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ARTICLE

Nonrelativistic and relativistic bound state solutions of the molecular Tietz potential via the improved asymptotic iteration method

W.A. Yahya, K. Issa, B.J. Falaye, and K.J. Oyewumi

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Abstract: We have obtained the approximate analytical solutions of the relativistic and nonrelativistic molecular Tietz potential using the improved asymptotic iteration method. By approximating the centrifugal term through the Greene–Aldrich approximation scheme, we have obtained the energy eigenvalues and wave functions for all orbital quantum numbers ℓ. Where necessary, we made comparison with the result obtained previously in the literature. The relative closeness of the two results reveal the accuracy of the method presented in this study. We proceed further to obtain the rotational-vibrational energy spectrum for some diatomic molecules. These molecules are CO, HCl, H_2, and LiH. We have also obtained the relativistic bound state solution of the Klein–Gordon equation with this potential. In the nonrelativistic limits, our result converges to that of the Schrödinger system.

Key words: molecular Tietz potential, Klein–Gordon equation, improved asymptotic iteration method, Greene–Aldrich approximation, Jacobi polynomials.

Résumé : Nous avons obtenu les solutions analytiques approximatives du potentiel moléculaire de Tietz relativiste et non relativiste en utilisant la méthode d'itération asymptotique améliorée. En approximant le terme centrifuge au moyen du modèle d'approximation de Greene–Aldrich, nous avons obtenu les valeurs propres d'énergie et les fonctions d'onde pour toutes les valeurs du nombre quantique azimutal ℓ. Au besoin, nous avons comparé nos résultat à ce publié antérieurement dans la littérature. La proximité relative des deux résultats témoigne de l'exactitude de la méthode présentée. Nous avons aussi obtenu les spectres de rotation-vibration de certaines molécules diatomiques, à savoir CO, HCl, H_2 et LiH. Enfin, nous avons obtenu la solution de l'équation de Klein–Gordon pour l'état lié relativiste en utilisant ce potentiel. Dans les limites non relativistes, notre résultat converge vers celui du système de Schrödinger. [Traduit par la Rédaction]

Mots-clés : potentiel moléculaire de Tietz, équation de Klein–Gordon, méthode d'itération asymptotique améliorée, approximation de Greene–Aldrich, polynômes de Jacobi.

Introduction

The solutions of the Schrödinger wave equations occupy a pole position in quantum mechanics[1] just as the Dirac and Klein–Gordon equations occupy pole positions in relativistic quantum mechanics. Different methods have been employed to solve the Schrödinger equation, Klein–Gordon equation, and Dirac equation for various potentials. The methods include the Nikiforov–Uvarov method,[2–15] asymptotic iteration method,[16–38] supersymmetry quantum mechanics,[39–54] Laplace integral transform,[55] factorization method,[56] proper quantization rule and exact quantization rule[57–61] among others. We shall employ in this paper the use of the improved asymptotic iteration method (improved AIM) introduced by Boztosun and Karakoc (2007)[62] to obtain the result of the Schrödinger equation and Klein–Gordon equation under the Tietz potential. In the three-dimensional case, the solutions of most potentials cannot be obtained analytically for any ℓ-state but by using an appropriate approximation scheme to deal with the centrifugal term. We shall make use of the Greene–Aldrich approximation scheme in this paper to deal with the centrifugal term. The Tietz potential we examine in this study is given as[63,64,65]

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

where D_e is the dissociation energy between two atoms in a solid and r_e is the equilibrium intermolecular separation. The molecular Tietz potential resembles Eckart or Möbius potentials for certain conditions.[63,65] An empirical potential energy function $V(r)$ for diatomic molecules should satisfy the following conditions:[66]

$$\begin{aligned} &\left.\frac{dV(r)}{dr}\right|_{r=r_e} = 0 \\ &V(\infty) - V(r_e) = D_e \\ &\left.\frac{d^2V(r)}{dr^2}\right|_{r=r_e} = k_e \end{aligned} \tag{2}$$

This molecular Tietz potential satisfies all of the conditions. It is worth mentioning that the solutions of the Dirac equation have been obtained for the Tietz–Hua potential in Hassanabadi et al.[39]

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and Ikot et al.[67] Also, the solution of the Schrödinger equation for the molecular Tietz molecular has been obtained recently by using the parametric form of the Nikiforov–Uvarov method.[63] The solutions of the Tietz–Wei potential have also been obtained for relativistic spin-zero particles.[68] In Jia et al.[69], the authors discussed the equivalence of the Wei potential model and Tietz potential model. They also showed that when parameter h in the Tietz potential function has the values 0, +1, and –1, the Tietz potential becomes the standard Morse, Rosen–Morse, and Manning–Rosen potentials, respectively. The aim of this paper is to obtain the approximate analytical solutions of the Schrödinger equation and Klein–Gordon equation for the molecular Tietz potential using the improved AIM.

The paper is organized as follows. In the next section, the improved AIM is presented. In the following section, we obtain the approximate analytical solutions of the nonrelativistic molecular Tietz potential and also compare our results with the ones obtained previously in literature. The subsequent section present the solutions of the relativistic Klein–Gordon equation for the potential. We also discuss the nonrelativistic limit. The concluding remarks are given in the final section.

Improved asymptotic iteration method

The asymptotic iteration method is proposed to solve the second-order differential equations in the form[62,70]

$$y''(r) = \lambda_0(r)y'(r) + s_0(r)y(r) \tag{3}$$

where $\lambda_0(r) \neq 0$ and $s_0(r)$ and $\lambda_0(r)$ are in $C_\infty(a,b)$. If we rearrange eq. 3 by introducing new forms for $\lambda_0(r)$ and $s_0(r)$, we have

$$\lambda_0(r) = -\frac{\tau(r)}{\sigma(r)}, s_0(r) = -\frac{\gamma_n}{\sigma(r)} \tag{4}$$

where τ and σ are new functions and γ_n is a constant with which we quantize the energy. Inserting them into eq. 3, the second-order differential equation takes the form

$$y'' = -\frac{\tau(r)}{\sigma(r)}y' - \frac{\gamma_n}{\sigma(r)}y \tag{5}$$

To obtain the energy eigenvalue, the following equation has been derived in Boztosun and Karakoc:[62]

$$\gamma_n = -n\tau'(r) - \frac{n(n-1)}{2}\sigma''(r) \tag{6}$$

This formula gives directly the energy eigenvalues for the differential eq. 5. It replaces the iterative calculations needed to find the energy eigenvalues in the original AIM formulation.[62] To obtain the eigenfunctions, we use

$$y_n(r) = \frac{1}{\rho(r)}\frac{d^n}{ds^n}[\sigma(r)^n\rho(r)], n = 0, 1, 2, 3, \ldots \tag{7}$$

where $\rho(r)$ has to satisfy[11,62,71]

$$[\sigma(r)\rho(r)]' = \tau(r)\rho(r) \tag{8}$$

In the next section, we apply this approach to find the approximate bound state solution of Schrödinger–Tietz problem.

Nonrelativistic bound sate solution of the Schrödinger equation with the Tietz potential

The Schrödinger equation in spherical polar coordinate can be written as[72]

$$-\frac{\hbar^2}{2\mu}\left\{\frac{\partial^2}{\partial r^2} + \frac{2}{r}\frac{\partial}{\partial r} + \frac{1}{r^2}\left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right] + V(r)\right\} \times \Psi_{n\ell\mu}(r,\theta,\phi) = E\Psi_{n\ell\mu}(r,\theta,\phi) \tag{9}$$

Defining $\Psi_{n\ell\mu}(r,\theta,\phi) = U_{n\ell}Y_{\ell\mu}(\theta,\phi)$, we obtain the radial part of the Schrödinger equation as

$$\left(\frac{d^2}{dr^2} + \frac{2}{r}\frac{d}{dr}\right)U_{n\ell}(r) - \frac{2\mu}{\hbar^2}\left(V(r) + \frac{\hbar^2\ell(\ell+1)}{2\mu r^2}\right)U_{n\ell} + \frac{2\mu E_{n\ell}}{\hbar^2}U_{n\ell} = 0 \tag{10}$$

If we define $U_{n\ell}(r) = \frac{R_{n\ell}(r)}{r}$, the radial equation appears as

$$\frac{d^2R_{n\ell}(r)}{dr^2} + \frac{2\mu}{\hbar^2}\left(E_{n\ell} - V(r) - \frac{\hbar^2\ell(\ell+1)}{2\mu r^2}\right)R_{n\ell}(r) = 0 \tag{11}$$

Substitution of the molecular Tietz potential in eq. 1 into eq. 11, we have

$$\frac{d^2R_{n\ell}(r)}{dr^2} + \frac{2\mu}{\hbar^2}\left\{E_{n\ell} - D_e\left(\frac{\sinh\left(\frac{r-r_e}{a}\right)}{\sinh\left(\frac{r}{a}\right)}\right)^2 - \frac{\hbar^2\ell(\ell+1)}{2\mu r^2}\right\} \times R_{nl}(r) = 0 \tag{12}$$

Using the Greene–Aldrich approximation scheme[72–75]

$$\frac{1}{r^2} \approx \frac{\alpha^2}{\sinh^2(\alpha r)} \tag{13}$$

to deal with the centrifugal term in eq. 12, we obtain

$$\frac{d^2R_{n\ell}(r)}{dr^2} + \frac{2\mu}{\hbar^2}\left\{E_{n\ell} - D_e\cosh^2(\alpha r_e) + 2D_e\cosh(\alpha r_e)\sinh(\alpha r_e)\coth(\alpha r) - D_e\sinh^2(\alpha r_e)\coth^2(\alpha r) - \frac{\hbar^2\alpha^2\ell(\ell+1)}{2\mu\sinh^2(\alpha r)}\right\}R_{n\ell}(r) = 0 \tag{14}$$

where $\alpha = 1/a$. The approximation used together with the centrifugal term have been plotted in Nikoofard et al.[63] It was observed that the approximation is a good one for small value of a. Now defining a new variable such as $z = e^{-2\alpha r}$ and using

$$\begin{aligned}\xi &= \frac{\mu(E_{n\ell} + D_e)}{2\alpha^2\hbar^2} - \frac{\mu D_e}{\alpha^2\hbar^2}(\cosh^2(\alpha r_e) - \cosh(\alpha r_e)\sinh(\alpha r_e))\\ \eta &= \frac{\mu(D_e - E_{n\ell})}{\alpha^2\hbar^2} - \ell(\ell+1)\\ \delta &= \frac{\mu(E_{n\ell} - D_e)}{2\alpha^2\hbar^2} + \frac{\mu D_e}{\alpha^2\hbar^2}(\cosh(\alpha r_e)\sinh(\alpha r_e) - \sinh^2(\alpha r_e))\end{aligned} \tag{15}$$

Equation 15 transforms to

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$$\frac{d^2R_{n\ell}(z)}{dz^2} + \frac{1}{z}\frac{dR_{n\ell}(z)}{dz} + \frac{1}{z^2(1-z)^2}(\xi z^2 + \eta z + \delta)R_{n\ell}(z) = 0 \tag{16}$$

To solve eq. 16 using the improved AIM, we propose the wave function ansatz of the form

$$R(z) = z^{-\sqrt{-\delta}}(1-z)^{\left(\frac{1}{2}+\sqrt{-\eta-\delta-\xi+\frac{1}{4}}\right)}P(z) \tag{17}$$

Inserting this wave function into eq. 16, we obtain

$$\begin{aligned}[4\delta + 2\eta + (-1+2\sqrt{-\delta})(1+\sqrt{1-4\delta-4\eta-4\xi})] \\ + [2-4\sqrt{-\delta} + z(-4+4\sqrt{-\delta}-2\sqrt{1-4\delta-4\eta-4\xi})]P'(z) \\ + 2z(1-z)P''(z) = 0\end{aligned} \tag{18}$$

Comparing eqs. 18 and 5, we obtain

$$\sigma(z) = 2z(1-z) \tag{19}$$

$$\tau(z) = 2 - 4\sqrt{-\delta} + z(-4+4\sqrt{-\delta}-2\sqrt{1-4\delta-4\eta-4\xi}) \tag{20}$$

$$\gamma_n = 4\delta + 2\eta + (-1+2\sqrt{-\delta})(1+\sqrt{1-4\delta-4\eta-4\xi}) \tag{21}$$

Substituting eqs. 19, 20, and 21 into eq. 6, we have

$$\begin{aligned}4\delta + 2\eta + (-1+2\sqrt{-\delta})(1+\sqrt{1-4\delta-4\eta-4\xi}) \\ + n(-4+4\sqrt{-\delta}-2\sqrt{1-4\delta-4\eta-4\xi}) - 2n(n-1) = 0\end{aligned} \tag{22}$$

or more explicitly:

$$\begin{aligned}\frac{1}{\hbar^2\alpha^2}\Bigg\{2\mu D_e(1-e^{-2\alpha r_e}) + \hbar^2\alpha^2\Bigg[-2\ell(\ell+1) - 2n^2 \\ + \left(-1+\sqrt{\frac{2\mu D_e e^{-2\alpha r_e} - 2\mu E_{n\ell}}{\hbar^2\alpha^2}}\right)\left(1+\sqrt{(1+2\ell)^2+\frac{8\mu D_e \sinh^2\alpha r_e}{\hbar^2\alpha^2}}\right) \\ - 2n\left(1-\sqrt{\frac{2\mu D_e e^{-2\alpha r_e} - 2\mu E_{n\ell}}{\hbar^2\alpha^2}} + \sqrt{(1+2\ell)^2+\frac{8\mu D_e \sinh^2\alpha r_e}{\hbar^2\alpha^2}}\right)\Bigg]\Bigg\} = 0\end{aligned} \tag{23}$$

from which we can obtain the energy eigenvalues. Equation 23 is the energy equation for the nonrelativistic molecular Tietz potential. To show the accuracy of our approximate method, in Table 1, we show the comparison of our result (improved AIM) with the result obtained previously in Nikoofard et al.[63] where the parametric Nikiforov–Uvarov method has been employed. As displayed in the table, the two results are in excellent agreement. Furthermore, by using the following values of the dissociation energy D_e, equilibrium intermolecular separation r_e, and range of potential a:

CO: $D_e = 10.845073641$ eV, $r_e = 1.1282$ Å, $\mu = 6.860586000$ amu, $a = 2.2994$ Å^{-1}
HCl: $D_e = 4.619030905$ eV, $r_e = 1.2746$ Å, $\mu = 0.9801045$ amu, $a = 1.8677$ Å^{-1}
H_2: $D_e = 4.7446$ eV, $r_e = 0.7416$ Å, $\mu = 0.50391$ amu, $a = 1.9425$ Å^{-1}
LiH: $D_e = 2.5152672118$ eV, $r_e = 1.5956$ Å, $\mu = 0.8801221$ amu, $a = 1.1280$ Å^{-1}

we obtain the rotational-vibrational energy spectrum for some few selected diatomic molecules. These parameters are taken from Oyewumi and Sen[77] We have also used the conversions $\hbar c = 1973.29$ eV Å^{-1} and 1 amu = 931.494028×10^6 eV c^{-2} throughout our numerical computation for the diatomic molecules. The results are displayed in Table 2. Let us now calculate the radial wave function. Substituting $\sigma(z)$ and $\tau(z)$ into eq. 8, we obtain

$$\rho(z) = (-1+z)^{\sqrt{1-4\delta-4\eta-4\xi}}z^{-2\sqrt{-\delta}} \tag{24}$$

Inserting eq. 24 into eq. 7, we have

$$\begin{aligned}y_n(z) = C_n(-1+z)^{-\sqrt{1-4\delta-4\eta-4\xi}}z^{2\sqrt{-\delta}}\frac{d^n}{ds^n} \\ \times\left[(2z(1-z))^n(-1+z)^{\sqrt{1-4\delta-4\eta-4\xi}}z^{-2\sqrt{-\delta}}\right]\end{aligned} \tag{25}$$

We then obtain the wave function as

$$R_{n\ell} = C_n z^{\sqrt{-\delta}}(1-z)^{\frac{1}{2}+\sqrt{-\eta-\delta-\xi+\frac{1}{4}}}P_n^{\left(2\sqrt{-\delta},2\sqrt{-\eta-\delta-\xi+\frac{1}{4}}\right)}(1-2z) \tag{26}$$

where

$$P_n^{(x,y)}(1-2z) = \frac{\Gamma(n+x+1)}{n!\Gamma(x+1)}\,{}_2F_1(-n,n+x+y+1,x+1;s) \tag{27}$$

Since $z = e^{-2\alpha r}$, therefore, eq. 26 can be written as

$$\begin{aligned}R_{n\ell} = C_n e^{-2\alpha r\sqrt{-\delta}}(1-e^{-2\alpha r})^{\frac{1}{2}+\sqrt{-\eta-\delta-\xi+\frac{1}{4}}}\frac{\Gamma(n+2\sqrt{-\delta}+1)}{n!\Gamma(1+2\sqrt{-\delta})} \\ \times\,{}_2F_1\left(-n,n+2\sqrt{-\delta}+2\sqrt{-\eta-\delta-\xi+\frac{1}{4}}+1;2\sqrt{-\delta}+1;e^{-2\alpha r}\right)\end{aligned} \tag{28}$$

where C_n is the normalization constant.

Relativistic bound state solution of the Klein–Gordon equation with Tietz potential

In relativistic quantum mechanics, the Klein–Gordon and Dirac wave equations are most frequently used to understand the dynamics of a particle in a large class of potentials. The time-independent Klein–Gordon equation with scalar $S(r)$ and vector $V(r)$ potentials, describing spin-zero particle of rest mass μ, can be written as[78–81]

$$\begin{aligned}-\hbar^2c^2\left[\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{r^2\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right]\Psi(\mathbf{r}) \\ = \{[E_R - V(r)]^2 - [\mu c^2 + S(r)]^2\}\Psi(\mathbf{r})\end{aligned} \tag{29}$$

where E_R refers to the energy spectrum and μ is the rest mass of the confined particle. By using the following variable-separation ansatz $\Psi(\mathbf{r}) = u(r)\Theta(\theta)\Phi(\phi)r^{-1}\sin^{-\frac{1}{2}}\theta$ for the stationary wave function, we obtain the radial part of the Klein–Gordon equation as

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Table 1. Energies of the nonrelativistic molecular Tietz (fm^{-1}) for μ = 5 fm^{-1}, $\hbar$ = 1, α = 0.01, and r_e = 2.

	D_e = 0.2		D_e = 0.4	
(n, ℓ)	Nikiforov–Uvarov ([63])	Improved AIM	Nikiforov–Uvarov ([63])	Improved AIM
(0,0)	0.059294	0.059294	0.088263	0.088263
(0,1)	0.083196	0.083196	0.118925	0.118925
(0,2)	0.112385	0.112385	0.164796	0.164796
(0,3)	0.135879	0.135879	0.210629	0.210629
(1,0)	0.116235	0.116235	0.190727	0.190727
(1,1)	0.127523	0.127523	0.207801	0.207801
(1,2)	0.142351	0.142351	0.234273	0.234273
(1,3)	0.155334	0.155334	0.261993	0.261993
(2,0)	0.144408	0.144408	0.249787	0.249787
(2,1)	0.150593	0.150593	0.260242	0.260242
(2,2)	0.159111	0.159111	0.276865	0.276865
(2,3)	0.167001	0.167001	0.294870	0.294870
(3,0)	0.160332	0.160332	0.286861	0.286861
(3,1)	0.164068	0.164068	0.293713	0.293713
(3,2)	0.169384	0.169384	0.304811	0.304811
(3,3)	0.174507	0.174507	0.317141	0.317141

Table 2. Energies of the nonrelativistic molecular Tietz (eV) for some diatomic molecules.

(n, ℓ)	CO	HCl	H_2	LiH
(0,0)	0.048793	0.070963	0.179989	0.033280
(0,1)	0.049231	0.073124	0.193329	0.034150
(0,2)	0.050107	0.077437	0.219733	0.035877
(0,3)	0.051420	0.083882	0.258660	0.038441
(1,0)	0.144942	0.203905	0.501052	0.086542
(1,1)	0.145372	0.205894	0.512652	0.087170
(1,2)	0.146232	0.209864	0.535611	0.088415
(1,3)	0.147522	0.215794	0.569461	0.090258
(2,0)	0.239349	0.326117	0.780238	0.123017
(2,1)	0.239771	0.327943	0.790323	0.123414
(2,2)	0.240616	0.331587	0.810285	0.124198
(2,3)	0.241882	0.337031	0.839714	0.125350

$$\left\{\frac{d^2}{dr^2}-\frac{\ell(\ell+1)}{r^2}+\frac{1}{\hbar^2c^2}[E-V(r)]^2-\frac{1}{\hbar^2c^2}[\mu c^2+S(r)]^2\right\}u(r)=0 \tag{30}$$

where the second term provides a centrifugal potential, which together with the third term comprises the effective resultant potential. Setting $V(r) = S(r)$, eq. 30 reduces to

$$\left\{\frac{d^2}{dr^2}-\frac{\ell(\ell+1)}{r^2}+\frac{1}{\hbar^2c^2}[E^2-\mu^2c^4]-\frac{1}{\hbar^2c^2}[E+\mu c^2]V(r)\right\}u(r)=0 \tag{31}$$

If we let $\varepsilon = E_R^2 - \mu^2c^4$ and $\beta = E_R + \mu c^2$ and make use of eqs. 1 and 13, eq. 31 can then be written as

$$\frac{d^2u(r)}{dr^2}+\frac{\varepsilon u(r)}{\hbar^2c^2}-\frac{\alpha^2\ell(\ell+1)u(r)}{\sinh^2(\alpha r)}+\frac{\beta D_e}{\hbar^2c^2}\times[\cosh(\alpha r_e)\sinh(\alpha r)\coth(\alpha r)-\cosh^2(\alpha r_e)-\sinh^2(\alpha r_e)\coth^2(\alpha r)]u(r)=0 \tag{32}$$

Defining a new variable $s = e^{-2\alpha r}$, we obtain

$$\frac{d^2u(s)}{ds^2}+\frac{1}{s}\frac{du(s)}{ds}+\frac{1}{s^2(1-s)^2}(As^2+Bs+C)u(s)=0 \tag{33}$$

Table 3. Energies of the relativistic molecular Tietz potential (fm^{-1}) for μ = 5 fm^{-1}, $\hbar$ = 1, α = 0.01, and r_e = 2.

(n, ℓ)	D_e = 0.2	D_e = 0.4	D_e = 0.6	D_e = 0.8
(0,0)	−5.02356496	−5.02231473	−5.02117740	−5.02013918
(0,1)	−7.68636672	−6.37406970	−5.92685203	−5.69964204
(0,2)	−12.7412173	−8.90157049	−7.60333917	−6.94781274
(0,3)	−20.2652810	−12.6549402	−10.0892781	−8.79602695
(1,0)	−5.00003928	−5.00003858	−5.00003790	−5.00003725
(1,1)	−5.20845412	−5.19774157	−5.18795050	−5.17897567
(1,2)	−10.8317383	−8.12923326	−7.18480953	−6.69463117
(1,3)	−18.5171621	−12.0413968	−9.81787923	−8.67818011
(2,0)	−5.00008837	−5.00008679	−5.00008527	−5.00008381
(2,1)	−5.00015710	−5.00015431	−5.00015161	−5.00014901
(2,2)	−5.56074853	−5.53356094	−5.50851281	−5.48538894
(2,3)	−14.1231970	−10.0493354	−8.60891598	−7.85228324

where

$$A=\frac{\varepsilon+\beta D_e}{4\alpha^2\hbar^2c^2}-\frac{\beta D_e}{2\alpha^2\hbar^2c^2}(\cosh^2(\alpha r_e)+\cosh(\alpha r_e)\sinh(\alpha r_e)) \tag{34}$$

$$B=\frac{\beta D_e-\varepsilon}{2\alpha^2\hbar^2c^2}-\ell(\ell+1) \tag{35}$$

$$C=\frac{\varepsilon-\beta D_e}{4\alpha^2\hbar^2c^2}+\frac{\beta D_e}{2\alpha^2\hbar^2c^2}(\cosh(\alpha r_e)\sinh(\alpha r_e)-\sinh^2(\alpha r_e)) \tag{36}$$

Solving eq. 33 using the improved AIM, we obtain the relativistic energy spectrum equation for a relativistic spin-zero particle in the molecular Tietz potential as

$$4C+2B+(-1+2\sqrt{-C})(1+\sqrt{1-4C-4B-4A})+n(-4+4\sqrt{-C}-2\sqrt{1-4C-4B-4A})-2n(n-1)=0 \tag{37}$$

or more explicitly as

$$\frac{1}{\hbar^2c^2\alpha^2}\left\{\beta D_e(1-e^{-2\alpha r_e})+\hbar^2c^2\alpha^2\left[-2\ell(\ell+1)-2n^2+\left(-1+\sqrt{\frac{\epsilon-\beta D_e e^{-2\alpha r_e}}{\hbar^2c^2\alpha^2}}\right)\left(1+\sqrt{(2\ell+1)^2+\frac{4\beta D_e\sinh^2\alpha r_e}{\hbar^2c^2\alpha^2}}\right)-2n\left(1-\sqrt{\frac{\epsilon-\beta D_e e^{-2\alpha r_e}}{\hbar^2c^2\alpha^2}}+\sqrt{(2\ell+1)^2+\frac{4\beta D_e\sinh^2\alpha r_e}{\hbar^2c^2\alpha^2}}\right)\right]\right\}=0 \tag{38}$$

from which the energy eigenvalues for the Klein–Gordon equation with the molecular Tietz potential can be obtained. The wave function is also obtained as

$$u_{n\ell}=N_n e^{-2\alpha r\sqrt{-C}}(1-e^{-2\alpha r})^{\frac{1}{2}+\sqrt{-B-C-A+\frac{1}{4}}}\frac{\Gamma(n+2\sqrt{-C}+1)}{n!\Gamma(1+2\sqrt{-C})}\times{}_2F_1\left(-n,n+2\sqrt{-C}+2\sqrt{-B-C-A+\frac{1}{4}}+1;2\sqrt{-C}+1;e^{-2\alpha r}\right) \tag{39}$$

where N_n is the normalization constant. By varying the dissociation energy, we obtain the relativistic energy spectrum for various n and ℓ in Table 3. Let us now obtain the nonrelativistic limit of eq. 37. In the nonrelativistic limit, we set $\frac{E_R^2-\mu^2c^4}{\hbar^2c^2}\to\frac{2\mu E_{NR}}{\hbar^2}$ and $\frac{E_R+\mu c^2}{\hbar^2c^2}\to\frac{2\mu}{\hbar^2}$; thus, eq. 32 is readily transformed to

$$\frac{d^2R_{n\ell}(r)}{dr^2} + \frac{2\mu}{\hbar^2}\left\{E_{n\ell} - D_e\cosh^2(\alpha r_e) + 2D_e\cosh(\alpha r_e)\sinh(\alpha r_e)\coth(\alpha r) - D_e\sinh^2(\alpha r_e)\coth^2(\alpha r) - \frac{\hbar^2\alpha^2\ell(\ell+1)}{2\mu\sinh^2(\alpha r)}\right\}R_{n\ell}(r) = 0 \quad (40)$$

which essentially coincides with eq. 15. Similarly, the wave function eq. 39 is transformed into eq. 28.

Conclusion

We have obtained the approximate analytical solutions of the nonrelativistic and relativistic molecular Tietz potential using the improved asymptotic iteration method. By using a Greene–Aldrich approximation scheme, we obtained the energy eigenvalues and wave functions for all orbital quantum numbers ℓ. Our results are compared with some existing ones and we found that they are in good agreement. We also obtained the rotational-vibrational energy spectrum for a few selected diatomic molecules by using various dissociation energies D_e, equilibrium intermolecular separations r_e, and a range of potential α. We also obtained the bound state solution of the relativistic Klein–Gordon equation in the presence of this potential. We also studied the effect of the dissociation energy on the relativistic energy spectrum. The energy spectrum increased with an increment in dissociation energy except for the *s*-wave case where $E_{n,0}(D_e) \approx E_{n,0}(D_e + 0.2)$. The nonrelativistic limit has also been discussed. In this limit, it was found that the result obtained for the Klein–Gordon system converges to that of the Shrödinger system. Finally, because of the accuracy and simplicity of the elegant method presented in this study, we recommend its application in finding bound state solutions of some other model potentials.

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