Rotational and vibrational diatomic molecule in the Klein-Gordon equation with hyperbolic scalar and vector potentials

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Abstract

We present an approximate analytic solution of the Klein-Gordon equation in the presence of equal scalar and vector generalized deformed hyperbolic potential functions by means of parametric generalization of the Nikiforov-Uvarov method. We obtain the approximate bound state rotational-vibrational (ro-vibrational) energy levels and the corresponding normalized wave functions expressed in terms of the Jacobi polynomial $P_{n}^{(\mu,\nu)}(x)$, where $\mu > -1$, $\nu > -1$ and $x \in [-1, +1]$ for a spin-zero particle in a closed form. Special cases are studied including the non-relativistic solutions obtained by appropriate choice of parameters and also the s-wave solutions.

Keywords: Bound states, Klein-Gordon equation, hyperbolic potential functions, deformation theory, Nikiforov-Uvarov method.

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I. INTRODUCTION

In nuclear, molecular and high energy physics [1,2], one of the interesting problems is to obtain exact solutions of the relativistic wave equations like Klein-Gordon (KG), Dirac and Salpeter wave equations for mixed vector and scalar potential. The KG equation has also been used to understand the motion of a spin-zero particle in large class of potentials using different methods. This allows us to introduce two types of potential coupling, which are the four-vector potential \((V)\) and the space-time scalar potential \((S)\).

For the case \(S = \pm V\), the solution of these wave equations with physical potentials has been studied recently. Furthermore, their exact solutions are possible only for certain central potentials such as Morse potential [3], Hulthén potential [4], Woods-Saxon potential [5], Pöschl-Teller potential [6], reflectionless-type potential [7], pseudoharmonic oscillator [8], ring-shaped harmonic oscillator [9], \(V_0 \tanh^2(r/r_0)\) potential [10], five-parameter exponential potential [11], Rosen-Morse potential [12], and generalized symmetrical double-well potential [13], etc by using different methods. It is remarkable that in most of these works, the scalar and vector potentials are almost taken to be equal (i.e., \(S = V\)) [2,14]. Recently, interest in the solutions of the KG equation for the case where \(S(r) = \pm V(r)\) has surged. It presents bounded solutions in the relativistic view, although the KG equation reduces to the Schrödinger-like problem in the nonrelativistic limit. However, the reduced equation can show the relativistic properties of the system. For the most recent contributions, one may consult the papers in [2,6,9,10] and references therein. Therefore, the choice \(S(r) = V(r)\) (positive energy states) produces a nontrivial nonrelativistic limit with a potential function \(\Sigma(r) = 2V(r)\), and not \(V(r)\). It represents the concept of the exact spin symmetry that occurs in nuclei (i.e., when the difference potential \(\Delta(r) = V(r) - S(r) = 0\)). In the negative energy states (corresponding to \(S(r) = -V(r)\)) the nonrelativistic limit is the trivial interaction free-mode. It represents the concept of the pseudospin symmetry (i.e., occurs when the sum potential \(\Sigma(r) = V(r) + S(r) = 0\)) [15]. The spin symmetry is relevant for mesons [16]. The pseudospin symmetry concept has been applied to many systems in nuclear physics and related areas [15-17] and used to explain features of deformed nuclei [18], the super-deformation [19] and to establish an effective nuclear shell-model scheme [17,20]. This, of course, does not diminish the importance of such problems. It only limits it’s contribution (with the proper physical interpretation) to the relativistic regime [14]. However, in some
few other cases, it is considered the case where the scalar potential is greater than the vector potential (in order to guarantee the existence of KG bound states) (i.e., $S > V$) [21-24].

Many authors have considered a more general transformation between the unequal vector and scalar potentials given by $V(r) = V_0 + \beta S(r)$ (or $S(r) \neq \pm V(r)$), where $V_0$ and $\beta$ being arbitrary constants of certain proportions have to be chosen after solving the problem under consideration (cf. Ref. [25] and references therein). Nonetheless, such physical potentials are very few. The bound state solutions for the last case is being obtained for the exponential potential with the s-wave ($l = 0$) KG equation when the scalar potential is greater than the vector potential [21].

The problems connected with the molecular structure provide interesting and instructive applications of quantum mechanics, since molecules are considerably more complex in structure than atoms. Two distinct problems arise in connection with molecular structure. The first is to obtain the electronic wave functions and potential energy functions of the nuclear coordinates. This problem can be solved analytically only in the simplest cases. The second is to obtain the solution of the nuclear motion equation. In this regard, the construction of a suitable potential function of a diatomic molecule is very important. It has been found that the potential-energy function for the lowest electronic states of actual diatomic molecules can be expressed by means of the Morse potential [26]:

$$V_M(r) = D \left[ 1 - \exp \left[ -\alpha(r - r_e) \right] \right]^2,$$

which has three adjustable positive parameters $\alpha$, $D$ and $r_e$. At $r = r_e$, it has a minimum value at zero and approaches $D$ exponentially for large $r$. If $\frac{1}{\alpha}$ is somewhat smaller than $r_e$, it becomes large (but not infinite) as $r \to 0$. This potential is important in the field of molecular physics describing the interaction between two atoms [26,27]. Overmore, progress has been made in the field of diatomic molecules and extensive use of the potential functions have been introduced [28,29]. At present the Morse potential is still one of the potential functions used most in molecular physics and quantum chemistry [30]. However, it has few asymptotic inaccuracies in the regions of small and large $r$. To avoid these inaccuracies, many works have been carried out in that direction to improve Morse potential [31]. In 1986, Schöberg [32] suggested hyperbolical (empirical) potential functions of the form:

$$V_{\pm}(r) = D \left\{ 1 - \sigma \left[ \coth(\alpha r) \right]^{\pm 1} \right\}^2,$$

where $\sigma = \pm 1$. These potential functions have been introduced in molecular physics [33].
where $D$, $\alpha$ and $\sigma$ are three adjustable positive parameters with $D = D_e/(1 - \sigma)^2$ ($D_e$ is the spectroscopic dissociation energy) and $\sigma \rightarrow \sigma/\delta$, $\delta \neq 0$ is a parameter. In contrast to the everywhere-regular Morse potential, $V_+(r)$ is highly singular at the origin with $1/r^2$ and $1/r$ singularities. The two potentials behave similarly near the extremum point $r = r_e$. It has the minimum value 0 at the point

$$r = r_e = \frac{1}{\alpha} \arctan h (\sigma)^{\pm 1},$$

(3)

and approaches $D$ exponentially for large $r$. Unlike the Morse potential (1), the empirical potential (EP) function $V_+(r)$ approaches infinity at the point $r = 0$. In the region of large $r$, it is closer to the experimental Rydberg-Klein-Rees (RKR) curve than the Morse potential for some diatomic molecules. For a diatomic molecular model instead of the nuclear model, we consider the reduced mass definition. If the nuclei have masses $m_1$ and $m_2$, the reduced mass is defined as $\mu = m_1 m_2/(m_1 + m_2)$ and at this point the diatomic molecular model can be included to the the pseudospin symmetry concept. In this context, it is worth noting that the energy of the nuclear motion (in $MeV$) is widely separated from the energy in atomic vibration and rotation (in $KeV$). That is why, one is able to separate the two motions and study the atomic vibration and rotation separately from the nuclear motion.

Lu et al [33] obtained an approximate solution for the Schrödinger equation of diatomic molecule oscillator with the positive sign EP functions given in Eq. (2) ($\delta = 1$ case) by means of the hypergeometric series method. Further, rigorous energy eigenvalues and eigenfunctions for the 1D Schrödinger equation are also obtained using a similar method. Since there are no exact analytical solutions for the EP functions ($l \neq 0$) without an approximation to the centrifugal term $\sim 1/r^2$, some approximation [34] was used to obtain these solutions. One of these approximations have been employed in solving the rotating Morse potential for any $l$-state [34,35]. The ro-vibrating energy eigenvalues of the EP functions were determined with a semiclassical (SC) procedure (the Bohr-Sommerfeld quantization condition) and a quantum-mechanical (QM) method (the Schrödinger equation) [33]. Furthermore, several approximation schemes have been developed to find better analytical formulas for Eq. (2) with $\delta = 1$ [33,36]. Overmore, Jia et al [37] have used the basic concepts of the super-symmetric quantum mechanics formalism and the functional analysis method to investigate approximately the pseudospin symmetric solutions of the Dirac equation for the arbitrary pseudo-orbital angular momentum number $\tilde{l}$ and to obtain the bound state solutions for the
nuclei in the relativistic EP as a diatomic molecular model. Very recently, the NU method [38-40] was applied to solve the radial Schrödinger wave equation with the EP functions for \( l \neq 0 \) case [41]. The analytic solution is used to obtain the ro-vibrating energy states for selected \( H_2 \) and \( Ar_2 \) diatomic molecules using the relevant potential parameters and spectroscopic constants given in Ref. [32].

Over the past years, the quantum deformation [42] has been the subject of interest because of its relevance with applications in nuclei [43-45], statistical quantum theory, string beam theory and conformal field theory [46-49]. Recently, some authors have introduced few potentials in terms of hyperbolic functions [50,51] in the view of \( q \)-deformation [52].

Encouraged with the high performance of the above inter-molecular potential, we write the EP functions as

\[
\begin{align*}
\left[ \coth \alpha (r - r_e) \right]^{\pm 1} &= \frac{e^{\alpha (r - r_e)} \pm e^{-\alpha (r - r_e)}}{e^{\alpha (r - r_e)} \mp e^{-\alpha (r - r_e)}} = \frac{1 \pm e^{-2\alpha (r - r_e)}}{1 \mp e^{-2\alpha (r - r_e)}} = \frac{1 \pm q e^{-2\alpha r}}{1 \mp q e^{-2\alpha r}} = \left[ \coth_q (\alpha r) \right]^{\pm 1}, \\
V_{\pm}(r, q) &= D \left\{ 1 - \sigma \left[ \coth \alpha (r - r_e) \right]^{\pm 1} \right\}^2 = D \left\{ 1 - \sigma \left[ \frac{1 \pm q e^{-2\alpha r}}{1 \mp q e^{-2\alpha r}} \right] \right\}^2,
\end{align*}
\]

(4a)

where \( q = e^{2\alpha r_e} \), giving a magnitude for \( q \) that is larger than one. For an inverse transformation \( q = e^{-2\alpha r_e} \), the magnitude for \( q \) varies between zero and one. In the context of the quantum deformation [52], the above form is similar to a \( q \)-deformed (perturbed) generalized deformed empirical potential (\( q \)-DEP/GDEP) functions. It is worth noting that the range of parameter \( q \) was taken as \( q > 0 \) in [50] and has been extended to \(-1 \leq q < 0 \) or \( q > 0 \) or even complex by Ref. [51]. Such \( q \)-deformed potential functions have been introduced for the first time by Arai [42] for real \( q \) values. When \( q \) is complex, these functions are called the generalized deformed potential functions. In this paper, we intend to find the analytic solution of the KG equation for the equal scalar and vector \( q \)-DEP/GDEP with any orbital angular quantum number (\( l \neq 0 \)). The specific choice of \( V(r) = S(r) \) allows one to make KG equation approximately soluble for it’s relativistic energy eigenvalues and wave functions. Further, it opens up a new approach of generating the non-relativistic solution which is found to coincide with the previous Schrödinger solution of Eq. (4). In the present calculations, we apply a parametric generalization procedures of the NU method which are making our calculations straightforward and simple.

The present paper is organized as follows. In sect. 2, we present a parametric generalization of the NU method which holds for the exponential-type potentials. In sect. 3,
we obtain an approximate analytic NU bound state solution of the (3 + 1)-dimensional KG equation for equal scalar and vector q-DEP/GDEP functions with arbitrary l-states. In sect. 4, we discuss two special cases, the vibrational (l = 0) and the non-relativistic limit (Schrödinger solution). In Sect. 5, we calculate the ro-vibrating energy states for selected $H_2$ and $Ar_2$ diatomic molecules in the non-relativistic approach. Section 6 contains the relevant conclusions.

II. NU METHOD

The NU method is briefly outlined here and the details can be found in [38]. This method was proposed to solve the second-order differential equation of the hypergeometric-type:

$$\sigma^2(z)g''(z) + \sigma(z)\tilde{\tau}(z)g'(z) + \tilde{\sigma}(z)g(z) = 0,$$

(5)

where $\sigma(z)$ and $\tilde{\sigma}(z)$ are at most second-degree polynomials and $\tilde{\tau}(s)$ is a first-degree polynomial. The primes denote derivatives with respect to z. To find a particular solution of Eq. (5), one can decompose the wave functions, $g_{nl}(z)$ as follows:

$$g(z) = \phi(z)y_n(z),$$

(6)

leading to recast (5) in the hypergeometric-type equation

$$\sigma(z)y''_n(z) + \tau(z)y'_n(z) + \lambda y_n(z) = 0,$$

(7)

where

$$\lambda = k + \pi'(z),$$

(8)

and $y_{nl}(z)$ satisfies the Rodrigues relation

$$y_n(z) = \frac{A_n}{\rho(z)} \frac{d^n}{dz^n} [\sigma^n(z)\rho(z)].$$

(9)

In the above equation, $A_n$ is a constant related to the normalization and $\rho(z)$ is the weight function satisfying the condition

$$[\sigma(z)\rho(z)]' = \tau(z)\rho(z),$$

(10)

with

$$\tau(z) = \tilde{\tau}(z) + 2\pi(z), \tau'(z) < 0.$$  

(11)
The weight function should be carefully chosen because it has an influence on the performance of orthogonal wave functions, orthogonal in the interval $[0, 1]$, of the type Laguerre $L_n^{(\gamma)}(z)$ and Jacobi $P_n^{(\alpha,\beta)}(z)$ polynomials etc. It is defined with a compact support often called domain of influence which can be spheres in three-dimensions. Generally speaking, the weight function commonly used is exponential function. Furthermore, the weighted integral and weighted average are defined by $h(z) = \int_{\Omega} f(z)\rho(z)dz$ and $g(z) = \int_{\Omega} f(z)\rho(z)dz/\int_{\Omega} \rho(z)dz$, if $f(z) : \Omega \in \mathbb{R}$, real-valued orthogonal polynomial functions, respectively, with $f(z) = \sigma(z)$ and $g(z) = P_n^{(\alpha,\beta)}(z)$, $L_n^{(\gamma)}(z)$, etc. Since $\rho(z) > 0$ and $\sigma(z) > 0$, the derivative of $\tau(z)$ needs to be negative [38] which is the essential condition in making the choice of particular solution relevant to the real bound state solution.

The other part of the wave functions in Eq. (6) is mainly the solution of the logarithmic derivative:

$$\frac{\phi'(z)}{\phi(z)} = \frac{\pi(z)}{\sigma(z)},$$

where

$$\pi(z) = \frac{1}{2} [\sigma'(z) - \tilde{\tau}(z)] \pm \sqrt{\frac{1}{4} [\sigma'(z) - \tilde{\tau}(z)]^2 - \tilde{\sigma}(z) + k\sigma(z)}.$$

is a polynomial of order one. The determination of $k$ is the essential point in the calculation of $\pi(z)$, for which the discriminant of the square root in the last equation is set to zero. This gives the polynomial $\pi(z)$ which is dependent on the transformation function $z(r)$. Also, the parameter $\lambda$ defined in Eq. (8) takes the form

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

In this regard, we can construct a parameteric generalization of the NU method valid for any central and non-central exponential-type potentials. We begin by comparing the following general hypergeometric equation

$$[z (1 - c_3 z)^2 g''(z) + [z (1 - c_3 z) (c_1 - c_2 z)] g'(z) + (-B_1 z^2 + B_2 z - B_3) g(z) = 0,$$

with it’s counterpart equation (5) to obtain

$$\tilde{\tau}(z) = c_1 - c_2 z,$$

$$\sigma(z) = z (1 - c_3 z),$$

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\[ \bar{\sigma}(z) = -B_1 z^2 + B_2 z - B_3. \]  

where the parameters \( c_i \) and \( B_i \) \((i = 1, 2, 3)\) are constants to be determined during the solution process. Thus, following the method, we may obtain all the analytic polynomials and their relevant constants necessary for the solution of a radial wave equation. These analytic expressions are given in Appendix A.

III. THE KG SOLUTION OF EQUAL SCALAR-VECTOR GDEP FUNCTIONS

In relativistic quantum mechanics, we usually use the KG equation for describing a scalar particle, i.e., the spin-0 particle dynamics. The discussion of the relativistic behavior of spin-zero particles requires understanding the single particle spectrum and the exact solutions to the KG equation which are constructed by using the four-vector potential \( A_\lambda (\lambda = 0, 1, 2, 3) \) and the scalar potential \( S \). In order to simplify the analytic solution of the KG equation, the four-vector potential can be written as \( A_\lambda = (A_0, 0, 0, 0) \). The first component of the four-vector potential is represented by a vector potential \( V \), i.e., \( A_0 = V \). In this case, the motion of a relativistic spin-0 particle in a potential is described by the KG equation with the potentials \( V \) and \( S \) [1]. For \( S = V \) case [39], the \((3 + 1)\)-dimensional KG equation is recasted to a Schrödinger-like equation and thereby the bound state solutions are easily obtained by using the well-known methods developed in nonrelativistic quantum mechanics [2].

Let us now consider the \((3 + 1)\)-dimensional time-independent KG equation describing a scalar particle (spin-0 particle) with Lorentz scalar \( S(r) \) and Lorentz vector \( V(r) \) potentials which takes the form [2,14,53]

\[
\left[ \mathbf{P}_{op}^2 - (V(r) - E_R)^2 + \left( S(r) + mc^2 \right)^2 \right] \psi_{KG}(\vec{r}) = 0 ,
\]

where \( m \) and \( E_R \) denote the reduced mass and relativistic binding energy of two interacting particles, respectively, with \( \mathbf{P}_{op} = -i\hbar \vec{\nabla} \) is the momentum operator. It would be natural to scale the potential terms in Eq. (17) so that in the nonrelativistic limit the interaction potential becomes \( V(r) \), not \( 2V(r) \). We follow Alhaidari \textit{et al} [14] to reduce the above equation to the form [54]

\[
\left\{ \nabla^2 + \frac{1}{\hbar^2 c^2} \left[ \left( \frac{1}{2} V(r) - E_R \right)^2 - \left( \frac{1}{2} S(r) + mc^2 \right)^2 \right] \right\} \psi_{KG}(\vec{r}) = 0 .
\]
Thus, after making use of the equal scalar and vector GDEP functions \((S_\pm(r; q) = V_\pm(r; q))\), Eq. (18) recasts to

\[
\left\{ \nabla^2 - \frac{1}{\hbar^2 c^2} \left[ \alpha^2_0 \left( \alpha^2_1 + V_\pm(r, q) \right) \right] \right\} \psi_{KG}(\vec{r}) = 0,
\]

\[
\nabla^2 = \frac{\partial^2}{\partial r^2} + \frac{2}{r} \frac{\partial}{\partial r} + \frac{1}{r^2} \left[ \frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \left( \sin \theta \frac{\partial}{\partial \theta} \right) + \frac{1}{\sin^2 \theta} \frac{\partial^2}{\partial \varphi^2} \right],
\]

\[r^2 = \sum_{j=1}^{3} x_j^2, \quad (19)\]

where \(\alpha^2_1 = mc^2 - E_R, \alpha^2_2 = mc^2 + E_R\). It is worth noting that the solution of the \((3 + 1)\)-dimensional KG equation can be reduced to the solution of the Schrödinger equation with the following appropriate choice of parameters: \(\alpha^2_1 \rightarrow -E_{NR}\) and \(\alpha^2_2/\hbar^2 c^2 \rightarrow 2\mu/\hbar^2\), where \(\mu = m_1m_2/(m_1 + m_2)\) is the reduced atomic mass for the diatomic molecular system [14,54].

In addition, we take the interaction potential as in (4) and decompose the total wave function \(\psi_{KG}(\vec{r})\), with a given angular momentum \(l\), as a product of a radial wave function \(R_l(r) = \frac{g(r)}{r}\) and the angular dependent spherical harmonic functions \(Y_{lm}(\hat{r})\): [53-56]

\[
\psi_{KG}(\vec{r}) = \frac{g(r)}{r} Y_{lm}(\hat{r}), \quad (20)
\]

with angular momentum quantum numbers being \(l\) and \(m\). This reduces Eq. (19) into the form

\[
\frac{d^2g(r)}{dr^2} - \frac{1}{\hbar^2 c^2} \left\{ \alpha^2_1 \alpha^2_2 + \alpha^2_2 D \left[ 1 - \sigma \left( \frac{1 \pm q \exp(-2\alpha r)}{1 \mp q \exp(-2\alpha r)} \right) \right]^2 + \frac{l(l+1)\hbar^2 c^2}{r^2} \right\} g(r) = 0, \quad q \neq 0,
\]

\[ (21)\]

where \(\frac{l(l+1)}{r^2}\) is the centrifugal potential and the boundary conditions \(g(0) = g(\infty) = 0\) as we are dealing with bound-state solutions. Moreover, if \(l\) is not too large, the case of the vibrations of small amplitude about the minimum, we can then use the approximate expansion of the centrifugal potential near the minimum point \(r = r_e\) as [33]

\[
\frac{l(l+1)}{r^2} \approx \frac{l(l+1)}{r_e^2} \left\{ A_0 + A_1 \frac{\pm \exp(-2\alpha r_e)}{1 \mp q \exp(-2\alpha r_e)} + A_2 \left[ \frac{\pm \exp(-2\alpha r_e)}{1 \mp q \exp(-2\alpha r_e)} \right]^2 \right\}, \quad (22)
\]

where

\[
A_0 = 1 - \left[ \frac{1 \mp \exp(-2\alpha r_e)}{2\alpha r_e} \right]^2 \left[ \frac{8\alpha r_e}{1 \mp \exp(-2\alpha r_e)} - 3 - 2\alpha r_e \right], \quad (23a)
\]

\[
A_1 = \pm 2 \left[ \exp(2\alpha r_e) \mp 1 \right] \left\{ 3 \left[ \frac{1 \mp \exp(-2\alpha r_e)}{2\alpha r_e} \right] - (3 + 2\alpha r_e) \left[ \frac{1 \mp \exp(-2\alpha r_e)}{2\alpha r_e} \right] \right\}, \quad (23b)
\]

\[
A_2 = \left[ \exp(2\alpha r_e) \mp 1 \right]^2 \left[ \frac{1 \mp \exp(-2\alpha r_e)}{2\alpha r_e} \right]^2 \left[ 3 + 2\alpha r_e - \frac{4\alpha r_e}{1 \mp \exp(-2\alpha r_e)} \right], \quad (23c)
\]
and higher-order terms are neglected. In fact, Eq. (22) is the approximate expansion of the centrifugal potential \( \frac{l(l+1)}{r^2} \) and is valid for all \( r \approx r_e \), the minimum point of \( V_{\pm}(r) \) since \( r \) is not singular there. However, the expansion is not valid near the singularity point \( r = 0 \). Overmore, it is a good approximation for small vibrations around the equilibrium separation \( r - r_e \). When \( l \neq 0 \), we have to use an approximation for the centrifugal term similar to the non-relativistic cases which is valid only for \( q = 1 \) value [33,53]. However, for \( s \)-waves, we remark that the problem can be solved exactly and the solution is valid for any deformation parameter \( q \). At this point, it is important to mention that very similar expressions to the above expression for the energy states have also been found over the past years for the hyperbolical (exponential-type) potentials with \( \delta \to 1 \) in Eq. (2) for \( V_{\pm}(r) \) (cf. Ikhdair and Sever in Ref. [36]). Very recently, a new improved approximation scheme [36,39] for the centrifugal potential term \( l(l+1)/r^2 \) was proposed which appears to be very different from the ones used by Refs. [33,53,54].

Putting \( z = \pm \exp(-2\alpha r) \in (\pm 1, 0) \) for \( V_{\pm}(r) \), and defining the parameters

\[
B_1 = q^2 \tilde{K}_{nl}^2 + \tilde{S}_l^2 - q^2 \tilde{Q}_l - \frac{q^2}{4}, \quad B_2 = 2q\tilde{K}_{nl}^2 - \tilde{Q}_l, \quad B_3 = \tilde{K}_{nl}^2, \tag{24a}
\]

with

\[
\tilde{K}_{nl} = \frac{1}{2\alpha \hbar c} \sqrt{\frac{\alpha^2 D (1 - \sigma)^2 + \frac{l(l+1)\hbar^2 c^2}{r_e^2} A_0 + \alpha_1^2 \alpha_2^2}{\alpha^2 \hbar^2 c^2}} > 0, \tag{25a}
\]

\[
\tilde{Q}_l = -\frac{q\alpha^2 D}{\alpha^2 \hbar^2 c^2} \sigma (1 - \sigma) + \frac{l(l+1)}{4\alpha^2 r_e^2} A_1, \tag{25b}
\]

\[
\tilde{S}_l = \frac{1}{2\alpha \hbar c} \sqrt{\frac{4q^2 \alpha^2 D \sigma^2 + \frac{l(l+1)\hbar^2 c^2}{r_e^2} A_2 + q^2 \alpha^2 \hbar^2 c^2}{\alpha^2 \hbar^2 c^2}} > 0. \tag{25c}
\]

we obtain the hypergeometric wave equation

\[
g''(z) + \frac{(1 - qz)}{z (1 - qz)} g'(z) + \frac{1}{z^2 (1 - qz)^2} \left\{ -B_1 z^2 + B_2 z - B_3 \right\} g(z) = 0, \tag{26}
\]

where \( g(z) = g(r) \). If we apply the previous transformations, the above expressions reduce into their non-relativistic limits:

\[
\tilde{K}_{nl} \to K_{nl} = \frac{1}{2\alpha \hbar} \sqrt{\frac{2\mu D (1 - \sigma)^2 + \frac{l(l+1)\hbar^2}{r_e^2} A_0 - 2\mu E_{NR}}{\alpha^2 \hbar^2 c^2}} > 0, \tag{27a}
\]

\[
\tilde{Q}_l \to Q_l = -\frac{2\mu q D}{\alpha^2 \hbar^2 c^2} \sigma (1 - \sigma) + \frac{l(l+1)}{4\alpha^2 r_e^2} A_1. \tag{27b}
\]
\[ \tilde{S}_l \to S_l = \frac{q}{2\alpha \hbar} \sqrt{8\mu D\sigma^2 + \frac{l(l+1)\hbar^2 A_2}{r_0^2}} + \alpha^2 \hbar^2 > 0, \quad (27c) \]

and also when the deformation parameter \( q = 1 \), the above equations reduce to their counterparts as in Refs. [33,41].

Now comparing Eq. (26) with Eq. (5), we obtain particular values for the set of constant parameters given in Section 2:

\[
\begin{align*}
    c_1 &= 1, \quad c_2 = c_3 = q, \quad c_4 = 0, \quad c_5 = -\frac{q}{2}, \quad c_6 = q^2 \tilde{K}_{nl}^2 + \tilde{S}_l^2 - q\tilde{Q}_l, \\
    c_7 &= -2q\tilde{K}_{nl}^2 + \tilde{Q}_l, \quad c_8 = \tilde{K}_{nl}^2, \quad c_9 = \tilde{S}_l^2, \\
    c_{10} &= 2\tilde{K}_{nl} = 2c_{12} > -1, \quad c_{11} = \frac{2}{q}\tilde{S}_l = 2c_{13} - 1 > -1, \\
    c_{12} &= \tilde{K}_{nl} > 0, \quad c_{13} = \frac{1}{q} \left( \tilde{S}_l + \frac{q}{2} \right) > 0.
\end{align*}
\]  

(28)

Using Eqs. (28) together with Appendix A, we find the following particular physical solutions for the parameters:

\[
\begin{align*}
    \pi(z) &= \tilde{K}_{nl} - \left( \frac{q}{2} + q\tilde{K}_{nl} + \tilde{S}_l \right) z, \\
               &= \tilde{K}_{nl} - \left( \frac{q}{2} \tilde{Q}_l \right) z, \\
    k &= -\tilde{Q}_l - 2\tilde{K}_{nl}\tilde{S}_l, \\
    \tau(z) &= 1 + 2\tilde{K}_{nl} - 2 \left( q + q\tilde{K}_{nl} + \tilde{S}_l \right) z, \\
    \tau'(z) &= \left( \frac{d\tau(z)}{dz} \right) = -2 \left( q + q\tilde{K}_{nl} + \tilde{S}_l \right) < 0 \text{ which gives possible real solutions.}
\end{align*}
\]

In what follows, from Appendix A, we find the ro-vibrational energy equation with the aid of (28) as

\[
2\tilde{K}_{nl} = \left( \frac{\tilde{S}_l}{q} \right)^2 - \frac{\tilde{Q}_l}{q} - \frac{1}{4} - \left( \frac{\tilde{S}_l}{q} + n + \frac{1}{2} \right)^2, \quad q \neq 0,
\]  

(32)

which can be written more explicitly as

\[
2 \sqrt{\left( mc^2 + E_R \right) D (1 - \sigma)^2 + \frac{l(l+1)\hbar^2 c^2}{r_0^2}} A_0 + m^2 c^4 - E_R^2 =
\]

\[
\frac{4 (mc^2 + E_R) D \sigma + \frac{l(l+1)\hbar^2 c^2}{r_0^2} \left( A_2 - \frac{A_1}{q} \right) - \left( \tilde{E} + \alpha \hbar c (2n+1) \right)^2}{\hat{E} + \alpha \hbar c (2n+1)}, \quad (33a)
\]

\[
\tilde{E} = \sqrt{4 (mc^2 + E_R) D \sigma^2 + \frac{l(l+1)\hbar^2 c^2 A_2}{q^2} + \alpha^2 \hbar^2 c^2}, \quad (33b)
\]

11
where \( n = 0, 1, 2, \cdots \) and \( l = 0, 1, 2, \cdots \) signify the usual vibrational and rotational angular momentum quantum numbers, respectively.

Let us now turn to the calculations of the corresponding wave functions for the potential under consideration. Thus, referring to the general model in Appendix A, the explicit form of the weight function reads

\[
\rho(z) = z^{2K_{nl}}(1-qz)^{\frac{1}{2}S_i},
\]

which gives the first part of the wave functions (6) as

\[
y_n(z) \rightarrow P_n^{(2K_{nl},\frac{2}{q}S_i)}(1 \mp 2qz), \quad \tilde{K}_{nl} > 0, \quad \tilde{S}_i > 0,
\]

with the essential requirement that \( 2\tilde{K}_{nl} > -1 \) and \( \frac{2}{q}\tilde{S}_i > -1 \). For example, if \( q > 0 \) then \( \tilde{S}_i > -\frac{q}{2} \) and if \( q < 0 \) then \( 0 < \tilde{S}_i < -\frac{q}{2} \). Also, the second part can be found as

\[
\phi^\pm(z) \rightarrow z^{\tilde{K}_{nl}}(1 \mp qz)^{\frac{1}{2}(\tilde{S}_i + \frac{q}{2})}, \quad \tilde{K}_{nl} > 0, \quad \frac{1}{q} \left( \tilde{S}_i + \frac{q}{2} \right) > 0,
\]

and, hence, the unnormalized wave functions are being expressed in terms of the Jacobi polynomials as

\[
g^\pm(z) = N_{nl}z^{\tilde{K}_{nl}}(1 \mp qz)^{\frac{1}{2}S_i + \frac{1}{2}}P_n^{(2\tilde{K}_{nl},\frac{2}{q}S_i)}(1 - 2qz), \quad z \in [0, 1/q]
\]

where \( N_{nl} \) being the normalization constants and

\[
P_n^{(2\tilde{K}_{nl},\frac{2}{q}S_i)}(1 - 2qz) = \frac{(2\tilde{K}_{nl+1})}{n!} _2F_1(-n, 2\tilde{K}_{nl} + 2\tilde{S}_i + n + 1, 2\tilde{K}_{nl} + 1; qz) \quad \text{with} \quad (m)_n = \frac{(m+n-1)!}{(m-1)!}
\]

is Pochhammer’s symbol. For example, if \( q \geq 1 \) then \( z \in [0, 1/q] \) and if \( q \leq -1 \) then \( z \in [1/q, 0] \) lie within or on the boundary of the interval \([-1, +1]\).

Hence, the total wave function of the \( q\)-DEP/GDEP functions is

\[
\psi^\pm(\vec{r}) = N_{nl}^{\pm} |\pm \exp(-2\alpha r)|^{\tilde{K}_{nl}} [1 \pm q \exp(-2\alpha r)]^{\frac{1}{2}S_i + \frac{1}{2}}
\]

\[
\times P_n^{(2\tilde{K}_{nl},\frac{2}{q}S_i)}(1 - \pm 2q \exp(-2\alpha r))Y_{lm}(\hat{r}).
\]

where the normalization constants \( N_{nl} \) are calculated explicitly in Appendix B.

**IV. DISCUSSIONS**

In this section, we are going to study two special cases of the energy eigenvalues given by Eq. (34). First, we consider the \( s \)-wave (\( l = 0 \)) vibrational energy equation:

\[
2\sqrt{(mc^2 + E_R)} D (1 - \sigma)^2 + m^2c^4 - E_R^2 =
\]
The relativistic limits for the vibrational energy states are obtained from the approximate Schrödinger solution of Eq. (2) for the ro-vibrational molecules. The non-relativistic limit is then:

\[ n \to n_{\text{max}} = \frac{1}{2} \left[ -1 - \sqrt{\frac{4D}{\alpha^2 \hbar^2 c^2} (mc^2 + E_R) \sigma^2 + 1 + \sqrt{\frac{4D}{\alpha^2 \hbar^2 c^2} (mc^2 + E_R) \sigma} \right], \]  

where \( n = 0, 1, 2, \cdots, n_{\text{max}} \), and \( n_{\text{max}} \) is the number of bound states for the whole bound spectrum near the continuous zone. \( n_{\text{max}} \) is the largest integer which is less than or equal to the value of \( n \) that makes the right side of Eq. (39) vanish, that is,

\[ E_{n_{\text{max}}}^{(R)} \to mc^2 + D_e, \]  

This represents the non-relativistic limit of the energy eigenvalues and wave functions in the non-relativistic limit. Obviously, the currently calculated KG solutions, under the previously mentioned transformations, can be reduced to their associated Schrödinger ones for the GDEP functions as

\[ R_{nl}^{(\pm)} (r) = N_n \frac{1}{r} \left[ \pm \exp(-2\alpha r) \left( 1 - q \exp(-2\alpha r) \right) \right]^{\frac{1}{4}} \left[ 1 - \pm q \exp(-2\alpha r) \right]^{\frac{1}{4}} \times P_n^{(2\alpha_n^2 + 1)} (1 - \pm 2q \exp(-2\alpha r)), \]  

where \( N_n \) are the normalization constants and calculated in Appendix B.

Second, we discuss the non-relativistic limit of the energy eigenvalues and wave functions for the GDEP functions as

\[ E_{nl}^{(N)} = E_{nl}^{(NR)} = D_e + \frac{l(l+1) \hbar^2}{2\mu r_e^2} A_0 \]

or more explicitly as

\[ E_{nl}^{(NR)} = D_e + \frac{l(l+1) \hbar^2}{2\mu r_e^2} A_0 \]

which is identical to Eq. (28) of Ref. [33] if one sets \( \delta = 1 \) and \( q = 1 \). This represents the approximate Schrödinger solution of Eq. (2) for the ro-vibrational molecules. The non-relativistic limits for the vibrational energy states \( (l = 0) \) read...
\[ E_{n}^{(NR)}(r) = D_{e} - \frac{\alpha^{2} \hbar^{2}}{2\mu} \left[ \frac{2\mu D}{h^2 \alpha^2} \sigma - \left( n + \frac{1}{2} + \sqrt{\frac{2\mu D}{h^2 \alpha^2} \sigma^2 + \frac{1}{4}} \right) \right]^2 \], \quad n = 0, 1, 2, \cdots, n_{\text{max}}. \quad (44)

and the corresponding unnormalized wave functions from Eq. (38) are

\[ \psi_{\pm}(\vec{r}) = N_{nl} \frac{1}{r} [\pm \exp(-2\alpha r)]^{K_{nl}} \left[ 1 - \pm q \exp(-2\alpha r) \right]^{\frac{1}{2} S_l + \frac{1}{2}} \times P_{n}^{(2K_{nl}, \frac{1}{2} S_l)} \left( 1 - \pm 2q \exp(-2\alpha r) \right) Y_{lm}(\hat{r}). \quad (45)\]

where \( K_{nl} \) and \( S_l \) are defined in Eq. (27) and the condition for \( n_{\text{max}} \) turns to become

\[ n \rightarrow n_{\text{max}} = \frac{1}{2} \left[ -1 - \sqrt{\frac{8\mu D}{h^2 \alpha^2} \sigma^2 + 1} + \sqrt{\frac{8\mu D}{h^2 \alpha^2} \sigma^2} \right], \quad E_{n_{\text{max}}}^{(NR)} \rightarrow D_{e}. \quad (46)\]

Thus, the finiteness of \( n_{\text{max}} \) is reflected in the above condition. If \( \sigma = 1 \), then \( n_{\text{max}} \rightarrow 0 \).

V. APPLICATIONS TO DIATOMIC MOLECULES

We have calculated the non-relativistic energy states for the two selected \( H_2 \) and \( Ar_2 \) diatomic molecules using energy equation (35) with \( q \rightarrow 1 \) and (23). The spectroscopic constants of these two molecules are given in Table 1. The vibrating ground state energy eigenvalues \( E_{+}^0 \) (in \( cm^{-1} \)) for the \( H_2 \) molecule in the non-deformed EP functions \( V_+ (r) \) are found using the NU method for the potential parameters given in Table 2. Our numerical results obtained in the present NU model are listed together with the numerical results obtained by using SC (as Semi-Classical) procedure and a QM (as Quantum-Mechanical) method mentioned in Ref. [32] for various potential parameters. Obviously, as shown in Table 2, the results obtained in the present model are in high agreement with those obtained by QM. However, the SC procedure is proportionally different. Therefore, the differences between our results and SC procedure are less than 0.01 \( cm^{-1} \), i.e., they are negligible because of these approximations: 1 \( a.m.u = 931.502 \, MeV/c^2 \), 1 \( cm^{-1} = 1.23985 \times 10^{-4} \) \( eV \) and \( \hbar c = 1973.29 \, eV.A^{\circ} \) [57]. The second application is applied to \( Ar_2 \) molecule. We confine our study to calculate the ro-vibrating energy states for the \( V_+ (r) \) potential using the following potential parameters: \( \sigma = 25.23 \), \( \delta = 41.75 \) and \( \alpha = 0.6604 \, (A^{\circ})^{-1} \) [32] together with the parameters given in Table 1. For the previously given set of physical parameters,
we plot the non-relativistic energy spectrum curve as a function of vibrational quantum number $n$ as seen in Figure 1. Obviously, in a reference to Figure 1, the energy spectrum of the diatomic molecule $Ar_2$ approaches the value of $D_e$ as $n$ approaches $n_{\text{max}} = 6.689$ or $n_{\text{max}} = 6$. This is also verified analytically from Eqs. (44) and (46). Moreover, a plot of the non-relativistic energy spectrum curve as a function of the potential strength $D_e$ for the above given set of physical parameters and $n = 0$ for $Ar_2$ molecule is shown in Figure 2. The relationship is noticed to be nearly linear for any arbitrary value of vibrational quantum number $n$. The attractive energy value increases with the increasing potential strength. The splittings of the energy states of $s$-waves $E_+ = E_+(n \neq 0) - E_+(n = 0)$ obtained by the NU method and SC procedures are presented in Table 3. The present results $\Delta E_+(\text{NU})$ from NU method and $\Delta E_+(\text{SC})$ obtained from the SC procedures are also compared with four-different experimental results labeled $\Delta E(a)$, $\Delta E(b)$, $\Delta E(c)$ and $\Delta E(d)$ taken from Ref. [32]. It is obvious from Table 3 that our results are very close with the experimentally determined values as well as the SC procedure results. Finally, the approximated rotating and vibrating energy states of the $V_+(r)$ given in Eq. (2) for the $Ar_2$ and $H_2$ molecules are also calculated for the $l \neq 0$ case. Table 4 shows the energy levels for vibrational ($n = 0, 1, 2, 3, 4, 5$) and rotational ($l = 0, 1, 2$) quantum numbers.

VI. CONCLUSIONS

To summarize, we have presented the approximate bound state energy eigenvalues and their corresponding normalized wave functions of the relativistic spin-0 particle in the radial $(3 + 1)$-dimensional KG equation with equal scalar and vector $q$-DEP/GDEP functions by means of the parametric generalization of the NU method. We point out that the KG wave functions are found in terms of the Jacobi polynomials. The analytic expressions for the relativistic energy expression and the corresponding wave functions of this molecular system can be reduced to the well-known non-relativistic solutions and to the $s$-waves solutions as well. The relativistic energy $E_R$ defined implicitly by Eq. (33) is rather a transcendental equation and it has many solutions for any arbitrarily chosen values of usual quantum numbers $n$ and $l$. The method presented in this paper is general and worth extending to the solution of other molecular interaction problems. The method is simple and useful in solving other complicated systems analytically without giving any restriction on the solution.
of some quantum systems as is the case in the other models. We have also seen that for the nonrelativistic model, the approximate energy spectrum can be obtained either by directly solving the Schrödinger equation [41] or rather by even applying appropriate transformations to the relativistic solution as currently shown. We should emphasize that the approximate bound state energy spectrum obtained in the present work might have some interesting applications in different branches like atomic and molecular physics and quantum chemistry. The present solution is describing the inter-molecular structures and interactions in diatomic molecules [32-36,41,58,59]. The present study is also useful in calculating the vibrating energy for different radial $n$ quantum numbers as well as the rotating energy for different orbital $l$ quantum numbers. To conclude, the proposed $q$-deformation potential with a flexible and fixed value $q$ (real or complex) can generate various potential models with various energy solutions.

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APPENDIX A: PARAMETERIZED VERSION OF THE NU METHOD

We complement the theoretical formulation of the NU method in presenting the essential polynomials, energy equation and wave functions together with their relevant constants as follows.

(i) The key polynomials:

$$\pi(z) = c_4 + c_5 z - \left[ (\sqrt{c_9} + c_3 \sqrt{c_8}) z - \sqrt{c_8} \right], \quad (A1)$$

$$k = -(c_7 + 2c_3c_8) - 2\sqrt{c_8c_9}, \quad (A2)$$

$$\tau(z) = 1 - (c_2 - 2c_5) z - 2 \left[ (\sqrt{c_9} + c_3 \sqrt{c_8}) z - \sqrt{c_8} \right], \quad (A3)$$

$$\tau'(z) = -2c_3 - 2 \left( \sqrt{c_9} + c_3 \sqrt{c_8} \right) < 0, \quad (A4)$$
(ii) The energy equation:

\[(c_2 - c_3) n + c_3 n^2 - (2n + 1) c_5 + (2n + 1) \left( \sqrt{c_9} + c_3 \sqrt{c_5} \right) + c_7 + 2c_3c_8 + 2\sqrt{c_8c_9} = 0. \quad (A5)\]

(iii) The wave functions:

\[\rho(z) = z^{c_{10}} (1 - c_3 z)^{c_{11}}, \quad (A6)\]

\[\phi(z) = z^{c_{12}} (1 - c_3 z)^{c_{13}}, \quad c_{12} > 0, \quad c_{13} > 0, \quad (A7)\]

\[y_n(z) = P_n^{(c_{10}, c_{11})}(1 - 2c_3 z), \quad c_{10} > -1, \quad c_{11} > -1, \quad z \in [0, 1/c_3], \quad (A8)\]

\[u(z) = N_n z^{c_{12}} (1 - c_3 z)^{c_{13}} P_n^{(c_{10}, c_{11})}(1 - 2c_3 z), \quad (A9)\]

where the Jacobi polynomial \(P_n^{(\mu, \nu)}(x)\) is defined only for \(\mu > -1, \nu > -1\), and for the argument \(x \in [-1, +1]\) and \(N_n^c\) is a normalizing factor. It can be expressed in terms of the hypergeometric function as

\[P_n^{(\mu, \nu)}(1 - 2s) = \frac{(\mu + 1)_n}{n!} {}_2F_1 \left(-n, 1 + \mu + \nu + n; \mu + 1; s\right), \quad (A10)\]

where \(s \in [0, 1]\) which lie within or on the boundary of the interval \([-1, 1]\). Also, the above wavefunctions can be expressed in terms of the hypergeometric function as

\[u(z) = N_n z^{c_{12}} (1 - c_3 z)^{c_{13}} {}_2F_1 \left(-n, 1 + c_{10} + c_{11} + n; c_{10} + 1; c_3 z\right), \quad (A11)\]

where \(c_{12} > 0, \quad c_{13} > 0\) and \(z \in [0, 1/c_3]\).

(iv) The relevant constants:

\[c_4 = \frac{1}{2} (1 - c_1), \quad c_5 = \frac{1}{2} (c_2 - 2c_3), \quad c_6 = c_5^2 + B_1, \quad (A12)\]

\[c_7 = 2c_4c_5 - B_2, \quad c_8 = c_4^2 + B_3, \quad c_9 = c_3 (c_7 + c_3c_8) + c_6, \quad (A12)\]

\[c_{10} = c_1 + 2c_4 + 2\sqrt{c_8} - 1 > -1, \quad c_{11} = 1 - c_1 - 2c_4 + 2 \frac{1}{c_3} \sqrt{c_9} > -1, \quad (A12)\]

\[c_{12} = c_4 + \sqrt{c_8} > 0, \quad c_{13} = -c_4 + 1 \frac{1}{c_3} (\sqrt{c_9} - c_5) > 0. \quad (A12)\]
APPENDIX B: NORMALIZATION OF THE RADIAL WAVE FUNCTION

In order to find the normalization factor $\mathcal{N}_{nl}$, we start by writing the normalization condition:

$$\frac{\mathcal{N}_{nl}^2}{2\alpha} \int_0^1 z^{2\bar{K}_{nl}-1}(1-z)^{2\bar{S}_l+1} \left[ P_n^{(2\bar{K}_{nl}, 2\bar{S}_l)}(1-2z) \right]^2 \, dz = 1,$$  \hspace{1cm} (B1)

where $q = 1$.Unfortunately, there is no formula available to calculate this key integration. Nevertheless, we can find the explicit normalization constant $\mathcal{N}_{nl}$. For this purpose, it is not difficult to obtain the results of the above integral by using the following formulas [59]

$$\int_0^1 (1-s)^{\mu-1} s^{\nu-1} \, _2F_1(\alpha, \beta; \gamma; a\, s) \, ds = \frac{\Gamma(\mu)\Gamma(\nu)}{\Gamma(\mu+\nu)} \, _3F_2(\nu, \alpha, \beta; \mu+\nu; \gamma; a),$$  \hspace{1cm} (B2)

and $\, _2F_1(\alpha, \beta; c; z) = \frac{\Gamma(c)}{\Gamma(\alpha)\Gamma(\beta)} \sum_{p=0}^{\infty} \frac{\Gamma(\alpha+p)\Gamma(\beta+p)}{\Gamma(c+p)} \frac{z^p}{p!}$. Following Ref. [59], we calculate the normalization constants:

$$\mathcal{N}_{nl} = \left[ \frac{\Gamma(2\bar{K}_{nl}+1)\Gamma(2\bar{S}_l+2)}{2\alpha\Gamma(n)} \sum_{m=0}^{\infty} \frac{(-1)^m (1 + n + 2(\bar{K}_{nl} + \bar{S}_l))}{m! (m + 2\bar{K}_{nl})! \Gamma(m + 2(\bar{K}_{nl} + \bar{S}_l + 1))} f_{nl} \right]^{-1/2},$$  \hspace{1cm} (B3)

where

$$f_{nl} = \, _3F_2 \left( 2\bar{K}_{nl} + m, -n, n + 1 + 2(\bar{K}_{nl} + \bar{S}_l); m + 2(\bar{K}_{nl} + \bar{S}_l + 1); 1 + 2\bar{K}_{nl}; 1 \right).$$  \hspace{1cm} (B4)

Furthermore, the normalization constants for the s-wave can be also found as

$$\mathcal{N}_n = \left[ \frac{\Gamma(2\bar{k}_n+1)\Gamma(2\bar{s}+2)}{2\alpha\Gamma(n)} \sum_{m=0}^{\infty} \frac{(-1)^m (1 + n + 2(\bar{k}_n + \bar{s}))}{m! (m + 2\bar{k}_n)! \Gamma(m + 2(\bar{k}_n + \bar{s} + 1))} g_n \right]^{-1/2},$$  \hspace{1cm} (B5)

where

$$g_n = \, _3F_2 \left( 2\bar{k}_n + m, -n, n + 1 + 2(\bar{k}_n + \bar{s}); m + 2(\bar{k}_n + \bar{s} + 1); 1 + 2\bar{k}_n; 1 \right),$$  \hspace{1cm} (B6)

and

$$\bar{k}_n = \frac{1}{2\alpha\hbar} \sqrt{(mc^2 + E_R) D(1 - \sigma)^2 + m^2c^4 - E_R^2},$$

$$\bar{s} = \frac{q}{2\alpha\hbar} \sqrt{4(mc^2 + E_R) D\sigma^2 + \alpha^2\hbar^2}, \quad n = 0, 1, 2, \cdots,$$  \hspace{1cm} (B7)

where $E_R$ is the solution of the transcendental equation (33).
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FIG. 1: A plot of the non-relativistic energy spectrum curve as a function of the vibrational quantum number $n$ for a given set of physical parameters for $Ar_2$ molecule.

FIG. 2: A plot of the non-relativistic energy spectrum curve as a function of the potential strength $D_e$ for a given set of physical parameters and vibrational ground state $n = 0$ for $Ar_2$ molecule.

TABLE I: The spectroscopic constants of the EP for $H_2$ and $Ar_2$ molecules [26].

| Parameters | $H_2$ | $Ar_2$ |
|------------|-------|--------|
| $D_e$ ($cm^{-1}$) | 38281 | 99.55 |
| $r_e$ ($A^\circ$) | 0.7414 | 3.759 |
| $\mu$ (a.m.u) | 0.50407 | 19.9812 |
TABLE II: The EP parameters of the $V_+(r)$ and the ground state energy, $E_+^{00}$ (in cm$^{-1}$) of the $H_2$ molecule.

| $\sigma$ | $\delta$ | $\alpha$ (A$^\circ$)$^{-1}$ | $E_+(SC)$ | $E_+(QM)$ | Present |
|----------|----------|-----------------|-----------|-----------|---------|
| 426.826  | 463.102  | 0.9327          | 2167.68   | 2168.93   | 2168.68 |
| 47.294   | 102.341  | 0.6146          | 2153.69   | 2164.83   | 2164.45 |
| 28.685   | 117.121  | 0.3826          | 2139.57   | 2157.69   | 2157.53 |
| 21.250   | 213.212  | 0.1762          | 2124.29   | 2148.40   | 2147.53 |

TABLE III: Comparisons of experimentally calculated s-states energy transition values $\Delta E_{n,0}$ (cm$^{-1}$) for $n \neq 0 \rightarrow n = 0$ together with the results of the SC procedure and the present NU method for the Ar$_2$ molecule.

| $n$ | Present | $\Delta E(a)$ | $\Delta E(b)$ | $\Delta E(c)$ | $\Delta E(d)$ | $\Delta E_+(SC)$ |
|-----|---------|---------------|---------------|---------------|---------------|------------------|
| 1   | 25.808  | 25.74         | 25.49         | 25.21         | 25.56         | 25.75            |
| 2   | 46.079  | 46.15         | 45.63         | 45.02         | 46.00         | 46.01            |
| 3   | 61.472  | 61.75         | 60.70         | 60.04         | 61.32         | 61.42            |
| 4   | 72.536  | 72.66         | 71.33         | 70.92         | 71.52         | 72.52            |
| 5   | 79.733  | 79.44         | -             | -             | -             | 79.79            |
| 6   | 83.453  | -             | -             | -             | -             | 83.59            |
| 7   | 84.026  | -             | -             | -             | -             | -                |
TABLE IV: Energy levels $E_{n,l}(cm^{-1})$ for $Ar_2$ and $H_2$ molecules in $V_+(r)$ using the NU method.

| n l  | $E_+ (Ar_2)$ | $E_+ (H_2)$ |
|------|--------------|--------------|
| 0 0  | 15.3828      | 2168.68      |
| 1 0  | 41.1910      | 6306.66      |
|      | 25.7584      | 6331.10      |
| 2 0  | 61.4619      | 10183.8      |
|      | 49.7874      | 10207.6      |
| 2 -  |             | 10255.2      |
| 3 0  | 76.8546      | 13802.1      |
|      | 68.3028      | 13825.2      |
|      | 19.9133      | 13871.5      |
| 4 0  | 87.9188      | 17163.2      |
|      | 82.0041      | 17185.7      |
|      | 46.4777      | 17230.7      |
| 5 0  | 95.1159      | 20269.1      |
|      | 91.4672      | 20291.0      |
|      | 66.5474      | 20334.8      |
This figure "Energy-vs-states.jpg" is available in "jpg" format from:

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