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The nonrelativistic molecular Tietz potential

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Abstract: We solve the 3-dimensional Schrödinger equation under the Tietz potential by an approximate analytical scheme. A Pekeris-type approximation and the Nikiforov–Uvarov technique are used in the calculations to report the arbitrary-state eigenfunctions and eigenvalues and we calculate some useful expectation values of the Tietz potential using the Hellmann–Feynman theorem and obtain the oscillator strength.

Key words: Schrödinger equation (SE), Tietz potential, Nikiforov–Uvarov (NU) method, oscillator strength

PACS: 21.60.Cs, 03.65.Ge, 02.30.Gp, 24.10.Ht.

1. Introduction

There is a rather lengthy list of potentials that can account for the observed experimental data in physical sciences. In the 3-dimensional cases, most of these potentials cannot be analytically solved unless an approximation is used. Within the approximate schemes, the Pekeris-type ones, which relate the exponential-type terms to inverse or inverse square ones (and vice versa), are frequently used due to their acceptable nature. Such approximations have been applied to almost all wave equations of quantum mechanics including the Schrödinger [1–7], Dirac [8], Klein–Gordon [9,10], Duffin–Kemmer–Petiau [11,12], and spinless Salpeter equations [13].

In addition, depending on the potential under consideration, various analytical tools have been used. The common methodologies include supersymmetry quantum mechanics (SUSYQM) [14–17], the Nikiforov–Uvarov (NU) technique [18–23], ansatz solution [24,25], iteration method [26 and references therein] etc. Our aim is to investigate the Schrödinger equation under the Tietz potential [27,28]. This potential resembles Eckart or Möbius potentials for certain conditions [28].

2. Schrödinger equation (SE)

We start from the radial Schrödinger equation [16]

$$\frac{-\hbar^2}{2m} \left(\frac{d^2}{dr^2} + \frac{2}{r} \frac{d}{dr} \right) R_{nl} + \left(V(r) + \frac{\hbar^2 l(l+1)}{2mr^2} \right) R_{nl} = E_{nl} R_{nl}, \quad (1)$$

where m , $E_{n,l}$, $V(r)$, and l respectively stand for the mass, energy, potential, and angular momentum. Using the transformation $R_{nl} = \frac{U_{nl}(r)}{r}$ the radial equation appears as [16]

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$$\frac{d^2 U_{nl}(r)}{dr^2} = \frac{-2m}{\hbar^2} (E_{nl} - V(r) - \frac{\hbar^2 l(l+1)}{2mr^2}) U_{nl}(r), \quad (2)$$

Substitution of the Tietz potential

$$V(r) = V_0 \left(\frac{\sinh(\frac{r-r_0}{a})}{\sinh(\frac{r}{a})} \right)^2, \quad (3)$$

brings us to

$$\frac{d^2 U_{nl}(r)}{dr^2} = \frac{-2m}{\hbar^2} (E_{nl} - V_0 \left(\frac{\sinh(\alpha r) \cosh(\alpha r_0) - \cosh(\alpha r) \sinh(\alpha r_0)}{\sinh(\alpha r)} \right)^2 - \frac{\hbar^2 l(l+1)}{2mr^2}) U_{nl}(r), \quad (4)$$

or, alternatively,

$$\frac{d^2 U_{nl}(r)}{dr^2} = \frac{-2m}{\hbar^2} \left\{ E_{nl} - V_0 (\cosh(\alpha r_0) - \sinh(\alpha r_0) \coth(\alpha r))^2 - \frac{\hbar^2 l(l+1)}{2mr^2} \right\} U_{nl}(r). \quad (5)$$

The latter cannot be exactly solved. Thus, we use the approximation [2]

$$\frac{1}{r^2} \approx \frac{\alpha^2}{\sinh^2(\alpha r)} = \alpha^2 \operatorname{csc}^2 h^2(\alpha r), \quad (6)$$

where $\alpha = \frac{1}{a}$. We plotted the approximation in Figure 1 to compare the behavior of both sides. Figure 2 depicts the Tietz potential for various α s. Replacing the centrifugal term in Eq. (5) by the above Pekeris-type approximation gives

$$\begin{aligned} \frac{d^2 U_{nl}(r)}{dr^2} + \frac{2m}{\hbar^2} \left\{ E_{nl} - V_0 \cosh^2(\alpha r_0) - V_0 \sinh^2(\alpha r_0) - V_0 \sinh^2(\alpha r_0) \operatorname{csc}^2 h^2(\alpha r) \right. \\ \left. + 2V_0 \cosh(\alpha r_0) \sinh(\alpha r_0) \coth(\alpha r) - \frac{\hbar^2 \alpha^2 l(l+1)}{2m} \operatorname{csc}^2 h^2(\alpha r) \right\} U_{nl}(r) = 0. \end{aligned} \quad (7)$$

In the next section, we briefly review the NU method.

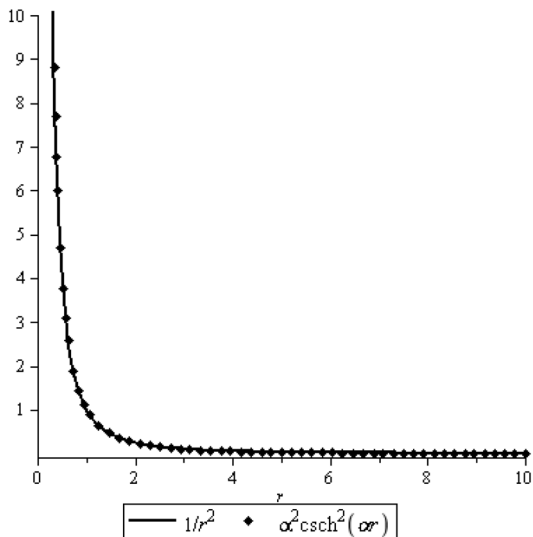


Figure 1. $\frac{1}{r^2}$ and its approximation for $\alpha = 0.01$.

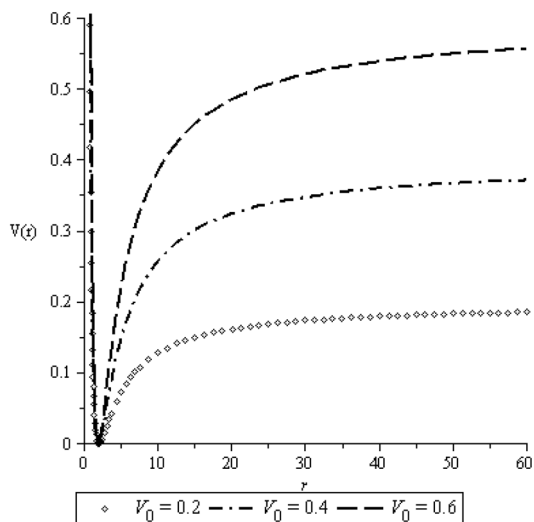


Figure 2. The Tietz potential for $\alpha = 0.01$, $r_0 = 2$.

3. The NU method

By the NU method [18–23], the solutions of

$$\left\{ \frac{d^2}{ds^2} + \frac{\alpha_1 - \alpha_2 s}{s(1 - \alpha_3 s)} \frac{d}{ds} + \frac{1}{[s(1 - \alpha_3 s)]^2} [-\xi_1 s^2 + \xi_2 s - \xi_3] \right\} \psi = 0, \quad (8)$$

are [23]

$$\psi(s) = s^{\alpha_{12}} (1 - \alpha_3 s)^{-\alpha_{12} - \frac{\alpha_{13}}{\alpha_3}} P_n^{(\alpha_{10}-1, \frac{\alpha_{11}}{\alpha_3} - \alpha_{10}-1)}(1 - 2\alpha_3 s), \quad (9)$$

where

$$\alpha_2 n - (2n + 1)\alpha_5 + (2n + 1)(\sqrt{\alpha_9} + \alpha_3 \sqrt{\alpha_8}) + n(n - 1)\alpha_3 + \alpha_7 + 2\alpha_3 \alpha_8 + 2\sqrt{\alpha_8 \alpha_9} = 0, \quad (10)$$

$$\alpha_4 = \frac{1}{2}(1 - \alpha_1), \quad \alpha_5 = \frac{1}{2}(\alpha_2 - 2\alpha_3), \quad \alpha_6 = \alpha_5^2 + \xi_1, \quad \alpha_7 = 2\alpha_4 \alpha_5 - \xi_2, \quad \alpha_8 = \alpha_4^2 + \xi_3$$

$$\alpha_9 = \alpha_3 \alpha_7 + \alpha_3^2 \alpha_8 + \alpha_6, \quad \alpha_{10} = \alpha_1 + 2\alpha_4 + 2\sqrt{\alpha_8},$$

$$\alpha_{11} = \alpha_2 - 2\alpha_5 + 2(\sqrt{\alpha_9} + \alpha_3 \sqrt{\alpha_8}), \quad \alpha_{12} = \alpha_4 + \sqrt{\alpha_8}, \quad \alpha_{13} = \alpha_5 - (\sqrt{\alpha_9} + \alpha_3 \sqrt{\alpha_8}). \quad (11)$$

In the rather more special case of $\alpha_3 = 0$,

$$\lim_{\alpha_3 \rightarrow 0} P_n^{(\alpha_{10}-1, \frac{\alpha_{11}}{\alpha_3} - \alpha_{10}-1)}(1 - 2\alpha_3 s) = L_n^{\alpha_{10}-1}(\alpha_{11} s), \quad (12a)$$

$$\lim_{\alpha_3 \rightarrow 0} (1 - \alpha_3 s)^{-\alpha_{12} - \frac{\alpha_{13}}{\alpha_3}} = e^{\alpha_{13} s}, \quad (12b)$$

and, from Eq. (9), we find for the wavefunction

$$\psi = s^{\alpha_{12}} e^{\alpha_{13} s} L_n^{\alpha_{10}-1}(\alpha_{11} s), \quad (13)$$

4. Exact solution of the Schrödinger equation

If we write Eq. (7) as

$$\begin{aligned} \frac{d^2 U_{nl}(r)}{dr^2} + \left\{ \frac{2mE_{nl}}{\hbar^2} - \frac{2mV_0}{\hbar^2} \cosh^2(\alpha r_0) - \frac{2mV_0}{\hbar^2} \sinh^2(\alpha r_0) - \frac{8mV_0 \sinh^2(\alpha r_0) e^{-2\alpha r}}{\hbar^2 (1 - e^{-2\alpha r})^2} \right. \\ \left. + \frac{4mV_0}{\hbar^2} \cosh(\alpha r_0) \sinh(\alpha r_0) \left(\frac{1 + e^{-2\alpha r}}{1 - e^{-2\alpha r}} \right) - \frac{4\alpha^2 l(l+1) e^{-2\alpha r}}{(1 - e^{-2\alpha r})^2} \right\} U_{nl}(r) = 0, \end{aligned} \quad (14)$$

and apply the transformation $z = e^{-2\alpha r}$, we find

$$\frac{d^2 U_{nl}(z)}{dz^2} + \frac{(1-z)}{z(1-z)} \frac{dU_{nl}(z)}{dz} + \frac{1}{(z(1-z))^2} (kz^2 + Lz + f) U_{nl}(z) = 0, \quad (15)$$

where

$$k = \frac{mE_{nl}}{2\alpha^2 \hbar^2} - \frac{mV_0}{2\alpha^2 \hbar^2} \cosh^2(\alpha r_0) - \frac{mV_0}{2\alpha^2 \hbar^2} \sinh^2(\alpha r_0) - \frac{mV_0}{\alpha^2 \hbar^2} \cosh(\alpha r_0) \sinh(\alpha r_0), \quad (16a)$$

$$L = -\frac{mE_{nl}}{\alpha^2 \hbar^2} + \frac{mV_0}{\alpha^2 \hbar^2} \cosh^2(\alpha r_0) + \frac{mV_0}{\alpha^2 \hbar^2} \sinh^2(\alpha r_0) - \frac{2mV_0}{\alpha^2 \hbar^2} \sinh^2(\alpha r_0) - l(l+1), \quad (16b)$$

$$f = \frac{mE_{nl}}{2\alpha^2\hbar^2} - \frac{mV_0}{2\alpha^2\hbar^2} \cosh^2(\alpha r_0) - \frac{mV_0}{2\alpha^2\hbar^2} \sinh^2(\alpha r_0) + \frac{mV_0}{\alpha^2\hbar^2} \cosh(\alpha r_0) \sinh(\alpha r_0), \quad (16c)$$

By comparing Eq. (16) with Eq. (11), we find

$$\begin{aligned} \alpha_1 = 1, \alpha_2 = 1, \alpha_3 = 1, \xi_1 = -k, \xi_2 = L, \xi_3 = -f, \\ \alpha_4 = 0, \alpha_5 = -\frac{1}{2}, \alpha_6 = \frac{1}{4} + \xi_1, \alpha_7 = -\xi_2, \alpha_8 = \xi_3, \alpha_9 = -\xi_2 + \xi_3 + \xi_1 + \frac{1}{4}, \\ \alpha_{10} = 1 + 2\sqrt{\xi_3}, \alpha_{11} = 2 + 2(\sqrt{-\xi_2 + \xi_3 + \xi_1 + \frac{1}{4}} + \sqrt{\xi_3}), \\ \alpha_{12} = \sqrt{\xi_3}, \alpha_{13} = -\frac{1}{2} - (\sqrt{-\xi_2 + \xi_3 + \xi_1 + \frac{1}{4}} + \sqrt{\xi_3}). \end{aligned} \quad (17)$$

Thus, by putting Eq. (17) in Eq. (10), we find

$$\begin{aligned} n + \frac{(2n+1)}{2} + (2n+1)(\sqrt{-\xi_2 + \xi_3 + \xi_1 + \frac{1}{4}} + \sqrt{\xi_3}) + n(n-1) - \xi_2 + 2\xi_3 \\ + 2\sqrt{-\xi_2\xi_3 + \xi_3^2 + \xi_1\xi_3 + \frac{\xi_3}{4}} = 0. \end{aligned} \quad (18)$$

The energy is plotted vs. the potential coefficient and mass in Figures 3 and 4. The Table contains numerical values of the energy for various states. Moreover, we compared our results by numerical method. The wavefunction, from Eq. (17) and Eq. (9), is then simply written as

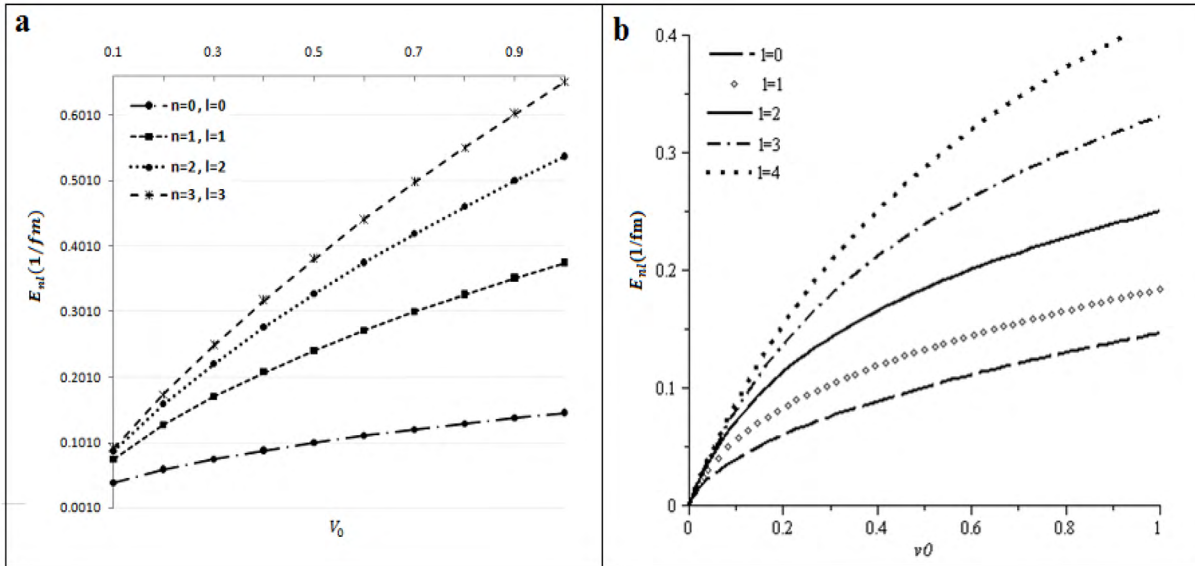


Figure 3. a) Energy vs. V_0 for $m = 5fm^{-1}$, $r_0 = 2$, $\alpha = 0.01$, $\hbar = 1$. b) Energy vs. V_0 for $n = 0$, $m = 5fm^{-1}$, $r_0 = 2$, $\alpha = 0.01$, $\hbar = 1$.

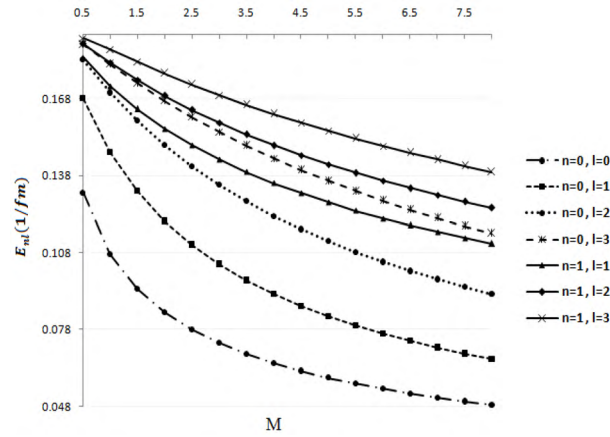


Figure 4. Energy vs. M for $V_0 = 0.2$, $r_0 = 2$, $\alpha = 0.01$, $\hbar = 1$.

Table. Eigenvalues of bound states for Tietz potential for $\alpha = 0.01$, $M = 5 fm^{-1}$, $r_0 = 2$, $\hbar = 1$.

| $ n, l\rangle$ | $E_{nl}(fm^{-1})$ | | | |
|----------------|-------------------|--|-------------|--|
| | $V_0 = 0.2$ | Numerical results before any approximation for $V_0 = 0.2$ | $V_0 = 0.4$ | Numerical results before any approximation for $V_0 = 0.4$ |
| $ 0, 0\rangle$ | 0.059294 | 0.059294 | 0.088263 | 0.088263 |
| $ 0, 1\rangle$ | 0.083196 | 0.083203 | 0.118925 | 0.118932 |
| $ 0, 2\rangle$ | 0.112385 | 0.112405 | 0.164796 | 0.164816 |
| $ 0, 3\rangle$ | 0.135879 | 0.135919 | 0.210629 | 0.210669 |
| $ 1, 0\rangle$ | 0.116235 | 0.116235 | 0.190727 | 0.190727 |
| $ 1, 1\rangle$ | 0.127523 | 0.127529 | 0.207801 | 0.207808 |
| $ 1, 2\rangle$ | 0.142351 | 0.142371 | 0.234273 | 0.234293 |
| $ 1, 3\rangle$ | 0.155334 | 0.155374 | 0.261993 | 0.262033 |
| $ 2, 0\rangle$ | 0.144408 | 0.144408 | 0.249787 | 0.249787 |
| $ 2, 1\rangle$ | 0.150593 | 0.150599 | 0.260242 | 0.260249 |
| $ 2, 2\rangle$ | 0.159111 | 0.159131 | 0.276865 | 0.276885 |
| $ 2, 3\rangle$ | 0.167001 | 0.167040 | 0.2948702 | 0.294910 |
| $ 3, 0\rangle$ | 0.160332 | 0.160332 | 0.286861 | 0.286861 |
| $ 3, 1\rangle$ | 0.164068 | 0.164074 | 0.293713 | 0.293720 |
| $ 3, 2\rangle$ | 0.169384 | 0.169405 | 0.304811 | 0.304831 |
| $ 3, 3\rangle$ | 0.174507 | 0.174573 | 0.317141 | 0.317118 |

$$U_{nl}(r) = N_{nl} e^{-2\alpha r \sqrt{\xi_3}} (1 - e^{-2\alpha r})^{\frac{1}{2} + (\sqrt{-\xi_2 + \xi_3 + \xi_1 + \frac{1}{4}})} P_n^{(2\sqrt{\xi_3}, 2\sqrt{-\xi_2 + \xi_3 + \xi_1 + \frac{1}{4}})} (1 - 2e^{-2\alpha r}), \quad (19)$$

where [18]

$$P_n^{(A,B)}(1 - 2x) = \frac{\Gamma(n + 1 + A)}{n! \Gamma(1 + A)} {}_2F_1(-n, n + A + B + 1; A + 1; x). \quad (20)$$

Therefore, Eq. (19) can be written more neatly as

$$U_{nl}(r) = e^{-2\alpha r \sqrt{\xi_3}} (1 - e^{-2\alpha r})^{\frac{1}{2} + (\sqrt{-\xi_2 + \xi_3 + \xi_1 + \frac{1}{4}})} \frac{\Gamma(n + 1 + 2\sqrt{\xi_3})}{n! \Gamma(1 + 2\sqrt{\xi_3})}$$

$${}_2F_1\left(-n, n + 2\sqrt{\xi_3} + 2\sqrt{-\xi_2 + \xi_3 + \xi_1 + \frac{1}{4}} + 1; 2\sqrt{\xi_3} + 1; e^{-2\alpha r}\right). \quad (21)$$

The wavefunction for 3 states is plotted in Figure 5. We now calculate some expectation values of the Tietz potential using the Hellmann–Feynman theorem (HFT) [29,30]. Assuming that the Hamiltonian H for a particular quantum system is a function of some parameters q , and denoting the eigenvalues and eigenfunctions of H , respectively, by $E_{n,l}(q)$ and $U_{n,l}(q)$, theoretically we have

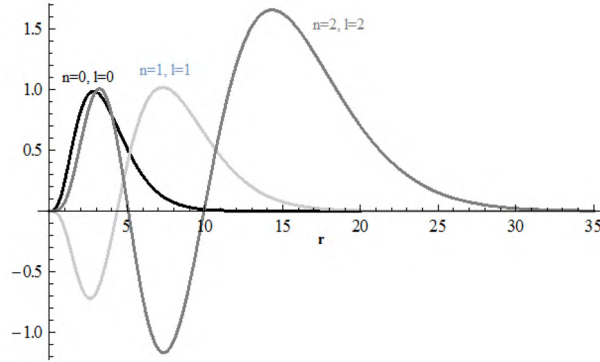


Figure 5. Wavefunction for $V_0 = 0.2$, $m = 5fm^{-1}$, $r_0 = 2$, $\alpha = 0.01$, $\hbar = 1$

$$\frac{\partial E_{n,l}(q)}{\partial q} = \left\langle U_{n,l}(q) \left| \frac{\partial H(q)}{\partial q} \right| \right\rangle, \quad (22)$$

The effective Hamiltonian of the hyper-radial function is given as

$$H = \frac{-\hbar^2}{2m} \frac{d^2}{dr^2} + \frac{\hbar^2}{2m} \frac{l(l+1)}{r^2} + V(r), \quad (23a)$$

or

$$H = \frac{-\hbar^2}{2m} \frac{d^2}{dr^2} + \frac{\hbar^2}{2m} \frac{l(l+1)}{r^2} + V_0 [\cosh(\alpha r_0) - \sinh(\alpha r_0) \coth(\alpha r)]^2, \quad (23b)$$

In order to calculate $\langle [\cosh(\alpha r_0) - \sinh(\alpha r_0) \coth(\alpha r)]^2 \rangle$, we set $q = V_0$ such that

$$\frac{\partial E_{n,l}(V_0)}{\partial V_0} = \langle U_{n,l}(V_0) | \frac{\partial H(V_0)}{\partial V_0} | U_{n,l}(V_0) \rangle = \langle [\cosh(\alpha r_0) - \sinh(\alpha r_0) \coth(\alpha r)]^2 \rangle, \quad (24)$$

Figures 6–9 show the behavior of $\langle [\cosh(\alpha r_0) - \sinh(\alpha r_0) \coth(\alpha r)]^2 \rangle$ versus α , M , V_0 , r_0 for some values of n and l .

Let us now use the results to calculate the oscillator strength. The strength of the change can be declared via a dimensionless quantity named oscillator strength P_{fi} . A transition from a lower state ψ_i to an upper state ψ_f is [31]

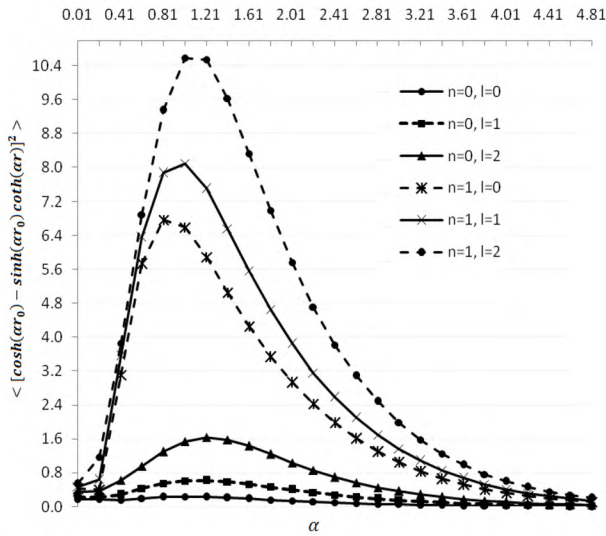


Figure 6. Behavior of $\langle [\cosh(\alpha r_0) - \sinh(\alpha r_0) \coth(\alpha r)]^2 \rangle$ versus α for some values of n, l . For $V_0 = 0.2$, $m = 5 fm^{-1}$, $r_0 = 2$, $\hbar = 1$.

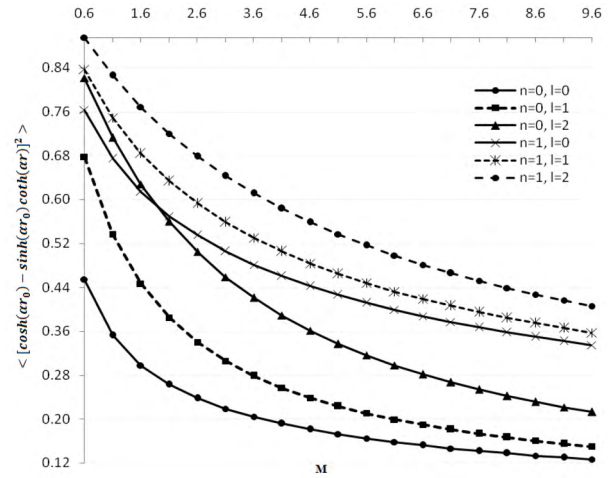


Figure 7. Behavior of $\langle [\cosh(\alpha r_0) - \sinh(\alpha r_0) \coth(\alpha r)]^2 \rangle$ versus M for some values of n, l . For $\alpha = 0.01$, $V_0 = 0.2$, $r_0 = 2$, $\hbar = 1$.

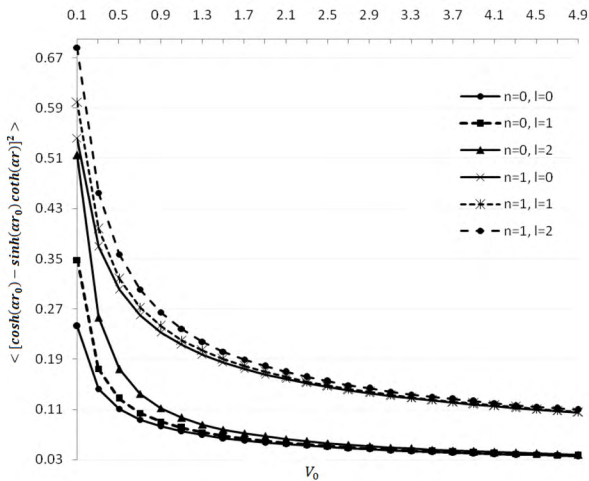


Figure 8. Behavior of $\langle [\cosh(\alpha r_0) - \sinh(\alpha r_0) \coth(\alpha r)]^2 \rangle$ versus V_0 for some values of n, l . For $\alpha = 0.01$, $m = 5$, $r_0 = 2$, $\hbar = 1$.

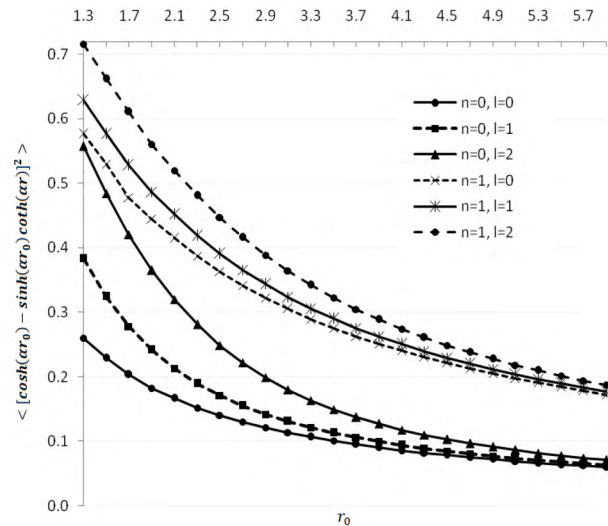


Figure 9. Behavior of $\langle [\cosh(\alpha r_0) - \sinh(\alpha r_0) \coth(\alpha r)]^2 \rangle$ versus r_0 for some values of n, l . For $\alpha = 0.01$, $V_0 = 0.2$, $m = 5$, $\hbar = 1$.

$$P_{fi} = \frac{2}{3}(E_f - E_i) |M_{fi}|^2. \quad (25)$$

where $M_{fi} = \langle \psi_i | R | \psi_f \rangle$ is the electric dipole moment of the transition. The oscillator strength gives additional information on the fine structure and selection rules of the optical absorption [32]. This quantity is in many cases an important part of scientific reports [33,34]. In Figure 10 we present the variation of the oscillator strength as a function of the coefficient V_0 . The fluctuation in the diagram is due to the numerical inaccuracy.

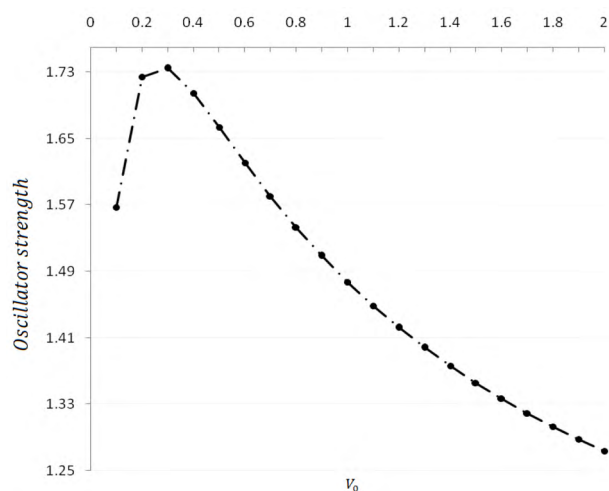


Figure 10. Variation in the oscillator strength versus the coefficient V_0 . For $\alpha = 0.01$, $x_0 = 2$, $m = 1$, $\hbar = 1$.

5. Conclusion

As the Schrödinger equation can be used for any particle, regardless of its spin, we considered this equation. For the potential, we picked the Tietz potential, which resembles the Eckart potential, and therefore is a useful molecular interaction. In contrast to most physical potentials, which have been investigated by more than one technique, the Tietz potential in its present form has not been investigated (at least to our knowledge). Instead of the rather vague and cumbersome numerical procedures, we used a Pekeris-type approximation, which looks quite logical. In our final step, using the established NU method, we reported the solutions of the system for an arbitrary quantum number. We obtained some useful expectation values via Feynman–Hellmann theorem as well as the oscillator strength. Our results can be used in related fields provided that the appropriate fits are executed. As we could not find a paper to make a comparison, we have included some numerical data for probable further studies.

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