinação dos potenciais constantes do tipo Kratzer e Mie, foi proposto como o potencial de interação. As soluções da equação de Schrödinger radial foram obtidas na presença da combinação de potenciais considerando uma barreira entre os potenciais. A equação de energia e as funções de onda correspondentes foram calculadas explicitamente. Os cálculos foram realizados utilizando a metodologia da mecânica quântica supersimétrica. Este método envolve a proposição da função superpotencial como uma solução para sua equação diferencial de Riccati. Resultados numéricos foram gerados para algumas moléculas diatômicas usando a equação de energia e os parâmetros do modelo diatômico. Alguns valores esperados para o potencial combinado foram calculados usando o teorema de Hellmann Feynman e o efeito da barreira sobre os valores esperados foram estudados numericamente. Pode-se observar que, quando uma partícula se move da extremidade inferior para a extremidade superior de uma barreira, ela absorve energia do sistema por alguns momentos. Esse mesmo comportamento também foi observado quando a partícula penetra por uma barreira. Assim, sua vibração dependerá apenas da energia inicial que absorveu. É igualmente visto que à medida que a largura da barreira se torna maior do que a altura, a energia do sistema diminui drasticamente.

Palavras-chave: *Eigen-soluções, equações de onda, potencial tipo Kratzer-Mie, moléculas diatômicas.*

ABSTRACT

Schrödinger equation was proposed in theoretical physics to provide information and the behavior of a system of particles. The Schrödinger equation was recently solved for a combination of different potentials using different traditional methodologies. The studies do not consider the effect of a barrier between the potentials. In reality, the barrier between the potentials has an effect on the energy eigenvalues. In the present work, a Kratzer-Mie-type potential, a combination of Kratzer and Mie-type-constant potentials, was proposed as the interacting potential. The solutions of the radial Schrödinger equation was obtained in the presence of the combined potentials by considering a barrier between the potentials. The energy equation and the corresponding wave functions were explicitly calculated. The calculations were performed by using the methodology of supersymmetric quantum mechanics. This method involves the proposition of superpotential function as a solution to its Riccati differential equation. Numerical results were generated for some diatomic molecules using the energy equation and the diatomic model parameters. Some expectation values for the combined potential were calculated using

Hellmann Feynman Theorem, and the effect of the barrier on the expectation values were numerically studied. It was observed that when a particle moves from the lower end to a higher end of a barrier, it absorbs energy from the system for some time. This same behavior was also noted when the particle penetrates through a barrier. Thus, its vibration will only depend on the initial energy, which is absorbed. It was equally seen that as the width of the barrier becomes larger than the height, the energy of the system decreases drastically.

Keywords: *Eigensolutions, Wave equations, Kratzer-Mie-type potential, diatomic molecules.*

1. INTRODUCTION:

The exact solutions of both the relativistic and nonrelativistic wave equations with some physical potential models are of great interest because the analysis of the solution makes a conceptual understanding of the state of the quantum and physical systems, such as the wave functions and eigenvalues. These solutions provide means to improve certain models and numerical methods for solving complicated physical systems (Flügge, 1974; Schiff, 1995) like Fisher information, Shannon entropy, and even some thermodynamic properties (mean energy, free energy, heat capacity, and entropy). The exact solutions of the wave equations are limited to a few numbers of physical potentials such as Harmonic oscillator, Coulomb potential, pseudoharmonic potential (Landau and Lifshitz, 1977; Ikhdair and Sever, 2007).

However, to make other potential models such as Frost-Musulin, Hellman, Yukawa, Inversely Quadratic Yukawa potentials relevant in the computation of Fisher information, Shannon entropy and thermodynamic properties, various traditional methods (analytic tools) have been developed by different authors to solve the wave equations in the presence of any physical potential models of interest. The traditional methods include supersymmetry quantum mechanics (Witten, 1981; Cooper *et al.*, 1995; Onate *et al.*, 2019), which involves the proposition of superpotential function based on the interacting potential. The superpotential function then relates to a Riccati equation where two partner potentials can be written. With some algebraic simplification and considering the negative partner potential, the energy equation can be obtained. The formula method for bound state problems (Falaye *et al.*, 2015) is another traditional method. This method involves a transformation of a variable for mathematical simplicity. The factorization method (Dong, 2007; Rahbar and Sadegh, 2016; Hoseein *et al.*, 2019) uses the formulation of independent variables. Nikiforov-Uvarov method (Nikiforov and Uvarov, 1988; Tezcan and Sever, 2009; Oluwadare *et al.*, 2012; Onate and Idiodi, 2016; Onyeaju *et al.*, 2017; Ikot *et al.*, 2018) involves the

reduction of a second-order linear differential equation to the generalized equation of the hypergeometric type. Asymptotic iteration method (Bayrak and Boztosun, 2007; Falaye, 2012; Falaye *et al.*, 2013; Oyewumi *et al.*, 2014), proposes variables that are sufficiently differentiable, which later leads to a recurrence relation where energy eigenvalues are obtained from the root of a quantized condition. The mathematical details of each of the methods can be found in the cited references and references therein. The most popular wave equations solved by these methods are Schrödinger equation, Dirac equation for spin and pseudospin symmetries, and Klien-Gordon equation. Under the Dirac equation, the solutions of both spin and pseudospin symmetries have been obtained in the presence of tensor interaction that brings about atomic stability as reported by Onate *et al.* (2017b; 2019), Ikot (2012), Hassanabadi *et al.* (2013) and others.

In bound state solutions of the Schrödinger equation, these methods have different approaches to the solutions but give each physical potential model an agreeable result. The energy equation obtained in most cases are used to generate energy eigenvalues (energy spectra) for some molecules. The generated eigenvalues are used to study the behaviour of different molecules with respect to the potential parameters under consideration. Different potential models have been combined and studied in terms of bound states. For instance, Edet *et al.* (2020) combined modified Kratzer potential and screened Coulomb potential and obtained bound state solutions in the domain of the nonrelativistic regime. Similarly, Okorie *et al.* (2020), combined Hyperbolic and Pöschl-Teller potentials to study the thermodynamic properties of a system. Other combinations of potentials were also reported. However, to the best of our knowledge, the effect of the boundary between these potentials on the bound state has not been investigated and reported yet. Motivated by this, the present study intends to investigate a one-dimensional radial Schrödinger equation with a combination of two different potentials. The two potential models to be considered in this work are the generalized Kratzer potential-type $V_1(r)$ and the Mie-type potential

$V_2(r)$. The Kratzer potential has played an important role in the history of quantum mechanics. So far, Kratzer potential has been used extensively to describe the molecular structure and interactions in the quantum domain.

As part of its applications, Bayrak *et al.* (2007), calculated the nonzero angular momentum solutions of the Schrödinger equation for the Kratzer potential and obtained the exact eigenvalues for different diatomic molecules, Ikot *et al.* (2019), obtained eigensolution, expectation values and thermodynamic properties of the screen Kratzer potential. Edet *et al.* (2020), in their own study, obtained bound state solutions of the Schrödinger equation for the modified Kratzer potential plus screened Coulomb potential. The generalized Kratzer potential and the Mie-type potentials are respectively given as

$$V_1(r) = D_e \left(\frac{r-r_e}{r} \right)^2 + \eta \quad (1)$$

$$V_2(r) = D_e \left[\frac{k}{j-k} \left(\frac{r_e}{r} \right)^j - \frac{j}{j-k} \left(\frac{r_e}{r} \right)^k \right], \quad (2)$$

The choice of potential in the present work is the interaction of Eq. (1) and Eq. (2) which is given as

$$V(r) = V_1(r) + V_2(r) = D_e \left(\frac{r-r_e}{r} \right)^2 + D_e \left[\frac{k}{j-k} \left(\frac{r_e}{r} \right)^j - \frac{j}{j-k} \left(\frac{r_e}{r} \right)^k \right] + \eta \quad (3)$$

In the above equation, D_e is a dissociation energy, r_e is the equilibrium bond length, r is the internuclear separation while j and k are potential parameters whose values are define later. The parameter η is a potential constant which can takes either negative or positive value. The potential can yield many results due to its subsets as will be seen later.

Thus, this study aimed to determine the effect of a barrier between two potential models on the energy eigenvalues.

2. MATERIALS AND METHODS:

2.1. Bound State Solutions

To obtain a one-dimensional Schrödinger equation, the original Schrödinger equation of the form is first considered as (Landau and Lifshitz, 1977; Schiff, 1995; Onate, 2016; Onate *et al.*, 2017a)

$$-\frac{\hbar^2}{2m} \left[\frac{1}{r^2} \frac{\partial}{\partial r} r^2 \frac{\partial}{\partial r} + \frac{1}{r^2 \sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial}{\partial \theta} \right) + \frac{1}{r^2 \sin^2 \theta} \frac{\partial^2}{\partial \phi^2} \right] \psi(r, \phi, \theta) = (E_{nl} - V(r)) \psi(r, \phi, \theta). \quad (4)$$

To solve the radial part of the Schrödinger equation above, the wave function is set as

$$\psi_{n,\ell}(r, \phi, \theta) = \frac{R_{n,\ell}(r) Y_{m,\ell}(\phi, \theta)}{r}, \quad (4a)$$

and therefore, Eq. (4) becomes

$$\left[-\frac{\hbar^2}{2m} \frac{d^2}{dr^2} + V_1(r) + V_2(r) - \left[\frac{\hbar^2 B_p}{2mr} + \frac{\hbar^2 \ell(\ell+1)}{2m r^2} \right] \right] R_{n\ell}(r) = E_{n\ell} R_{n\ell}(r), \quad (5)$$

where $\hbar$ is the reduced Planck's constant, m is the mass of the particle, $E_{n\ell}$ is the nonrelativistic energy of the system and $R_{n\ell}(r)$ is the wave function. In Eq. (5), the centrifugal term $\frac{\ell(\ell+1)}{r^2}$

and a barrier system $\frac{B_p}{r}$ have been introduced.

Substituting Eq. (3) into Eq. (5), we have a second order differential equation of the form

$$\frac{d^2 R_{n\ell}(r)}{dr^2} - \frac{2m(D_e + \eta - E_{n\ell})}{\hbar^2} = \left[\frac{4mD_e r_e^2 - 8mrD_e r_e - B_p r + \ell(\ell+1)}{\hbar^2 r^2} + \frac{2m(D_e + \eta - E_{n\ell})}{\hbar^2} \right] R_{n\ell}(r), \quad (6)$$

where $j = 2k$ and $k = 1$. To obtain energy equation of Eq. (6), the methodology of

supersymmetric quantum mechanics formalism and shape invariance technique is adopted (Gendenshtein, 1983; Cooper and Freedman, 1983; Comtet *et al.*, 1985; Jia *et al.*, 2007; Hassanabadi *et al.*, 2012a; Onate *et al.*, 2017b), to solve the calculations. Following the theory of calculations via supersymmetric approach for a state when $n = 0$, Eq. (6) can first be written as

$$R_{0,\ell}(r) = \exp\left(-\int W(r)dr\right), \quad (7)$$

where $W(r)$ is regarded as a superpotential function in supersymmetric quantum mechanics, which enables us to propose a solution to the differential equation of Eq. (6). Considering the potential function under consideration in Eq. (3), a superpotential function is given as

$$W(r) = \rho_0 - \frac{\rho_1}{r}. \quad (8)$$

The parameters ρ_0 and ρ_1 are two constants of the superpotential function whose values will be determine later. Substituting Eq. (7) into Eq. (6) results to a Riccati equation of the form

$$W^2(r) - \frac{dW(r)}{dr} = \frac{4mD_e r_e^2 - 8mrD_e r_e - \frac{ar}{w} + \ell(\ell+1)}{\hbar^2 r^2} + \frac{2m(D_e + \eta - E_{n\ell})}{\hbar^2}. \quad (9)$$

By substituting Eq. (8) into Eq. (9), the two parameters ρ_0 and ρ_1 in Eq. (8) can be determine as

$$\rho_0^2 = \frac{2m(D_e + \eta - E_{n\ell})}{\hbar^2}, \quad (10)$$

$$\rho_1 = -\frac{1}{2} \pm \sqrt{\left(\frac{1}{2} + \ell\right)^2 + \frac{4mD_e r_e^2}{\hbar^2}}, \quad (11)$$

$$\rho_0 = \frac{4mD_e r_e}{\hbar^2} \left(\frac{1}{\rho_1}\right), \quad (12)$$

$$B_p = \frac{a}{w}, \quad (13)$$

where a is the height of the barrier and w is the width of the barrier. In this work, the consideration of the bound state is ideal when the radial part of the wave function $\psi(r)$ clearly satisfies the boundary conditions that $R_{n,\ell}(r)/r$ becomes zero

as r tends to infinity and $R_{n,\ell}(r)/r$ is finite as r is zero. In order to make $R_{n,\ell}(r)/r$ satisfy the regularity conditions in this work, the value $\rho_0 > 0$ is obtained.

This is manifested in the energy equation. To achieve every desirable result, a pair of partner potentials is constructed (Witten, 1981; Cooper *et al.*, 1995; Wei and Dong, 2010; Hassanabadi *et al.*, 2011a; Onate, 2014) using the superpotential function of Eq. (8).

$$V_+(r) = \rho_0^2 - \frac{2\rho_0\rho_1}{r} + \frac{\rho_1(\rho_0+1)}{r^2}, \quad (14)$$

$$V_-(r) = \rho_0^2 - \frac{2\rho_0\rho_1}{r} + \frac{\rho_1(\rho_0-1)}{r^2}. \quad (15)$$

Comparing Eqs. (14) and (15), it reveals that the partner potentials satisfied the shape invariance potential and therefore, the shape invariance holds after a mapping of the form $\rho_1 \rightarrow \rho_1 - n$ as the following recurrence relations have been observed: $a_1 = a_0 - 1$, $a_2 = a_0 - 2$, $a_3 = a_0 - 3$. Therefore, the two partner potentials connect with a simple formula of the form:

$$R(a_1) = \frac{4mD_e r_e}{\hbar^2} \left(\frac{1}{a_0} - \frac{1}{a_1}\right), \quad (16)$$

$$R(a_2) = \frac{4mD_e r_e}{\hbar^2} \left(\frac{1}{a_1} - \frac{1}{a_2}\right), \quad (17)$$

$$R(a_3) = \frac{4mD_e r_e}{\hbar^2} \left(\frac{1}{a_2} - \frac{1}{a_3}\right), \quad (18)$$

$$R(a_n) = \frac{4mD_e r_e}{\hbar^2} \left(\frac{1}{a_{n-1}} - \frac{1}{a_n}\right). \quad (19)$$

In the above equations, a_1 is a new set of parameters uniquely determined from an old set of parameters a_0 (Wei and Dong, 2009; Oyewumi and Akoshile, 2010; Hassanabadi *et al.*, 2011b; Jia *et al.*, 2013). Considering the negative partner potential, the deduction of the energy equation begins as

$$E_{n\ell} = \sum_{k=1}^n R(a_k) = \frac{4mD_e r_e}{\hbar^2} \left(\frac{1}{a_0} - \frac{1}{a_1} \right), \quad (20)$$

which can fully be written as

$$E_{n\ell} = D_e + \eta - \frac{\hbar^2}{2m} \left(\frac{4mr_e D_e}{\hbar^2} + \frac{a}{2w} \right)^2 \times \left[n + \frac{1}{2} + \sqrt{\left(\frac{1}{2} + \ell \right)^2 + \frac{4mD_e r_e^2}{\hbar^2}} \right]^{-2}. \quad (21)$$

The corresponding wave function is given as

$$R(s) = N_{n,\ell} s^{\sqrt{\ell(\ell+1) + \frac{4mD_e r_e^2}{\hbar^2}}} e^{\frac{1}{\hbar} \sqrt{2m(D_e + \eta - E_{n,\ell})} s} \times L_n^{2\sqrt{\ell(\ell+1) + \frac{4mD_e r_e^2}{\hbar^2}} - 1} \left(\frac{2}{\hbar} \sqrt{2m(D_e + \eta - E_{n,\ell})} s \right), \quad (22)$$

where a simple transformation of the form $s = r$ was made.

2.1.1. Special Cases

2.1.1.1. Generalized Kratzer Potential

When $j = \eta = 0$, the interacting potential given in Eq. (3) results to a generalized Kratzer potential as

$$V_{GK}(r) = D_e \left(\frac{r - r_e}{r} \right)^2, \quad (23)$$

The energy equation for the generalized Kratzer potential is obtained as

$$E_{n\ell} = D_e - \frac{2mr_e^2 D_e^2}{\hbar^2} [n + \delta_T]^{-2} \quad (24)$$

$$\delta_T = \frac{1}{2} + \sqrt{\left(\frac{1}{2} + \ell \right)^2 + \frac{2mD_e r_e^2}{\hbar^2}}. \quad (24a)$$

2.1.1.2. The Kratzer-Fues potential

The Kratzer-Fues potential. The Kratzer-Fues potential is obtain when $r - r_e = \eta = 0$, $j = 1$ and $k = 2$. Thus, potential (3) turns to

$$V_{KF}(r) = D_e \left(\frac{r_e^2}{r^2} - \frac{2r_e}{r} \right). \quad (25)$$

The energy equation is given as

$$E_{n\ell} = -\frac{2mr_e^2 D_e^2}{\hbar^2} [n + \delta_T]^{-2}. \quad (26)$$

2.1.1.3. The Constant potential

The constant potential is obtained when $D_e = 0$. Thus,

$$V_C(r) = \eta. \quad (27)$$

This potential has energy equation as

$$E_{n\ell} = \eta - \frac{\hbar^2 (1 + n + \ell)}{2m}. \quad (28)$$

2.2. Expectation Values

In this section, some expectation values V , p^2 and r^{-2} of the interacting potential are calculated via the Hellmann Feynman Theorem (Feynman, 1939; Dong *et al.*, 2005; Hassanabadi *et al.*, 2012b; Falaye *et al.*, 2014). The Hellmann Feynman Theorem states that if a non-degenerate or degenerate energy eigenvalue and the corresponding eigenfunction of a Hamiltonian depends on a certain parameter, then the energy eigenvalue varies with respect to that parameter according to the following formula

$$\frac{\partial E_{n,\ell}(v)}{\partial v} = \left\langle R_{n\ell}(v) \left| \frac{\partial H(v)}{\partial v} \right| R_{n\ell}(v) \right\rangle, \quad (29)$$

provided that the associated normalized eigenfunction is continuous with respect to the parameter v . The effective Hamiltonian for our interacting potential radial wave function is given by

$$H = -\frac{\hbar^2}{2\mu} \frac{d^2}{dr^2} + \frac{\hbar^2}{2\mu} \frac{\ell(\ell+1)}{r^2} + \frac{A - Be^{-\alpha(r-r_e)}}{(1 - qe^{-\alpha(r-r_e)})} + \frac{k(C - De^{-\alpha(r-r_e)})^2}{(1 - qe^{-\alpha(r-r_e)})}. \quad (30)$$

According to the theorem, once the spatial distribution of the electrons has been determined by solving the Schrödinger equation, all forces in

the system can be calculated using classical electrostatics. This theorem finds some of its applications in the calculation of intramolecular forces in molecules. Having determined the effective Hamiltonian, the expectation values of the stated parameters can be calculated. The expectation value of V , p^2 and r^{-2} respectively can be obtain by setting $q = D_e$, $q = \mu$ and $q = \ell$.

(i): For V , then,

$$\langle V \rangle_{n,\ell} = D_e - \frac{\left[\frac{4\mu r_e^2 D_e^2}{\hbar^2} - \frac{2a r_e D_e \hbar^2}{w} \right]}{\left(n + \frac{1}{2} + \sqrt{\left(\ell + \frac{1}{2} \right)^2 + \frac{4\mu D_e r_e^2}{\hbar^2}} \right)^2} + \frac{\left[\frac{8\mu r_e^2 D_e^2}{\hbar^2} + \frac{a^2 \hbar^2}{8\mu w^2} - \frac{2a D_e r_e^2 \hbar^2}{w} \right] \left[\frac{4\mu D_e r_e^2}{\hbar^2} + \delta \right]}{\left(n + \frac{1}{2} + \sqrt{\left(\ell + \frac{1}{2} \right)^2 + \frac{4\mu D_e r_e^2}{\hbar^2}} \right)^4}. \quad (31)$$

$$\delta = \frac{\frac{2\mu D_e r_e^2}{\hbar^2} (2n+1)}{\sqrt{\left(\ell + \frac{1}{2} \right)^2 + \frac{4\mu D_e r_e^2}{\hbar^2}}}. \quad (32)$$

(ii): For p^2 , then,

$$\langle p^2 \rangle_{n,\ell} = \frac{\left[\frac{8\mu r_e^2 D_e^2}{\hbar^2} + \frac{a^2 \hbar^2}{8\mu w^2} - \frac{2a D_e r_e^2 \hbar^2}{w} \right] \left[\frac{4D_e r_e^2}{\hbar^2} + \delta_1 \right]}{\delta_p^4} - \frac{\left[\frac{8r_e^2 D_e^2}{\hbar^2} - \frac{a^2 \hbar^2}{8\mu^2 w^2} \right] \delta_p^2}{\delta_p^4}, \quad (33)$$

$$\delta_p = n + \frac{1}{2} + \sqrt{\left(\ell + \frac{1}{2} \right)^2 + \frac{4\mu D_e r_e^2}{\hbar^2}}. \quad (33a)$$

$$\delta_1 = \frac{\frac{2D_e r_e^2}{\hbar^2} (2n+1)}{\sqrt{\left(\ell + \frac{1}{2} \right)^2 + \frac{4\mu D_e r_e^2}{\hbar^2}}}. \quad (34)$$

(iii): For r^{-2} , then,

$$\langle r^{-2} \rangle = \frac{\frac{2\mu}{\hbar^2 (2\ell+1)} \left[\frac{8\mu r_e^2 D_e^2}{\hbar^2} + \frac{a^2 \hbar^2}{8\mu w^2} - \frac{2a D_e r_e \hbar^2}{w} \right]}{\left(n + \frac{1}{2} + \sqrt{\left(\ell + \frac{1}{2} \right)^2 + \frac{4\mu D_e r_e^2}{\hbar^2}} \right)^2} \times \frac{\left[2\ell+1 + \frac{2\ell+1}{2\sqrt{\left(\ell + \frac{1}{2} \right)^2 + \frac{4\mu D_e r_e^2}{\hbar^2}}} (2n+1) \right]}{\left(n + \frac{1}{2} + \sqrt{\left(\ell + \frac{1}{2} \right)^2 + \frac{4\mu D_e r_e^2}{\hbar^2}} \right)^2}. \quad (35)$$

3. RESULTS AND DISCUSSION:

Figure 1 shows the shape of generalized-Mie-type-constant potential. In Figure 2, the variation of the ground state energy $E_{0\ell}$ with the equilibrium bond length r_e for five values of ℓ was shown. The variation was studied with the length of the barrier greater than the width of the barrier. For all five values of the angular momentum quantum number, the ground state energy decreases as the equilibrium bond length increases. In Figure 3, the behaviour of the energy with respect to the dissociation energy was examined. In the observations, the energy of the system increases as the dissociation energy increases.

The energies for $\ell=1,2,3$ tends to decrease as $D_e > 100$. In Figure 4, the plot of energy against the height a of the barrier was shown. At the beginning of the height of the barrier (0 to 10), there is a sharp increase in the energy of the system. This energy tends to be constant as the height of the barrier increases above 10. This shows that a particle moving from the lower end of a barrier to the higher end of the barrier requires more energy at the beginning of its movement as it goes up until the particle is fully energized at a particular point, then, little or no additional energy is requires to get to the top.

In Figure 5, the plot of energy against the width of the barrier was shown. It can be observed that as the width of the barrier increases, the energy of the system initially decreases, and at a point, it remains constant. This indicates that the particle requires energy at the initial stage for a

particle to penetrate the barrier. After some times, the particle gains sufficient energy to penetrate the barrier without further consuming the energy of the system. The variation of the energy of each potential against the equilibrium bond length for the ground state and the first two excited states are shown in Figures 6 and 7 using equations (24) and (26) respectively. In each case, the energy of the system goes down as the equilibrium bond length increases. The energy, however, increases as the quantum number increases. Though the Figures have the same pattern, but the energy of the generalized kratzer potential are higher than that of the kratzer-Fues potential at every value of the equilibrium bond length. It was also noted that the energies of the kratzer-Fues potential were bounded.

Table 1 presented the model parameters (constants) for six diatomic molecules. In Tables 2 and 3, the numerical results of the energy eigenvalues for some diatomic molecules were presented. It is seen that the energy decreases as the quantum number n increases for the whole molecules considered. Similarly, the energy increases as the angular momentum quantum number ℓ increases. The numerical values of the calculated expectation values in Eqs. (31), (33) and (35) are presented in Tables 4(a) and 4(b) for various values of the height and width of the barrier. It was noted that an increase in the height of the barrier leads to an increase in each of the calculated expectation value while an increase in the width of the barrier decreases each of the calculated expectation value.

4. CONCLUSIONS:

The solutions of the one-dimensional Schrödinger equation obtained in the presence of a potential barrier for a combination of generalized Kratzer potential and Mie-type potentials revealed that the energy for the generalized Kratzer potential has the same behavior as the energy of the Kratzer-Fues potential. It was observed that the presence of a potential barrier affects the energy of a system. The energy eigenvalues in the presence of the potential barrier reduces as the width of the barrier increases but increases as the height of the barrier goes up. A particle moving up in this system absorbed more energy from the system at the beginning of its movement. The absorption of energy reduces as the particle goes up, and before it gets to the top, the particle requires little or no energy.

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Table 1. Spectroscopic parameters used in this work for the diatomic molecules taken from the paper of Falaye et al. (2014).

Molecules	$\mu/10^{-23}(g)$	$r_e(\text{\AA})$	$D_e(\text{cm}^{-1})$
$O_2(X^3\Sigma_g^+)$	1.337	1.207	42041
$I_2(X(O_g^+))$	10.612	2.666	12547
$H_2(X^1\Sigma_g^+)$	0.084	0.741	38318
$N_2(X^1\Sigma_g^+)$	1.171	1.097	79885
$NO^+(X^1\Sigma^+)$	1.239	1.063	88694
$CO(X^1\Sigma^+)$	1.146	1.128	90531

Table 2. Bound state eigenvalues of diatomic molecules for various n and ℓ with $\hbar c = 1973.29\text{eV}$.

n	ℓ	$O_2(X^3\Sigma_g^+)$	$I_2(X(O_g^+))$	$H_2(X^1\Sigma_g^+)$
0	0	1.359716716	1.030965494	1.381798095
1	0	1.404079134	1.089610643	1.382833900
	1	1.412718834	1.103060691	1.383025962
2	0	1.412967209	1.106749164	1.383026085
	1	1.416063865	1.112282505	1.383093345
	2	1.417608584	1.116431061	1.383124532
3	0	1.416170011	1.113998241	1.383093397
	1	1.417620807	1.116793887	1.383124537
	2	1.418462410	1.119116908	1.383141480
	3	1.418976038	1.120694311	1.383151698
4	0	1.417675579	1.117727020	1.383124564
	1	1.418469499	1.119331756	1.383141483
	2	1.418977981	1.120761888	1.383151699
	3	1.419311654	1.121796155	1.383158331
	4	1.419541372	1.122537576	1.383162879
5	0	1.418501361	1.119894384	1.383141498
	1	1.418982452	1.120899440	1.383151701
	2	1.419312957	1.121841810	1.383158332
	3	1.419541883	1.122556411	1.383162879
	4	1.419706266	1.123089175	1.383166132
	5	1.419828125	1.123491837	1.383168538
6	0	1.419002592	1.121264431	1.383151710
	1	1.419315956	1.121935114	1.383158333
	2	1.419542799	1.122588688	1.383162879
	3	1.419706639	1.123102961	1.383166132
	4	1.419828304	1.123498604	1.383168538
	5	1.419921007	1.123805607	1.383170369
	6	1.419993228	1.124047354	1.383171794

Table 3. Bound state eigenvalues of diatomic molecules for various n and ℓ with $\hbar c = 1973.29 \text{ eV}$.

n	ℓ	$N_2(X^1\Sigma_g^+)$	$NO^+(X^1\Sigma^+)$	$CO(X^1\Sigma^+)$
0	0	1.647845814	1.705229227	1.710414495
1	0	1.757261120	1.836475239	1.850885506
	1	1.778894376	1.862562517	1.878903057
2	0	1.779739343	1.863681707	1.880177315
	1	1.787554530	1.873132958	1.890347181
	2	1.791550260	1.878008462	1.895624478
3	0	1.787917231	1.873614143	1.890895625
	1	1.791593650	1.878066823	1.895691605
	2	1.793773007	1.880727120	1.898571934
	3	1.795108957	1.882360591	1.900342482
4	0	1.791781305	1.878316024	1.895975823
	1	1.793798193	1.880761006	1.898610918
	2	1.795115900	1.882369953	1.900353267
	3	1.795984086	1.883431626	1.901504134
	4	1.796582713	1.884164090	1.902298444
5	0	1.793907552	1.880906328	1.898776733
	1	1.795131795	1.882391344	1.900377879
	2	1.795988743	1.883437905	1.901511368
	3	1.796584543	1.884166559	1.902301291
	4	1.797012976	1.884690809	1.902869828
	5	1.797330806	1.885079824	1.903291784
6	0	1.795201009	1.882483362	1.900482907
	1	1.795999408	1.883452261	1.901527888
	2	1.796587816	1.884170973	1.902306376
	3	1.797014311	1.884692610	1.902871904
	4	1.797331446	1.885080688	1.903292780
	5	1.797573252	1.885376662	1.903613822
	6	1.797761705	1.885607365	1.903864090

Table 4 (a). Expectation values for various values of the barrier height with $n = \ell = \mu = \hbar = w = 1$, $r_e = 0.2$ and $D_e = 0.55$.

a	$\langle V \rangle_{n,\ell}$	$\langle p^2 \rangle_{n,\ell}$	$\langle r^{-2} \rangle_{n,\ell}$
0.2	0.549713029	-0.002356946	0.004376939
0.4	0.554521427	-0.001927517	0.004668735
0.6	0.559350533	-0.001199653	0.005431170
0.8	0.564200347	-0.000173354	0.006664243
1.0	0.569070869	0.001151379	0.008367955
1.2	0.573962100	0.002774547	0.010542305
1.4	0.578874038	0.004696151	0.013187294
1.6	0.583806684	0.006916188	0.016302922
1.8	0.588760039	0.009434660	0.019889188
2.0	0.593734101	0.012251568	0.023946093

Table 4 (b). Expectation values for various values of the barrier width with $n = \ell = \mu = \hbar = a = 1$, $r_e = 0.2$ and $D_e = 0.55$.

w	$\langle V \rangle_{n,\ell}$	$\langle p^2 \rangle_{n,\ell}$	$\langle r^{-2} \rangle_{n,\ell}$
0.2	0.670830012	0.090317349	0.141276299
0.4	0.606259856	0.020599488	0.036147399
0.6	0.585455502	0.007722519	0.017446051
0.8	0.575188143	0.003226970	0.011159430
1.0	0.569070869	0.001151379	0.008367955
1.2	0.565010663	0.000026710	0.006915512
1.4	0.562119320	-0.000649739	0.006078154
1.6	0.559955627	-0.001087686	0.005559566
1.8	0.558275609	-0.001387191	0.005221067
2.0	0.556933392	-0.001600889	0.004991123

Figure 1. Generalized-Mie-type constant potential. This is the shape of the interacting potential given in Eq. (3)

Figure 2. Ground state energy against the equilibrium bond length in the presence of a barrier with $m = \hbar = \ell = \eta = 1$, $a = 2.5$, $w = 0.1$ and $D_e = 0.5$.

Figure 3. Ground state energy against the dissociation energy in the presence of a barrier with $m = \hbar = \ell = \eta = 1$, $a = 2.5$, $w = 0.1$.

Figure 4. Ground state energy against the height of the barrier with $m = \hbar = \ell = \eta = 1$, $w = 0.1$ and $D_e = 0.5$.

Figure 5. Ground state energy against the width of the barrier with $m = \hbar = \ell = \eta = 1$, $a = 2.5$ and $D_e = 0.5$.

Figure 6. Energy against the equilibrium bond length for Generalized kratzer potential with $m = \hbar = \ell = 1$, and $D_e = 0.1$.

Figure 7. Energy against the equilibrium bond length for kratzer-Fues potential with $m = \hbar = \ell = 1$, and $D_e = 0.1$.