Path integral discussion of the improved Tietz potential

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Abstract

An improved form of the Tietz potential for diatomic molecules is discussed in detail within the path integral formalism. The radial Green’s function is rigorously constructed in a closed form for different shapes of this potential. For \( |q| \leq 1 \), and \( \frac{1}{2\beta} \ln |q| < r < +\infty \), the energy spectrum and the normalized wave functions of the bound states are derived for the \( l \) waves. When the deformation parameter \( q \) is \( 0 < |q| < 1 \) or \( q > 0 \), it is found that the quantization conditions are transcendental equations that requires numerical solutions. In the limit \( q \to 0 \), the energy spectrum and the corresponding wave functions for the radial Morse potential are recovered.

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1 Introduction

As an advantageous alternative to the Morse potential for fitting certain diatomic interactions potential energy curves, Tietz \[1\] suggested, in 1963, a potential energy function given by

\[
U(r) = D e \left[ 1 + \frac{(a + b) e^{-2\beta r} - be^{-\beta r}}{(1 + ce^{-\beta r})^2} \right]
\]

which continues to stimulate numerous theoretical works \[2\] \[13\] made within the framework of various algebraic methods. In 2012, Jia et al \[14\] proposed an improved version of this potential having the form:

1
\[ V_T(r) = D_e \left( 1 - \frac{e^{2\alpha r_e} + q}{e^{2\alpha r} + q} \right)^2, \]  

in which \( D_e \) denotes the dissociation energy of the diatomic molecule, \( r_e \) is the equilibrium bond length, \( \alpha^{-1} \) is the range of the potential and \( q \) is a real deformation parameter. The introduction of the parameter \( q \) can serve as an additional parameter in describing inter-atomic interactions, and especially in three-dimensional problems, it allows to establish the center of mass location of a molecule at a certain distance from the coordinate origin. This potential has received a considerable attention immediately afterwards. The equivalence between the deformed Rosen-Morse potential and the Tietz potential for diatomic molecules has been studied \[15,16\]. Note also that the improved Tietz potential and the modified Rosen-Morse potential have been investigated from different points of view in these last years \[17–21\]. Another interesting case, which despite appearances, presents some kinship with the potentials above is the new deformed Schöberg-type potential introduced by Mustafa \[22\] to calculate the ro-vibrational energy levels of some diatomic molecules in the context of the supersymmetric quantum mechanics. This potential has also been discussed in an approach based on the Feynman path integral \[23\].

The potential function \( V_T \) contains three kinds of potentials namely the deformed modified Manning-Rosen potential \[24\] for \( q < 0 \), the deformed modified Rosen-Morse potential \[25\] when \( q > 0 \) and the Morse potential \[26\] at the limit \( q \to 0 \). Therefore, it is clear that the parameter \( q \) will have an influence on the form of the solutions of the problem. For \( q \neq 0 \), we will consider each case separately using the path integral method.

Our paper is organized as follows. In section 2, we shortly formulate the path integral for the Green’s function associated with the spherically symmetric potential \( V_T(r) \). In section 3, we examine the problem for \( q < 0 \) by distinguishing two cases: \( q \leq -1 \) and \(-1 < q < 0 \). When \( q \leq -1 \) and \( \frac{1}{2\alpha} \ln |q| < r < +\infty \), we calculate the radial Green’s function associated with the deformed modified Manning-Rosen potential for a state of orbital momentum \( l \) by using a proper approximation to the centrifugal potential term to find the energy spectrum and the normalized wave functions. For \(-1 < q < 0 \), the \(|q|\)–deformed Manning-Rosen potential is converted into the standard Manning-Rosen potential defined in the half-space \( \xi > \frac{1}{2\alpha} \ln |q| \). Following the procedure used in our earlier works \[27,29\], it is then fairly simple to write down the radial Green’s function for the \( s \)–waves in a closed form and deduce from it a transcendental equation for the energy levels and the non-normalized wave functions. In section 4, the potential \( V_T \), for \( q > 0 \), is worked out in a similar way. We first transform it into a \( q \)–deformed modified Rosen-Morse potential and consequently into the standard Rosen-Morse potential defined in the half-space \( u > \frac{1}{2\alpha} \ln q \). We construct the radial Green’s function in a closed form from which we also obtain a transcendental equation for the \( s \)–state energy levels and the non-normalized wave functions. In the limit \( q \to 0 \), we recover the results of the radial Morse potential problem for the Green’s function, energy spectrum and wave functions.
in section 5. In section 6, we briefly discuss some special cases and compare our results with those given in the literature by other authors. Section 7 will be a conclusion.

## 2 Green’s function

The energy-dependent Green’s function for a particle of mass $M$, moving in the potential $V(r)$ can be expanded into partial waves \cite{30} in spherical coordinates

$$G(r'', r'; E) = \frac{1}{r'' r'} \sum_{l=0}^{\infty} \frac{2l + 1}{4\pi} G_l(r'', r'; E) P_l(\cos \Theta), \quad (3)$$

in which the radial Green’s function is given by

$$G_l(r'', r'; E) = \int_0^\infty dt \exp \left( \frac{i}{\hbar} E T \right) \langle r'' | \exp \left( -\frac{i}{\hbar} \hat{H}_l T \right) | r' \rangle, \quad (4)$$

and $P_l(\cos \Theta)$ is the Legendre polynomial of degree $l$ in $\cos \Theta = \frac{r''_1 - r'_1}{r'' r'} = \cos \theta'' \cos \theta' + \sin \theta'' \sin \theta' \cos (\phi'' - \phi')$. The Hamiltonian operator $\hat{H}_l$ is defined by

$$\hat{H}_l = \frac{\hat{P}_r^2}{2M} + \frac{\hbar^2 l(l + 1)}{2Mr^2} + V_T(r), \quad (5)$$

where $\hat{P}_r = -i\hbar (\partial / \partial r) r$ is the radial momentum operator.

In the path integral formalism, the integrand $\langle r'' | \exp \left( -\frac{i}{\hbar} \hat{H}_l T \right) | r' \rangle$ is explicitly given by the Hamiltonian path integral,

$$\langle r'' | \exp \left( -\frac{i}{\hbar} \hat{H}_l T \right) | r' \rangle = \lim_{N \to \infty} \prod_{n=1}^{N} \left[ \int dr_n \prod_{n=1}^{N+1} \left[ \int d(P_r)_n \right] \right] \times \exp \left\{ \frac{i}{\hbar} \sum_{n=1}^{N+1} \mathcal{A}_n \right\}, \quad (6)$$

where the short-time action is

$$\mathcal{A}_n = (P_r)_n \Delta r_n - \varepsilon \left( \frac{(P_r)_n^2}{2M} + \frac{\hbar^2 l(l + 1)}{2Mr_n^2} + V_T(r_n) \right). \quad (7)$$

Note that $(P_r)_n = P_r(t_n)$, $r_n = r(t_n)$, $\Delta r_n = r_n - r_{n-1}$, $\varepsilon = t_n - t_{n-1}$ and $T = (N + 1) \varepsilon$. The momentum integrations can be carried out and we obtain
the Lagrangian path integral,
\[
\langle r''| \exp \left( -\frac{i}{\hbar} \hat{H}T \right) |r' \rangle = \lim_{N \to \infty} \left( \frac{M}{2\pi \hbar \varepsilon} \right)^{\frac{N+1}{2}} \prod_{n=1}^{N} \left[ \int dr_n \right] 
\times \exp \left\{ \frac{i}{\hbar} \sum_{n=1}^{N+1} \left[ \frac{M}{2\varepsilon} \left( \Delta r_n \right)^2 - \varepsilon \left( \frac{\hbar^2 l(l + 1)}{2Mr_n^2} + V_T(r_n) \right) \right] \right\}.
\]
(8)

To construct the radial Green’s function for \( V_T(r) \) via (4) in terms of the path integral formalism \[31\], three cases may be distinguished according to the real values of the parameter \( q \).

3 Deformed modified Manning-Rosen potential

When the deformation parameter \( q \) is negative, the improved Tietz potential is equivalent to the deformed modified Manning-Rosen potential

\[
V_{|q|}(r) = U_0 - U_1 \coth_{|q|}(ar) + U_2 \coth_{|q|}^2(ar),
\]
where \( U_0, U_1 \) and \( U_2 \) are the real constants given by

\[
\begin{align*}
U_0 &= D_e \left( \frac{e^{2ar_{|q|}}}{|q|} + 1 \right)^2, \\
U_1 &= D_e \left( \frac{e^{2ar_{|q|}}}{|q|} + 1 \right) \left( \frac{e^{2ar_{|q|}}}{|q|} - 1 \right), \\
U_2 &= D_e \left( \frac{e^{2ar_{|q|}}}{|q|} - 1 \right)^2.
\end{align*}
\]
(10)

The potential (9) is obtained by using a \( q \)-deformation of the usual hyperbolic functions denoted by

\[
\sinh_q x = \frac{e^x - q e^{-x}}{2}, \quad \cosh_q x = \frac{e^x + q e^{-x}}{2}, \quad \tanh_q x = \frac{\sinh_q x}{\cosh_q x}, \quad \coth_q x = \frac{\cosh_q x}{\sinh_q x}.
\]
(11)

These functions have been introduced for first time by Arai \[32\], with the real parameter \( q > 0 \). The deformation parameter \( q \) can be extended to the cases of \( q < 0 \) and the complex number \[33\].

Now, the energy-dependent Green’s for the deformed modified Manning-Rosen potential is given by

\[
G_{i|q|}^{\prime|q|}(r'', r'; E) = \int_0^\infty dT \exp \left( \frac{i}{\hbar} ET \right) K_{i|q|}^{\prime|q|}(r'', r'; T),
\]
(12)

where the propagator \( K_{i|q|}^{\prime|q|}(r'', r'; T) \) is formally written as:

\[
K_{i|q|}^{\prime|q|}(r'', r'; T) = \int Dr(t) \exp \left\{ \frac{i}{\hbar} \int_0^T \left[ \frac{M}{2} r^2 - \left( \frac{\hbar^2 l(l + 1)}{2Mr^2} + V_{|q|}(r) \right) \right] dt \right\}.
\]
(13)
In order to evaluate (12), we have to distinguish two cases: \(|q| \geq 1\) and \(0 < |q| < 1\).

### 3.1 First case: \(|q| \geq 1\) and \(r_0 < r < \infty\)

When \(|q| \geq 1\), the potential (9) has a strong singularity at the point \(r_0 = \frac{1}{2\alpha r}\ln|q|\), creating an impenetrable barrier. In this case, there are two distinct regions, one is defined by the interval \([0, r_0]\) and the other by the interval \([r_0, \infty]\).

As in the first interval, the calculation of the Green’s function is without physical interest, we will construct the latter only in the second interval for a state of orbital momentum \(l\) by using the following approximation to deal with the centrifugal potential term [35]:

\[
\frac{1}{r^2} \approx C_0 + \frac{B_0}{e^{2\alpha r} - |q|} + \frac{A_0}{(e^{2\alpha r} - |q|)^2}, \quad \text{for} \quad \alpha r \ll 1 \quad \text{and} \quad |q| \geq 1, \tag{14}
\]

where \(C_0 = \frac{\alpha^2}{4}, B_0\) and \(A_0\) are two adjustable parameters. If we take \(C_0 = 0, B_0 = \frac{A_0}{|q|}, A_0 = \alpha^2 |q|^2\) and \(|q| = 1\), Eq. (14) is reduced to the approximation proposed by Greene and Aldrich [35].

With (14) and (11), the effective potential is written as:

\[
V_{\text{eff}}(r) = \frac{\hbar^2 l(l+1)}{2Mr^2} + V_{|q|}(r)
\approx V_0^l - V_1^l \coth|q|(\alpha r) + \frac{V_2^l}{\sinh^2|q|(\alpha r)}, \tag{15}
\]

where

\[
\begin{align*}
V_0^l &= \frac{\hbar^2 l(l+1)}{2M} \left[ C_0 + \frac{1}{2|q|} \left( \frac{A_0}{|q|} - B_0 \right) \right] + U_0 + U_2, \\
V_1^l &= \frac{\hbar^2 l(l+1)}{4M|q|} \left( \frac{A_0}{|q|} - B_0 \right) + U_0 + U_2, \\
V_2^l &= \frac{\hbar^2 l(l+1)}{8M|q|} + |q| U_2.
\end{align*}
\]

Then, changing \(\alpha r\) into \(\xi = \alpha r - \frac{1}{4} \ln|q|\) and \(\varepsilon\) into \(\alpha^{-2} \varepsilon_s\), we can rewrite the Green’s function (12) in the form

\[
G_{\xi, \xi'}^{|q| \geq 1}(r'', r'; E) = \frac{1}{\alpha} G_{MR}^{\xi, \xi'} (\xi'', \xi'; E_l), \tag{17}
\]

where

\[
G_{MR}^{\xi, \xi'} (\xi'', \xi'; E_l) = \int_0^\infty dS \exp \left( \frac{i}{\hbar} \frac{E_l}{\alpha^2} S \right) P_{MR}^l (\xi'', \xi'; S), \tag{18}
\]

with

\[
E_l = E - \left( U_0 + U_2 + \frac{\hbar^2 l(l+1)}{2M} \left[ C_0 + \frac{1}{2|q|} \left( \frac{A_0}{|q|} - B_0 \right) \right] \right), \tag{19}
\]

and

\[
P_{MR}^l (\xi'', \xi'; S) = \int D\xi(s) \exp \left\{ \frac{i}{\hbar} \int_0^S \left[ \frac{M}{2} \xi^2 - V_{MR}(\xi) \right] ds \right\}. \tag{20}
\]
We can thus write down the solution of (18) immediately in a closed form as:
\[ V_{MR}^l(\xi) = -\frac{V^l_1}{\alpha^2} \coth \xi + \frac{V^l_2}{\alpha^2 |q| \sinh^2 \xi} : \xi > 0, \]  
(21)
which has been discussed in the literature by means of the path integral \[36\].
Substituting (22) into (17) and going back to the old variable we get
\[ G_{||q|\geq 1}^{l,MR}(\xi'', \xi'; \tilde{E}_l) = -\frac{iM}{\hbar} \frac{\Gamma(M_1 - L_E) \Gamma(L_E + M_1 + 1)}{\Gamma(M_1 + M_2 + 1) \Gamma(M_1 - M_2 + 1)} \times \left( \frac{2}{\coth \xi' + 1 \coth \xi'' + 1} \right)^{M_2 + M_1 + 1} \times \left( \frac{\coth \xi' - 1 \coth \xi'' - 1}{\coth \xi' + 1 \coth \xi'' + 1} \right)^{M_2 - M_1} \times 2F_1 \left( \frac{M_1 - L_E, L_E + M_1 + 1, M_1 - M_2 + 1; \coth \xi'' - 1}{\coth \xi' + 1} \right) \times \frac{2}{\coth \xi'' + 1} \right), \]
(22)
where the symbols \( \xi'' \) and \( \xi' \) denote \( \max(\xi'', \xi') \) and \( \min(\xi'', \xi') \) respectively.
\( 2F_1(\alpha, \beta; \gamma; z) \) is the hypergeometric function and the quantities \( L_E, M_1 \) and \( M_2 \) are defined by
\[ \begin{align*}
L_E &= -\frac{1}{2} + \frac{1}{\sqrt{2}} \sqrt{\frac{2M}{\hbar^2}} (U_0 + U_1 + U_2 - E) + l(l + 1) \left( C_0 + \frac{A_0}{|q|} - \frac{B_0}{|q|^2} \right), \\
M_1 &= \delta_l + \frac{1}{2\alpha} \sqrt{\frac{2M}{\hbar^2}} (U_0 - U_1 + U_2 - E) + l(l + 1)C_0, \\
M_2 &= \delta_l - \frac{1}{2\alpha} \sqrt{\frac{2M}{\hbar^2}} (U_0 - U_1 + U_2 - E) + l(l + 1)C_0,
\end{align*} \]
(23)
with
\[ \delta_l = \frac{1}{2} \sqrt{1 + \frac{8MU_2}{\hbar^2 \alpha^2} + \frac{l(l + 1)}{\alpha^2 |q|^2}}. \]
(24)
Substituting (22) into (17) and going back to the old variable we get
\[ G_{||q|\geq 1}(r'', r'; E) = -\frac{iM}{\hbar \alpha} \frac{\Gamma(M_1 - L_E) \Gamma(L_E + M_1 + 1)}{\Gamma(M_1 + M_2 + 1) \Gamma(M_1 - M_2 + 1)} \times \left[ \left( 1 - |q| e^{-2\alpha' r'} \right) \left( 1 - |q| e^{-2\alpha'' r''} \right) \right]^{M_2 + M_1 + 1} \times \left[ \left| q \right|^2 e^{-2\alpha (r'' + r')} \right]^{\frac{M_2 - M_1}{2}} \times 2F_1 \left( M_1 - L_E, L_E + M_1 + 1, M_1 - M_2 + 1; |q| e^{-2\alpha r''} \right) \times 2F_1 \left( M_1 - L_E, L_E + M_1 + 1, M_1 + M_2 + 1; 1 - |q| e^{-2\alpha r'} \right). \]
(25)
The poles of the radial Green’s function (25) in the complex energy-plane corresponding to the bound states are all contained in the first gamma function in the numerator. From the condition

$$M_1 - L_E = -n_r, \quad n_r = 0, 1, 2, \ldots,$$

and after inserting the expressions of $L_E$ and $M_1$ in (23), we find the following expression for the vibrational and the rotational energy levels of the diatomic molecule that has the value $l$ of the orbital quantum number, and $n_r$ of the radial quantum number:

$$E_{n_r,l}^{[\geq 1]} = U_0 + U_2 + \frac{\hbar^2 l(l+1)}{2M} \left( \frac{A_0}{2|q|^2} - \frac{B_0}{2|q|} + C_0 \right) - \frac{\hbar^2 \alpha^2}{2M} \left( N_r^2 + \frac{\lambda^2}{N_r^2} \right),$$

(27)

where

$$N_r = n_r + \delta l + \frac{1}{2},$$

(28)

and

$$\lambda_l = \frac{MU_l}{\hbar^2 \alpha^2} + \frac{l(l+1)}{4\alpha^2} \left( \frac{A_0}{|q|^2} - \frac{B_0}{|q|} \right).$$

(29)

To obtain the reduced radial wave functions, we approximate the gamma function $\Gamma (M_1 - L_E)$ near the poles $M_1 - L_E = -n_r$ as follows:

$$\Gamma (M_1 - L_E) \approx \frac{(-1)^{n_r}}{n_r!} \frac{1}{M_1 - L_E + n_r}$$

$$= \frac{(-1)^{n_r+1}}{n_r!} \frac{\hbar^2 \alpha^2}{N_r M} \left( \frac{\Delta \alpha}{N_r} - N_r \right) \frac{E - E_{n_r,l}^{[\geq 1]}}{E},$$

(30)

and take into account the Gauss’s transformation formula (see Ref. 37, p. 1043, Eq. (9.131.2))

$$2F_1(a, b, c; z) = \frac{\Gamma(c)\Gamma(c - a - b)}{\Gamma(c - a)\Gamma(c - b)} 2F_1(a, b, a + b - c + 1; 1 - z)$$

$$+ \frac{\Gamma(c)\Gamma(a + b - c)}{\Gamma(a)\Gamma(b)} (1 - z)^{c-a-b} 2F_1(c - a, c - b, c - a - b + 1; 1 - z),$$

(31)

in which, in this case, the second term is null because the gamma function $\Gamma(a)$ is infinite ($a = M_1 - L_E = -n_r \leq 0$). Thus, we arrive at an expression in the form of a spectral expansion for the radial Green’s function (25),

$$G_{[\geq 1]}^{[\geq 1]}(r'', r', E) = i\hbar \sum_{n_r=0}^{n_{r_{\text{max}}}} \frac{\lambda_{n_r,l}^{[\geq 1]}(r'')\lambda_{n_r,l}^{[\geq 1]}(r')}{E - E_{n_r,l}^{[\geq 1]}},$$

(32)

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where the reduced (normalized) radial wave functions are given by
\[ \chi_{n_{r},l}^{|q| \geq 1}(r) = C_{n_{r},l} \left( 1 - |q| e^{-2\alpha r} \right)^{\delta_{l}+\frac{1}{2}} \left( |q| e^{-2\alpha r} \right)^{\frac{1}{2}} \left( \frac{\lambda_{l}}{N_{r}} - N_{r} \right) \times 2F_{1} \left( -n_{r}, \frac{\lambda_{l}}{N_{r}} + N_{r} - n_{r}, \frac{\lambda_{l}}{N_{r}} - N_{r} + 1; |q| e^{-2\alpha r} \right), \] (33)
with the correct normalization factor
\[ C_{n_{r},l} = \left[ \frac{\alpha}{N_{r}} \left( \frac{\lambda_{l}}{N_{r}} + N_{r} \right) \Gamma \left( \frac{\lambda_{l}}{N_{r}} + N_{r} - n_{r} \right) \Gamma \left( 1 + n_{r} + \frac{\lambda_{l}}{N_{r}} - N_{r} \right) \right]^{\frac{1}{2}}. \] (34)

Using the connecting formula (see Ref. [37], p.952, Eq. (8.406.1))
\[ P_{n}^{(\alpha,\beta)}(t) = \frac{\Gamma(n + \alpha + 1)}{n! \Gamma(\alpha + 1)} 2F_{1} \left( -n, n + \alpha + \beta + 1, \alpha + 1; \frac{1 - t}{2} \right), \] (35)
between the hypergeometric function and the Jacobi polynomial \( P_{n}^{(\alpha,\beta)}(t) \), we can express (33) in the form
\[ \chi_{n_{r},l}^{|q| \geq 1}(r) = \left[ \frac{\alpha}{N_{r}} \left( \frac{\lambda_{l}}{N_{r}} + N_{r} \right) \Gamma \left( \frac{\lambda_{l}}{N_{r}} + N_{r} - n_{r} \right) \Gamma \left( 1 + n_{r} + \frac{\lambda_{l}}{N_{r}} - N_{r} \right) \right]^{\frac{1}{2}} \times \left( |q| e^{-2\alpha r} \right)^{\frac{1}{2}} \left( \frac{\lambda_{l}}{N_{r}} - N_{r} \right) \left( 1 - |q| e^{-2\alpha r} \right)^{\delta_{l}+\frac{1}{2}} \times P_{n_{r}}^{\left( \delta_{l}, 2\delta_{l} \right)}(2 - 2 |q| e^{-2\alpha r}). \] (36)

Now, for them to be physically acceptable, the wave functions \( \chi_{n_{r},l}^{|q| \geq 1}(r) \) must satisfy the boundary conditions
\[ \lim_{r \to r_{0}} \chi_{n_{r},l}^{|q| \geq 1}(r) = 0, \] (37)
and
\[ \lim_{r \to \infty} \chi_{n_{r},l}^{|q| \geq 1}(r) = 0. \] (38)

When \( r \to r_{0} \), it is obvious that (36) fulfills the boundary condition (37), but, by letting \( r \to \infty \) in (36), we obtain the asymptotic behavior
\[ \chi_{n_{r},l}^{|q| \geq 1}(r) \sim e^{-\alpha r} \left( \frac{\lambda_{l}}{N_{r}} - N_{r} \right), \] (39)
from which we must impose the restriction that only the wave functions with \( \left( \frac{\lambda_{l}}{N_{r}} - N_{r} \right) > 0 \) fulfill the boundary condition (38) and therefore the value of \( n_{r \max} \) in (32) is given by \( n_{r \max} = \left\{ \sqrt{\lambda_{l}} - \delta_{l} \right\} \) which denotes the largest integer \( n_{r} \in \mathbb{N} \) with \( n_{r} < \left( \sqrt{\lambda_{l}} - \delta_{l} \right) \). This condition provides a finite number of energy levels of the physical system.
3.2 Second case: $0 < |q| < 1$ and $r \in \mathbb{R}^+$

In this case, we limit ourselves to the evaluation of the Green’s function associated with the $s$-waves ($l = 0$). Making the change of variable defined by
\[
\xi = \alpha r - \frac{1}{2} \ln |q|, \quad (\xi \in \mathbb{R}, \xi_0 = -\frac{1}{2} \ln |q|)
\]
and performing the time transformation $d\tau = \frac{1}{\alpha} \, d\xi$, we can rewrite (12), for $l = 0$, as
\[
G_{0}^{0<|q|<1}(r', r'; E) = \frac{1}{\alpha} \tilde{G}(\xi''; \xi'; \tilde{E}_0)
= \frac{1}{\alpha} \int_{\xi'}^{\infty} dS \exp \left( i \frac{1}{\alpha} \tilde{E}_0 S \right) K_{0}^{0<|q|<1}(\xi'', \xi'; S), \quad (40)
\]
where
\[
\tilde{E}_0 = \frac{1}{\alpha^2} [E - (U_0 + U_2)], \quad (41)
\]
and
\[
K_{0}^{0<|q|<1}(\xi'', \xi'; S) = \int D\xi(s) \exp \left\{ i \frac{1}{\alpha} \int_0^S \left( \frac{M \alpha^2}{2} - \tilde{V}(\xi) \right) ds \right\}, \quad (42)
\]
with
\[
\tilde{V}(\xi) = -\frac{U_1}{\alpha} \coth \xi + \frac{U_2}{\alpha^2 \sinh^2 \xi}; \quad \xi > \xi_0. \quad (43)
\]

Note that the expression (43) is that of the Manning-Rosen potential [24] in the range $\xi > \xi_0$. This means that the kernel $K_{0}^{0<|q|<1}(\xi'', \xi'; S)$ is the propagator describing the motion of a particle subjected to the Manning-Rosen potential defined in the half-space $\xi > \xi_0$. As a direct path integration is not possible, we can construct the corresponding Green’s function in terms of the Green’s function in the interval $\mathbb{R}^+$ with the help of the perturbation expansion method discussed in detail in the literature [27,28,36] and it is not necessary to repeat here. We find, all calculations done, that
\[
G^{0<|q|<1}(\xi'', \xi'; \tilde{E}_0) = G_{MR}(\xi'', \xi'; \tilde{E}_0) - \frac{G_{MR}(\xi'', \xi_0; \tilde{E}_0)G_{MR}(\xi_0, \xi'; \tilde{E}_0)}{G_{MR}(\xi_0, \xi_0; \tilde{E}_0)}, \quad (44)
\]
where $G_{MR}(\xi'', \xi'; \tilde{E}_0)$ is the Green’s function (22), for $l = 0$.

The energy spectrum is determined by the poles of the Green’s function (44), i.e. by the equation $G_{MR}(\xi_0, \xi_0; \tilde{E}_0) = 0$, or as well by the transcendental equation
\[
_2F_1 \left( M_1 - L_{E_n}, L_{E_n} + M_1 + 1, M_1 - M_2 + 1; |q| \right) = 0, \quad (45)
\]
where
\[
\begin{aligned}
L_{E_n} &= -\frac{1}{2} + \frac{1}{2\alpha} \sqrt{2M \left( \frac{D_e^{2\alpha r}}{|q|^2} - E_n \right)}, \\
M_1 &= \delta_0 + \frac{1}{2\alpha} \sqrt{2M \left( D_e - E_n \right)}, \\
M_2 &= \delta_0 - \frac{1}{2\alpha} \sqrt{2M \left( D_e - E_n \right)}, \\
\delta_0 &= \frac{1}{2} \sqrt{1 + \frac{2M \delta_0^{2\alpha r}}{R^2}}.
\end{aligned}
\quad (46)
\]
The transcendental equation (45) can be solved numerically to determine the energy levels. The corresponding reduced radial wave functions are of the form:

\[
\chi_{\alpha n_r}^{0<|q|<1}(r) = C \left( 1 - |q| e^{-2\alpha r} \right)^{\delta_{0r} + \frac{1}{2}} \left( |q| e^{-2\alpha r} \right)^{\frac{1}{2\alpha}} \sqrt{2M(D_{\alpha} - E_{\alpha r})} \times 2F_1 \left( M_1 - L_{E_{\alpha r}}, L_{E_{\alpha r}} + M_1 + 1, M_1 - M_2 + 1; |q| e^{-2\alpha r} \right),
\]

where \( C \) is a constant factor.

4 Deformed modified Rosen-Morse potential

For \( q > 0 \), the improved Tietz potential is analogous to the deformed modified Rosen-Morse potential

\[
V_0(r) = V_0 + V_1 \tanh_q (\alpha r) + V_2 \tanh_q^2 (\alpha r).
\]

The constants \( V_0, V_1 \) and \( V_2 \) are given by

\[
\begin{align*}
V_0 &= \frac{D_e}{4} \left( \frac{e^{2\alpha r}}{q} - 1 \right)^2, \\
V_1 &= \frac{D_e}{2} \left( 1 + \frac{e^{2\alpha r}}{q} \right) \left( 1 - \frac{e^{2\alpha r}}{q} \right), \\
V_2 &= \frac{D_e}{4} \left( \frac{e^{2\alpha r}}{q} + 1 \right)^2.
\end{align*}
\]

As the approximation to the centrifugal potential term adopted above does not apply to the case of the Rosen-Morse potential (see, for example, the discussion of the validity of an approximation of this type in our previous work [29]), we will be satisfied with the study of the \( s \)-waves \( (l = 0) \) by evaluating the Green’s function in order to find the energy levels and the corresponding wave functions of the bound states. In this case, the radial Green’s function (4) is written

\[
G^{q>0}_0(r'', r'; E) = \int_0^\infty dT \exp \left( \frac{i}{\hbar} ET \right) K^{q>0}_0(r'', r'; T),
\]

where the propagator \( K^{q>0}_0(r'', r'; T) \) is given by

\[
K^{q>0}_0(r'', r'; T) = \int Dr(t) \exp \left\{ \frac{i}{\hbar} \int_0^T \left( \frac{M}{2} r^2 - V_q(r) \right) dt \right\}.
\]

To evaluate the Green’s function [50], we perform the coordinate- and time transformations \( u = \alpha r - \frac{1}{2} \ln q, (u \in ]u_0, \infty[, u_0 = -\frac{1}{2} \ln q) \) and \( \frac{du}{dt} = \frac{1}{\alpha} \). As a result of these transformations, the Green’s function [50] takes the form

\[
G^{q>0}_0(r'', r'; E) = \frac{1}{\alpha} G^{q>0}_0(u'', u'; E_0)
= \frac{1}{\alpha} \int_0^\infty dS \exp \left( \frac{i}{\hbar} S\beta_0 \right) I^{q>0}_0(u'', u'; S),
\]

\( \beta_0 = M_1 - M_2 + 1 \).
where
\[ E_0 = \frac{1}{\alpha^2} [E - (V_0 + V_2)], \]
and
\[ P_0^{q>0}(u'', u'; S) = \int D\omega(s) \exp \left\{ \frac{i}{\hbar} \int_0^S \left( \frac{M}{2} \dot{u}^2 - V(u) \right) ds \right\}, \]
with
\[ V(u) = \frac{V_1}{\alpha^2} \tanh u - \frac{V_2}{\alpha^2 \cosh^2 u}; \quad u > u_0. \]
Due to the fact that \( V(u) \) is the Rosen-Morse potential defined in the half-space \( u > u_0 \), the Green’s function (52) can be constructed in terms of the Green’s function in the entire \( \mathbb{R} \), by a method similar to that used in the literature [27, 28, 36]. Hence the solution of (52) is easily found to be
\[ G_{q>0}(u'', u'; E_0) = G_{RM}(u'', u'; E_0) - \frac{G_{RM}(u'', u_0; E_0)G_{RM}(u_0, u'; E_0)}{G_{RM}(u_0, u_0; E_0)}, \]
with the Green’s function \( G_{RM}(u'', u'; E_0) \) given by
\[ G_{RM}(u'', u'; E_0) = -\frac{iM}{\hbar} \frac{\Gamma(M_1 - L_{E_0}) \Gamma(L_{E_0} + M_1 + 1)}{\Gamma(M_1 + M_2 + 1) \Gamma(M_1 - M_2 + 1)} \times \left( \frac{1 - \tanh u' - \tanh u''}{2} \right) \frac{M_1 + M_2}{M_1 - M_2} \times \left( \frac{1 + \tanh u' + \tanh u''}{2} \right) \frac{M_1 - M_2}{M_1 + M_2} \times 2F_1 \left( M_1 - L_{E_0}, L_{E_0} + M_1 + 1, M_1 + M_2 + 1; \frac{1 + \tanh u_<}{2} \right) \times 2F_1 \left( M_1 - L_{E_0}, L_{E_0} + M_1 + 1, M_1 + M_2 + 1; \frac{1 - \tanh u_>}{2} \right). \]

Here we have used the abbreviations
\[ \begin{aligned}
L_{E_0} &= -\frac{1}{2} + \sqrt{\frac{1}{4} + \frac{2MV_2}{\hbar^2\alpha^2}}, \\
M_1 &= \frac{1}{2\alpha^2} \left( \sqrt{2M(V_0 + V_1 + V_2 - E)} + \sqrt{2M(V_0 - V_1 + V_2 - E)} \right), \\
M_2 &= \frac{1}{2\alpha^2} \left( \sqrt{2M(V_0 + V_1 + V_2 - E)} - \sqrt{2M(V_0 - V_1 + V_2 - E)} \right).
\end{aligned} \]

The bound state energy levels \( E_{n_r} \) can be obtained from the poles of the radial Green’s function (56) and are determined by the transcendental equation
\[ 2F_1 \left( M_1 - L_{E_0}, L_{E_0} + M_1 + 1, M_1 + M_2 + 1; \frac{q}{1 + q} \right) = 0; \quad \text{for } E = E_{n_r}, \]
which can be solved numerically. The reduced radial wave functions with $E = E_n$ are readily obtained to be

$$\chi^{q>0}_n(r) = C \left( \frac{q}{e^{2\alpha r} + q} \right) \frac{1}{\sqrt{2M(D_e - E)}} \left( \frac{1}{1 + qe^{-2\alpha r}} \right) \frac{1}{\sqrt{2M}} e^{\frac{2q}{\alpha} e^{2\alpha r} - E}$$

$$\times \ 2F1 \left( M_1 - L\varepsilon_0, L\varepsilon_0 + M_1 + 1, M_1 + M_2 + 1; \frac{q}{e^{2\alpha r} + q} \right),$$

(60)

where $C$ is a constant factor.

## 5 Morse potential

When $q = 0$, the Tietz potential given by Eq. (2) turns to the Morse potential

$$V_M(r) = D_e \left( 1 - e^{-2\alpha (r - r_e)} \right)^2.$$  (61)

In this case, it can be seen from Eqs. (58) that

$$\begin{align*}
L\varepsilon_0 &\approx q \to 0 - \frac{1}{4} + \lambda \left( 1 + \frac{2\alpha r_e}{q} \right), \\
M_1 &\approx q \to 0 \mu + \lambda \frac{2\alpha r_e}{q}, \\
M_2 &\approx q \to 0 \mu - \lambda \frac{2\alpha r_e}{q},
\end{align*}$$

(62)

where we have identified

$$\mu = \frac{\sqrt{2M(D_e - E)}}{2\hbar \alpha},$$

(63)

and

$$\lambda = \frac{\sqrt{2MD_e}}{2\hbar \alpha}.$$  (64)

Using the Gauss’s transformation formula (31) together with the property of the hypergeometric function (38)

$$\lim_{\beta \to \infty} 2F1(\alpha, \beta, \gamma; \frac{2}{\beta}) = \ 1F1(\alpha, \gamma; \frac{1}{\beta}),$$

(65)

the relation between the confluent hypergeometric function and the Whittaker functions (see Ref. [37], p. 1059, Eqs. (9.220.2) and (9.220.3))

$$M_{\lambda, \mu}(z) = z^{\frac{1}{2} + \frac{\lambda}{2}} e^{-\frac{z}{2}} \ 1F1 \left( \frac{1}{2} - \lambda + \mu, 1 + 2\mu; z \right),$$

(66)
\[
M_{\lambda,-\mu}(z) = z^{-\mu + \frac{1}{2}} e^{-\frac{z}{2}} \frac{1}{\Gamma(\frac{1}{2} - \lambda - \mu, 1 - 2\mu; z)}, \tag{67}
\]
and the formula (see Ref. [37], p. 1059, Eq. (9.220.4))
\[
W_{\lambda,\mu}(z) = \frac{\Gamma(-2\mu)}{\Gamma(\frac{1}{2} - \lambda - \mu)} M_{\lambda,\mu}(z) + \frac{\Gamma(2\mu)}{\Gamma(\frac{1}{2} - \lambda + \mu)} M_{\lambda,\mu}(z), \tag{68}
\]
it can be shown that, after some simple calculation, the Green’s function (56) reduces to the well known Green’s function associated with the radial Morse potential
\[
G_M(r''; r'; E_0) = -\frac{iM}{\hbar} \frac{\Gamma\left(\frac{1}{2} - \lambda + \mu\right)}{\Gamma\left(2\mu + 1\right)} e^{z'' + z'} M_{\lambda,\mu}(z') W_{\lambda,\mu}(z''); \quad z'' > z', \tag{69}
\]
where \( z = 2\lambda e^{-2\alpha(r-r_e)} \).

From (59), it follows that
\[
\lim_{q \to 0} 2F_1 \left( M_1 - L \epsilon_0 - M_1 + 1, M_1 + M_2 + 1; \frac{q}{1 + q} \right) = 0. \tag{70}
\]

Following Flügge [39], this transcendental equation can be solved approximately. Since, in general, the values of \( \lambda e^{2\alpha r_e} \gg 1 \) for the standard diatomic molecules, the asymptotic behavior of the confluent hypergeometric function (70) can be taken into consideration to show that
\[
\frac{1}{2} - \lambda + \mu = -n_r, \quad n_r = 0, 1, 2, \ldots. \tag{71}
\]
Upon inserting the values of \( \lambda \) and \( \mu \) in (71), one finds the well-known energy levels for the radial Morse potential:
\[
E_{n_r} = -\frac{2\hbar^2 \alpha^2}{M} \left( n_r + 1 \right)^2 \left( n_r + 1 \right) \left( \sqrt{2MD_e} \hbar \alpha \right), \tag{72}
\]
with \( n_{r_{\text{max}}} = \left\{ \frac{2\sqrt{2MD_e \hbar \alpha}}{2\hbar \alpha} - 1 \right\} \).

The corresponding wave functions are found, in the limiting case \( q \to 0 \), from (59) to be
\[
\chi^{q=0}_{n_r}(r) = \mathcal{N} \exp \left[ -\frac{\sqrt{2MD_e}}{2\hbar \alpha} e^{-2\alpha(r-r_e)} \left( e^{-2\alpha(r-r_e)} \right)^{n_r + \frac{1}{2}} \times \frac{1}{\Gamma\left(2n_r + \sqrt{2MD_e \hbar \alpha} - 2; \sqrt{2MD_e \hbar \alpha} e^{-2\alpha(r-r_e)} \right)}, \tag{73}
\]
where \( \mathcal{N} \) is the normalization constant.
6 Discussions

Firstly, it should be noted that there are several special cases of improved Tietz potential that have been analyzed through different methods. For \( q = 1 \), the deformed modified Rosen-Morse potential (49) becomes the general radial Rosen-Morse potential

\[
V(r) = V_0 + V_2 + V_1 \tanh(\alpha r) - \frac{V_2}{\cosh^2(\alpha r)}
\]

which is similar to that of the Natanzon potential. The results obtained by Natanzon in Ref. \[40\] using a transformation of the Schrödinger equation into a hypergeometric equation and by Wu et al. \[41\] in a work based on the group theory approach are not satisfactory. When \( V_1 = 0 \), and \( V_0 = -V_2 \), the potential \[74\] reduces to the radial Rosen-Morse potential (also called radial modified Pöschl-Teller potential) for which the Schrödinger equation has been solved by Nieto in Ref. \[42\], for the \( s \)-waves from that with the symmetric Rosen-Morse potential by imposing that the general wave function must have continuous derivatives at the origin to keep only the odd solutions. Given the results obtained, it is concluded that this is a bad idea.

Secondly, to obtain closed-form expressions for anharmonicity constants \( \omega_x, x \) and \( \omega_y, y \) in terms of the energy spectrum expression, Sun et al. \[16\] have established the equivalence, for the three-dimensional case, between the deformed modified Rosen-Morse potential and the Tietz potential. However, they have inappropriately adapted the expression of the vibrational energy levels associated with the one-dimensional deformed modified potential \[43\] to that of the Tietz potential.

Finally, It is well known that the supersymmetry approach in quantum mechanics is based on the factorization method that applies to problems for which wave equations admit orthogonal polynomials as solutions. Therefore, the problem solution of a new deformed Schöberg-type potential is partially correct \((q < -1)\) via this method contrary to what is claimed by Mustafa \[22\]. For \(-1 < q < 0 \) or \( q > 0 \), we have a problem with Dirichlet boundary conditions. In this case, the solutions of the Schrödinger equation are hypergeometric series \( \text{$_2F_1(a, b, c, z)$} \) with transcendental equations for energy levels. The same potential has been treated within the path integral approach by Amrouche et al. \[23\] without incorporating the Dirichlet boundary conditions into the path integral. Likewise, their solutions for the cases \(-1 < q < 0 \) and \( q > 0 \) must be discarded as that of Mustafa.

7 Conclusion

In the above, we have presented a method to solve completely an improved form of the Tietz potential in terms of the path integral formalism. As we have shown, the path integral for the Green’s function associated with this potential can not be constructed for any deformation parameter \( q \) in a unified way because
the parameter $q$ characterizes various shapes of the potential. This potential has a strong singularity at $r = r_0 = \frac{1}{2\alpha} \ln |q|$ when $q < 0$ and the limiting case $q = 0$. Contrary to what has been reported in the literature, the quantum treatment of the problem with this potential by any method requires to consider three cases separately. When $|q| \geq 1$ and $\frac{1}{2\alpha} \ln |q| < r < +\infty$, by adopting a suitable approximation for the centrifugal potential term and formulating the path integral in terms of the standard Manning-Rosen potential, the radial Green’s function for any $l$ wave is stated in a closed form, from which the energy spectrum and the normalized wave functions are extracted. For $|q| < 1$, the path integral for the Green function associated with the $s$ waves is also formulated in terms of the Manning-Rosen potential defined in the half-space $\xi > -\frac{1}{2\alpha} \ln |q|$ and when $q > 0$, it is expressed in terms of the Rosen-Morse potential in the half-space $u > -\frac{1}{2\alpha} \ln q$. In both cases, we have shown that the $s$ state energy levels are determined by a transcendental equation involving the hypergeometric function. Naturally, in the limit $q \to 0$, our results can be reduced to those for the radial Morse potential.

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