Complete non-relativistic bound state solutions of the Tietz-Wei potential via the path integral approach

A. Khodja, A. Kadja, F. Benamira and L. Guechi
Laboratoire de Physique Théorique, Département de Physique,
Faculté des Sciences Exactes, Université des frères Mentouri,
Route d’Ain El Bey, Constantine, Algeria

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Abstract

In this work, the bound state problem of some diatomic molecules in the Tietz-Wei potential with varying shapes is correctly solved by means of path integrals. Explicit path integration leads to the radial Green’s function in closed form for three different shapes of this potential. In each case, the energy equation and the wave functions are obtained from the poles of the radial Green’s function and their residues, respectively. Our results prove the importance the optimization parameter $c_h$ in the study of this potential which has been completely ignored by the authors of the papers cited below. In the limit $c_h \to 0$, the energy spectrum and the corresponding wave functions for the radial Morse potential are recovered.

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Corresponding author, e-mail: guechilarbi@yahoo.fr

1 Introduction

The four-parameter potential function so-called Tietz-Wei potential [1][3] introduced to describe the bond-stretching vibrations of diatomic molecules is defined by

$$V_{TW}(r) = D \left[ \frac{1 - e^{-b_h(r-r_e)}}{1 - c_h e^{-b_h(r-r_e)}} \right]^2; \quad b_h = \beta (1 - c_h),$$

(1)

where $r$ is the internuclear distance, $D$ and $r_e$ represent the depth of the potential well and the length of the molecular bond, respectively. For physical
reasons, the optimization parameter $c_h$ is a dimensionless constant chosen such that $|c_h| < 1$ and $\beta$ is the Morse constant. This potential is much more realistic than the Morse potential in the description of molecular dynamics. Since 1990, it continues to interest physicists and chemists if we judge by the impressive number of works done on its applications in molecular physics and quantum chemistry. Using the Hamilton-Jacobi theory and the Bohr-Sommerfeld quantization rule, the rotation-vibration energy levels of diatomic molecules [4] as well as radial probability distributions of some diatomic molecules in excited rotation-vibration states [5] were obtained. In a three-dimensional space, the analytical solution of the radial Schrödinger equation with this potential was recently given for $s(l = 0)$—waves in a formulation based on the Nikiforov-Uvarov method [6] and for the $l$—waves using the approximation of Pekeris to replace the centrifugal potential term [7]. The approximate analytical solutions of the Schrödinger, Klein-Gordon and Dirac equations were also proposed by adopting the Pekeris approximation [8] and by applying three types of techniques namely the asymptotic iteration method, the functional analysis approach and the supersymmetry in quantum mechanics [9]. In another study, the construction of Ladder operators by the algebraic approach and coherent states in the context of supersymmetry in quantum mechanics for the Tietz-Wei anharmonic potential was discussed [10]. The method based on the appropriate quantization rule has recently been applied to determine the energy spectrum of a set of diatomic molecules in the presence of the Tietz-Wei potential [11] and the modified Tietz-Wei potential [12]. The Schrödinger equation has been solved by adopting the Pekeris approximation for the centrifugal term. Finally, we find in a very recent work done in a space with $D$ dimensions the solutions of the Schrödinger equation with the Tietz-Wei potential obtained by using a Pekeris approximation and supersymmetry in quantum mechanics [13].

As in the articles quoted above, the parameter $c_h$ does not seem to have any influence on the solutions of the problem, we will devote the rest of this paper to a rigorous discussion by the path integral approach considering all the existing cases and prove the importance of $c_h$ to solve the problem properly.

In the second section, we express the radial Green’s function with respect to the potential $V_{TW}(r)$ in the form of a path integral, emphasizing that the problem of its construction is presented differently according to the value that takes the parameter $c_h$. We establish the correspondence between the Tietz-Wei potential and the deformed Manning-Rosen potential when $0 < c_h < 1$ in the third section. For $e^{-b_k r_e} \leq c_h < 1$, by replacing the centrifugal potential term with an appropriate approximation, we compute, in a closed form, the radial Green’s function associated with the $l$—waves. From this we deduce the energy spectrum and the appropriately normalized wave functions of the bound states by indicating the minimum values of the parameter $c_h$ from which the numerical values of the energy spectrum for certain diatomic molecules can be obtained. When $0 < c_h < e^{-b_k r_e}$, we limit ourselves to the study of $s(l = 0)$—waves and we calculate the Green’s function through the technique used to solve problems with Dirichlet boundary conditions described in our previous work [14] that it is not necessary to repeat here. In the fourth section, we consider the case
where \(-1 < c_h < 0\). The potential (11) is reduced to the deformed Rosen-Morse potential. We evaluate the Green’s function associated with the \(s(l = 0)\)–waves in the same way as before. In these last two cases, we explicitly obtain the wave functions and we find a transcendental equation to determine the energy spectrum. At the limit where \(c_h \to 0\), we recover the Green’s function, the energy spectrum and the wave functions for the Morse potential in the fifth section. The sixth section will be a conclusion.

2 Green’s function

Since the potential (11) has spherical symmetry, the radial Green’s function is defined by

\[
G_l (r'', r'; E) = \int_0^\infty dT \langle r'' | \exp \left\{ \frac{i}{\hbar} [E - H_l] T \right\} | r' \rangle ,
\]

(2)

where \(H_l\) is the Hamiltonian

\[
H_l = \frac{P^2}{2\mu} + V_{\text{eff}}(r),
\]

(3)

with the effective potential

\[
V_{\text{eff}}(r) = \frac{\hbar^2 l(l + 1)}{2\mu r^2} + V_{\text{TW}}(r).
\]

(4)

In the context of Feynman’s path integral approach [10], it is easy to express (2) as a path integral,

\[
G_l (r'', r'; E) = \int_0^\infty dT \exp \left( \frac{i}{\hbar} E T \right) K_l (r'', r'; T),
\]

(5)

with

\[
K_l (r'', r'; T) = \lim_{N \to \infty} \prod_{n=1}^N \left[ \int dr_n \prod_{n=1}^{N+1} \left[ \int d(P_r)_n \right] \right] \exp \left\{ \frac{i}{\hbar} \sum_{n=1}^{N+1} \left[ (P_r)_n \Delta r_n - \varepsilon \left( \frac{(P_r)_n^2}{2\mu} + V_{\text{eff}}(r_n) \right) \right] \right\}.
\]

(6)

Then, by integrating on the variables \((P_r)_n\), we obtain the path integral in the configuration space,

\[
G_l (r'', r'; E) = \int_0^\infty dT \exp \left( \frac{i}{\hbar} E T \right) \tilde{K}_l (r'', r'; T),
\]

(7)
where the propagator \( \tilde{K}_l (r'', r'; T) \) is explicitly defined by

\[
\tilde{K}_l (r'', r'; T) = \lim_{N \to \infty} \left( \frac{\mu}{2i\pi \varepsilon} \right)^{N+1} \prod_{n=1}^{N} \int dr_n \left[ \frac{1}{2} \sum_{\varepsilon}^{N+1} \left[ \frac{\mu}{2\varepsilon} (\Delta r)^2 - \varepsilon V_{\text{eff}}(r_n) \right] \right].
\]

(8)

To construct the radial Green’s function (7), two cases occur depending on whether \( \chi \) is in the interval \( ]0, 1[ \) or in the interval \( ]-1, 0[ \).

3 Deformed Manning-Rosen potential

If \( 0 < \chi < 1 \), the Tietz-Wei potential turns into the Manning-Rosen potential defined in terms of the \( \chi \)–deformed hyperbolic functions by

\[
V_{\text{TW}} (r) = V_0 - V_1 \coth_{\chi} \left( \frac{b_h}{2} (r - r_e) \right) + \frac{V_2}{\sinh_{\chi}^2 \left( \frac{b_h}{2} (r - r_e) \right)},
\]

(9)

where \( V_0, V_1 \) and \( V_2 \) are the real constants given by

\[
\begin{align*}
V_0 &= \frac{D}{2} \left( 1 + \frac{1}{\chi^2} \right), \\
V_1 &= \frac{D}{2} \left( \frac{1}{\chi} + 1 \right) \left( \frac{1}{\chi} - 1 \right), \\
V_2 &= \frac{D}{4} \chi \left( \frac{1}{\chi} - 1 \right)^2.
\end{align*}
\]

(10)

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

\[
\begin{align*}
\sinh_{\chi} x &= e^{x-\chi e^{-x}}, & \cosh_{\chi} x &= e^{x+\chi e^{-x}}, \\
\tanh_{\chi} x &= \frac{e^{x-\chi e^{-x}}}{\cosh_{\chi} x}, & \coth_{\chi} x &= \frac{e^{x+\chi e^{-x}}}{\sinh_{\chi} x}.
\end{align*}
\]

(11)

These functions have been introduced for first time by Arai [16], with the real parameter \( \chi > 0 \).

To evaluate the radial Green’s function associated to the potential (9), we have to distinguish two cases: \( e^{-b_h r_e} \leq \chi < 1 \) et \( 0 < \chi < e^{-b_h r_e} \).

3.1 First case: \( e^{-b_h r_e} \leq \chi < 1 \)

The potential \( V_{\text{TW}} (r) \) has a strong singularity at the point \( r = r_0 = r_e + \frac{1}{b_h} \ln \chi \).

In this case, there are two distinct regions, the first is defined by the interval \( ]0, r_0[ \) and the second by the interval \( ]r_0, +\infty[ \). We will be interested in the calculation of the path integral for this potential only in the interval \( ]r_0, +\infty[ \), since, in the other interval, the problem can not be solved analytically and moreover, its solution does not have a physical interest worthy of note. In
Figs. 1 and 2, the potential (11) is plotted in the interval \( |r_0, +\infty| \) for different choices of the parameter \( c_h \) of H\(_2\)(X\(^1\Sigma^+_g\)) and I\(_2\)(O\(^1\Sigma^+_g\)) molecules in the range \( e^{-b_h r_c} \leq c_h < 1 \).

Now, to calculate the radial Green’s function for a state with an orbital quantum number \( l \), we adopt the expression [17]:

\[
\frac{1}{r^2} \approx C_0 + \frac{B_0}{e^{b_h (r - r_e)} - c_h} + \frac{A_0}{(e^{b_h (r - r_e)} - c_h)^2}
\]

(12)
as an approximation of the term \( \frac{1}{r^2} \) contained in the centrifugal potential term when \( b_h (r - r_e) \ll 1 \). Here \( C_0 = \frac{b_h}{12} \), \( B_0 \) and \( A_0 \) are two adjustable parameters. If we take \( C_0 = 0, B_0 = \frac{A_0}{c_h} \), \( A_0 = b_h c_h^2 \) and \( c_h = 1 \), the equation (12) is reduced to the approximation proposed by Greene and Aldrich [13]. Thus, after some simple calculation, we can write the expression of the effective potential (11) in the form:

\[
V_{eff}(r) \approx V_0^l - V_1^l \coth_{c_h} \left( \frac{b_r}{2} (r - r_e) \right) + \frac{V_2^l}{\sinh_{c_h}^2 \left( \frac{b_r}{2} (r - r_e) \right)},
\]

(13)
where the parameters \( V_0^l, V_1^l \) and \( V_2^l \) are defined by

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

(14)

Then, by introducing the new variable \( \xi = \frac{1}{2} \left[ b_h (r - r_e) - \ln c_h \right] \) and putting \( \varepsilon = \frac{b_h^2}{4} \xi_s \), the Green’s function (7) is written

\[
G_l (r'', r'; E) = \frac{2}{b_h} G_{MR} (\xi'', \xi'; \tilde{E}_l),
\]

(15)
where

\[
G_{MR} (\xi'', \xi'; \tilde{E}_l) = \int_0^{\infty} dS \exp \left( \frac{i}{\hbar} \frac{\tilde{E}_l}{b_h} S \right) P_l (\xi'', \xi'; S),
\]

(16)
is an expression in which the kernel \( P_l (\xi'', \xi'; S) \) has the explicit form:

\[
P_l (\xi'', \xi'; S) = \frac{b_h}{2} \lim_{N \to -\infty} \left( \frac{\mu}{2\pi^2 \hbar \varepsilon_s} \right)^{\frac{N+1}{2}} \prod_{n=1}^{N} \left[ \frac{\mu}{\hbar} \int d\xi_n \right] \exp \left\{ \frac{i}{\hbar} \sum_{n=1}^{N+1} \left[ \frac{\mu}{2\varepsilon_s} (\Delta \xi)_n^2 \right. \right.
\]
\[
+ \left. \frac{4\varepsilon_s}{b_h^2} \left( V_1^l \coth \xi_n - \frac{V_2^l}{c_h \sinh^2 \xi_n} \right) \right\},
\]

(17)
and
\[ \bar{E}_l = 4 \left( E - V_0' \right). \]  

The expression (17) is the one of the propagator for the standard Manning-Rosen potential [19] which has been discussed in the literature by means of the path integral [20]. We can thus write down the solution of (16) immediately in a closed form as:

\[
G_{MR}(\xi'', \xi'; \bar{E}_l) = \frac{i\mu}{\hbar} \frac{\Gamma(M_1 - L_E) \Gamma(L_E + M_1 + 1)}{\Gamma(M_1 - M_2 + 1) \Gamma(M_1 + M_2 + 1)} \times \left( \frac{2}{1 + \coth \xi} \frac{2}{1 + \coth \xi''} \right)^{M_1 + M_2} \times 2F_1 \left( M_1 - L_E, L_E + M_1 + 1, M_1 - M_2 + 1; \frac{\coth \xi - 1}{\coth \xi + 1} \right) \\
\times 2F_1 \left( M_1 - L_E, L_E + M_1 + 1, M_1 + M_2 + 1; \frac{2}{\coth \xi + 1} \right),
\]

where the parameters \( L_E, M_1 \) and \( M_2 \) have in the present case the following values:

\[
\begin{align*}
L_E &= -\frac{1}{2} + \frac{1}{\hbar\mu} \sqrt{2\mu \left( V_0' + V_1' - E \right)}, \\
M_1 &= \delta_l + \frac{1}{\hbar\mu} \sqrt{2\mu \left( V_1' - V_0' - E \right)}, \\
M_2 &= \delta_l - \frac{1}{\hbar\mu} \sqrt{2\mu \left( V_1' - V_0' - E \right)},
\end{align*}
\]

with
\[
\delta_l = \sqrt{\frac{8\mu V_2}{\hbar^2 \mu^2 c_h^2} + \frac{l(l + 1)}{\delta_b^2 c_h^2}} A_0 + \frac{1}{4}.
\]

So, going back to the old variable, the radial Green’s function (15) has for expression:

\[
G_l (r'', r'; E) = -\frac{2i\mu}{\hbar \mu} \frac{\Gamma(M_1 - L_E) \Gamma(L_E + M_1 + 1)}{\Gamma(M_1 - M_2 + 1) \Gamma(M_1 + M_2 + 1)} \times \left( 1 - c_h e^{-b_h (r'' - r_1)} \right) \left( 1 - c_h e^{-b_h (r'' - r_3)} \right) \times \left( c_h^2 e^{-b_h (r'' - r_3)} \right) \times 2F_1 \left( M_1 - L_E, L_E + M_1 + 1, M_1 - M_2 + 1; \frac{2}{c_h e^{-b_h (r'' - r_3)}} \right) \\
\times 2F_1 \left( M_1 - L_E, L_E + M_1 + 1, M_1 + M_2 + 1; \frac{1}{c_h e^{-b_h (r'' - r_3)}} \right),
\]

The energy spectrum for the bound states can be obtained from the poles of the radial Green’s function (22). These poles are those of the gamma function...
\[ (M_1 - L_E) \text{ that we find when its argument is a negative integer or zero, i.e. when} \]
\[ M_1 - L_E = -n_r, \quad n_r = 0, 1, 2, 3, \ldots \quad \text{(23)} \]

Taking into account (20), the eigenvalues of energy are then given by
\[ E_{n_r,l} = V_0 + \frac{\hbar^2 l(l+1)}{2\mu} \left[ C_0 + \frac{1}{2c_h} \left( \frac{A_0}{c_h} - B_0 \right) \right] - \frac{\hbar^2 b_h^2}{8\mu} \left( N_r^2 + \frac{\lambda_l^2}{N_r^2} \right), \quad \text{(24)} \]
with the notation
\[ N_r = n_r + \delta_l + \frac{1}{2}, \quad \text{(25)} \]
and
\[ \lambda_l = \frac{4\mu V_1}{\hbar^2 b_h^2} + \frac{l(l+1)}{b_h^2 c_h} \left( \frac{A_0}{c_h} - B_0 \right). \quad \text{(26)} \]

Now expressing the radial Green’s function (22) in the form of a spectral expansion as follows:
\[ G_l (r'', r'; E) = i\hbar \sum_{n_r=0}^{n_r_{\text{max}}} \frac{\chi_{n_r,l} (r'') \chi_{n_r,l} (r')}{E - E_{n_r,l}}, \quad \text{(27)} \]
we find for the wave functions \( \chi_{n_r,l} (r) \), suitably normalized, the values:
\[ \chi_{n_r,l} (r) = N_{n_r,l} \left( 1 - c_h e^{-b_h (r-r_e)} \right)^{N_r-n_r} \left( c_h e^{-b_h (r-r_e)} \right)^{-\frac{1}{2}} \left( \frac{\lambda_l}{N_r} - N_r \right) \]
\[ \times \binom{-n_r, N_r + \frac{\lambda_l}{N_r} - n_r, \frac{\lambda_l}{N_r} - N_r + 1; c_h e^{-b_h (r-r_e)}}{2}. \quad \text{(28)} \]

where the normalization factor \( N_{n_r,l} \) is
\[ N_{n_r,l} = \left[ \frac{b_h}{2N_r} \left( \frac{\lambda_l}{N_r} + N_r \right) \left( \frac{\lambda_l}{N_r} - N_r \right) \frac{\Gamma \left( N_r - n_r + \frac{\lambda_l}{N_r} \right) \Gamma \left( 1 - N_r + n_r + \frac{\lambda_l}{N_r} \right)}{n_r! \Gamma (2N_r - n_r)} \right]^\frac{1}{2} \]
\[ \times \frac{1}{\Gamma \left( \frac{\lambda_l}{N_r} - N_r + 1 \right).} \quad \text{(29)} \]

Here note that \( n_r = 0, 1, 2, \ldots, n_{r_{\text{max}}} < \sqrt{\lambda_l - \delta_l} - \frac{1}{2}, \) with \( n_{r_{\text{max}}} \) the maximum number of bound states.

In calculating energy values from the equation (24), for some molecules, it should be noted that the parameter \( c_h \) must be greater than or equal to the values in the table below and less than unity, unlike what is claimed in the literature [9].
Minimal values of the parameter $c_h$ for obtaining the energy levels from Equation (24).

| molecule              | $b_h \left( \hat{A}^{-1} \right)$ | $r_c (\hat{A})$ | $c_h$          |
|-----------------------|-----------------------------------|-----------------|----------------|
| HF($X^+\Sigma^+$)     | 1.942 07                         | 0.917           | 0.168 490 115  |
| Cl$_2$(X+$\Sigma^+$)  | 2.200 354                        | 1.987           | 0.012 624 657  |
| I$_2$(O$_2^+$)         | 2.123 43                         | 2.666           | 0.003 478 812  |
| H$_2$(X+$\Sigma^+$)   | 1.618 90                         | 0.741           | 0.301 313 237  |
| O$_2$(X+$\Sigma^+$)   | 2.591 03                         | 1.207           | 0.043 832 785  |
| N$_2$(X+$\Sigma^+$)   | 2.785 85                         | 1.097           | 0.047 071 975  |
| CO(X+$\Sigma^+$)      | 2.204 81                         | 1.128           | 0.083 156 934  |
| NO(X+$\Pi^+$)          | 2.715 59                         | 1.151           | 0.043 908 643  |
| O$_2^+$($X^2\Pi^+$)   | 2.869 87                         | 1.116           | 0.040 649 248  |
| NO$_2^+$($X^1\Sigma^+$)| 2.733 49                         | 1.063           | 0.054 710 486  |
| N$_2^+$($X^2\Sigma^+$)| 2.708 30                         | 1.116           | 0.048 681 178  |

3.2 Second case: $0 < c_h < e^{-b_h r_c}$

In this case, the potential (11) is defined in the interval $\mathbb{R}^+$. Figs. 3 and 4 represent the shape of the potential (11) for different values of $c_h$ in the range $0 < c_h < e^{-b_h r_c}$ for $H_2(X^1\Sigma^+_g)$ and $I_2(X^1\Sigma^+_g)$ molecules. The transformation $r = r_c + \frac{1}{b_h} (2\xi + \ln c_h)$ converts $r \in [0, +\infty]$ into $\xi \in [-\frac{1}{2} (b_h r_c + \ln c_h), +\infty[$. This means that the kernel (17) for $l = 0$, is the propagator that describes the evolution of a particle in the presence of a potential of the Manning-Rosen type in the half-space $\xi > \xi_0 = -\frac{1}{2} (b_h r_c + \ln c_h)$.

Now, by performing the time transformation $\varepsilon = \frac{4\varepsilon_s}{\hbar}$, or $dT = \frac{4dS}{\hbar}$, we can rewrite (7), for $l = 0$, as

$$G_0(r'', r'; E) = \frac{2}{b_h} \tilde{G}_{MR} \left( \xi', \xi''; \tilde{E}_0 \right),$$

with

$$\tilde{G}_{MR} \left( \xi', \xi''; \tilde{E}_0 \right) = \int_0^\infty dS \exp \left( \frac{i}{\hbar} \tilde{E}_0 S \right) P_0(\xi'', \xi'; S),$$

where

$$\tilde{E}_0 = 4 (E - V_0),$$

and

$$P_0(\xi'', \xi'; S) = \frac{b_h}{2} \lim_{N \to -\infty} \left( \frac{\mu}{2\pi\hbar^2\varepsilon_s} \right)^{N+1} \prod_{n=1}^N \left[ \int d\xi_n \right] \exp \left\{ \frac{i}{\hbar} \sum_{n=1}^{N+1} \left[ \frac{\mu}{2\varepsilon_s} (\Delta \xi)_n^2 + \frac{4\varepsilon_s}{b_h^2} \left( V_1 \coth \xi_n - \frac{V_2}{c_h \sinh^2 \xi_n} \right) \right] \right\}.$$
Note that the kernel \( \tilde{G} \) represents the propagator relative to the Manning-Rosen potential defined in the half-space \( \xi > \xi_0 \). The details concerning the evaluation of the Green’s function \( G \) in terms of the Green’s function in the interval \( \mathbb{R}^+ \) through the perturbation expansion method discussed in the literature \([22–24]\) are similar to those presented in our previous work on the vector and scalar deformed radial Rosen-Morse-potentials \([14]\). Hence we obtain

\[
\tilde{G}_{MR}(\xi'', \xi'; \tilde{E}_0) = G_{MR}^0(\xi'', \xi'; \tilde{E}_0) - \frac{G_{MR}(\xi_0, \xi_0'; \tilde{E}_0) G_{MR}^0(\xi_0, \xi'; \tilde{E}_0)}{G_{MR}(\xi_0, \xi_0; \tilde{E}_0)}, \tag{34}
\]

where \( G_{MR}^0(\xi'', \xi'; \tilde{E}_0) \) is the Green’s function \( (19) \) associated with the standard Manning-Rosen potential, for the \( s^- \)-waves \( (l = 0) \) and \( 0 < c_h < e^{-b_h r_e} \).

The poles of the Green’s function \( G \) yield the energy eigenvalues \( E_{nr} \). These poles are determined by the equation \( G_{MR}^0(\xi_0, \xi_0; \tilde{E}_0) = 0 \) which immediately leads to the following transcendental equation

\[
2\text{F}1 \left( M_1 - L_{E_{nr}}, L_{E_{nr}} + M_1 + 1, M_1 - M_2 + 1; c_h e^{b_h r_e} \right) = 0, \tag{35}
\]

where the quantities \( L_{E_{nr}}, M_1 \) and \( M_2 \) are defined by

\[
\begin{cases}
L_{E_{nr}} = -\frac{1}{2} + \frac{1}{\hbar b_h} \sqrt{2\mu (V_0 + V_1 - E_{nr})}, \\
M_1 = \delta_0 + \frac{1}{\hbar b_h} \sqrt{2\mu (V_0 - V_1 - E_{nr})}, \\
M_2 = \delta_0 - \frac{1}{\hbar b_h} \sqrt{2\mu (V_0 - V_1 - E_{nr})},
\end{cases} \tag{36}
\]

with

\[
\delta_0 = \sqrt{\frac{1}{4} + \frac{8\mu V_2}{\hbar^2 b_h^2 c_h}}. \tag{37}
\]

The energy levels \( E_{nr} \) of the molecule are given by the solutions of the transcendental equation \( (35) \), which are to be found from numerical method and the corresponding wave functions will have the form

\[
\chi_{nr}^{0 < c_h < e^{-b_h r_e}}(r) = \mathcal{N} \left( 1 - c_h e^{-b_h (r-r_e)} \right) \delta_0^{L_{E_{nr}}} \left( e^{b_h (r-r_e)} \right) \times 2\text{F}1 \left( M_1 - L_{E_{nr}}, L_{E_{nr}} + M_1 + 1, M_1 - M_2 + 1; c_h e^{-b_h (r-r_e)} \right), \tag{38}
\]

where \( \mathcal{N} \) is a constant factor. Note that these wave functions satisfy the boundary conditions:

\[
\chi_{nr}^{0 < c_h < e^{-b_h r_e}}(r) \rightarrow 0, \quad r \rightarrow 0, \tag{39}
\]

and

\[
\chi_{nr}^{0 < c_h < e^{-b_h r_e}}(r) \rightarrow 0, \quad r \rightarrow \infty. \tag{40}
\]
4 Deformed Rosen-Morse potential

When $-1 < c_h < 0$, the Tietz-Wei potential matches the form of the Rosen-Morse potential expressed in terms of the $c_h$-deformed hyperbolic functions by

$$V_{TW}(r) = U_0 + U_1 \tanh|c_h| \left[ \frac{b_h}{2} (r - r_e) \right] - \frac{U_2}{\cosh^2|c_h| \left[ \frac{b_h}{2} (r - r_e) \right]},$$  \hspace{1cm} (41)

where the constants $U_0, U_1$ and $U_2$ are defined by

$$\begin{align*}
U_0 &= \frac{D}{2} \left( 1 + \frac{1}{|c_h|} \right), \\
U_1 &= \frac{D}{2} \left( 1 - \frac{1}{|c_h|} \right) \left( 1 + \frac{1}{|c_h|} \right), \\
U_2 &= \frac{D}{4} |c_h| \left( \frac{1}{|c_h|} + 1 \right)^2.
\end{align*}$$  \hspace{1cm} (42)

The potential (11) is plotted in Figs. 5 and 6 for different values of $c_h$ in the range $-1 < c_h < 0$ for $H_2(X^1\Sigma_g^+)$ and $I_2(X(O^1_g))$ molecules.

In this case, the radial Green’s function associated with the waves $s(l = 0)$ is written

$$G(r'', r'; \mathcal{E}_0) = \int_0^\infty dT \exp \left( \frac{i}{\hbar} \mathcal{E}_0 T \right) K_0(r'', r'; T)$$  \hspace{1cm} (43)

with

$$\mathcal{E}_0 = E - U_0,$$  \hspace{1cm} (44)

and

$$K_0(r'', r'; T) = \int \mathcal{D}r(t) \left\{ \frac{i}{\hbar} \int_0^T \left[ \frac{\mu}{2} \dot{r}^2 - \left( U_1 \tanh|c_h| \left[ \frac{b_h}{2} (r - r_e) \right] \right. \right. \right.$$

$$\left. \left. - \frac{U_2}{\cosh^2|c_h| \left[ \frac{b_h}{2} (r - r_e) \right]} \right) \right\} dt \right\}. \hspace{1cm} (45)

Now, by applying the spatial transformation $r \in \mathbb{R}^+ \rightarrow x \in ]x_0, +\infty[$ defined by

$$x = \frac{b_h}{2} (r - r_e) - \frac{1}{2} \ln |c_h|,$$  \hspace{1cm} (46)

accompanied by the time transformation

$$\varepsilon = \frac{4}{b_h^2} \varepsilon_s \hspace{0.5cm} \text{ou} \hspace{0.5cm} T = \frac{4}{b_h^2} S,$$  \hspace{1cm} (47)

we can thus rewrite the function of Green (13) in the following form:

$$G(r'', r'; \mathcal{E}_0) = \frac{2}{b_h} G(x'', x'; \mathcal{E}_0),$$  \hspace{1cm} (48)
with
\[ \tilde{G} (x'', x'; E_0) = \int_0^\infty dS \exp \left( \frac{4i}{\hbar b h} E_0 S \right) K_0 (x'', x'; E_0) , \] (49)

where
\[ K_0 (x'', x'; E_0) = \int Dx(s) \exp \left\{ \frac{i}{\hbar} \int_0^S \left[ \frac{\mu}{2} x^2 - \frac{4}{b h} \left( U_1 \tanh x - \frac{U_2}{|c_h| \cosh^2 x} \right) \right] ds \right\} ; \quad x > x_0 \] (50)
is the propagator associated with a particle that moves in the half-space \( x > x_0 = -\frac{1}{2} \left( (b_h r_c + \ln |c_h|) \right) \), under the action of the standard Rosen-Morse potential [25]. Since the propagator (50) is defined in the half-space \( x > x_0 \), we have to construct the corresponding Green’s function (49) in terms of the Green’s function for that potential in all the space \( \mathbb{R} \) by proceeding as in the previous case. All calculations done, we obtain
\[ \tilde{G} (x'', x'; E_0) = G_{RM} (x'', x'; E_0) - \frac{G_{RM} (x'', x_0; E_0) G_{RM} (x_0, x'; E_0)}{G_{RM} (x_0, x_0; E_0)} , \] (51)

where \( G_{RM} (x'', x'; E_0) \) is the Green’s function relative to the standard Rosen-Morse potential [26] given by

\[
G_{RM} (x'', x'; E_0) = -\frac{i \mu}{\hbar} \frac{\Gamma (M_1 - L_{E_0}) \Gamma (L_{E_0} + M_1 + 1)}{\Gamma (M_1 + M_2 + 1) \Gamma (M_1 - M_2 + 1)} \times \left( \frac{1 - \tanh x' - 1 - \tanh x''}{2} \right)^{\frac{M_1 + M_2}{2}} \times \left( \frac{1 + \tanh x' + 1 + \tanh x''}{2} \right)^{\frac{M_1 - M_2}{2}} \times 2F_1 \left( M_1 - L_{E_0}, L_{E_0} + M_1 + 1, M_1 - M_2 + 1; \frac{1 + \tanh x_<}{2} \right) \times 2F_1 \left( M_1 - L_{E_0}, L_{E_0} + M_1 + 1, M_1 + M_2 + 1; \frac{1 - \tanh x_>}{2} \right). \] (52)

Here we have used the following abbreviations
\[
\begin{align*}
L_{E_0} &= -\frac{1}{2} + \sqrt{\frac{1}{4} + \frac{8 \mu U_2}{\hbar^2 b^2 |c_h|^2}}, \\
M_1 &= \frac{1}{\hbar b_0} \sqrt{2 \mu (D - E)} + \frac{1}{\hbar b_0} \sqrt{2 \mu \left( \frac{D}{|c_h|^2} - E \right)}, \\
M_2 &= \frac{1}{\hbar b_0} \sqrt{2 \mu (D - E)} - \frac{1}{\hbar b_0} \sqrt{2 \mu \left( \frac{D}{|c_h|^2} - E \right)}. \end{align*} \] (53)

The bound states with the energy \( E_{n_r} \) are determined from the poles of the
Green’s function $G_{RM}(x_0, x_0; E_0)$ by the transcendental equation

$$2F_1 \left( M_1 - L_{E_0}, L_{E_0} + M_1 + 1, M_1 + M_2 + 1; \frac{|c_h|}{e^{-b_h r_e} + |c_h|} \right) = 0 \quad \text{for } E = E_{n_r},$$

(54)

which can also be solved numerically and the corresponding wave functions have the form:

$$\chi_{{n_r}}(r) = N \left( \frac{|c_h|}{|c_h| + e^{b_h (r-r_e)}} \right) \frac{2\sqrt{2\mu(D-E_{n_r})}}{\sqrt{2\mu |c_h|^2}} \times 2F_1 \left( M_1 - L_{E_0}, L_{E_0} + M_1 + 1, M_1 + M_2 + 1; \frac{|c_h|}{e^{b_h (r-r_e)} + |c_h|} \right),$$

(55)

where $N$ is a constant factor.

## 5 Morse potential

By making $|c_h| = 0$ in the expression (1), we obtain the radial Morse potential

$$V_M(r) = D \left( 1 - e^{-\beta (r-r_e)} \right)^2.$$  

(56)

In this case, we can show from the equations (55) that

$$\begin{align*}
L_{E_0} & \underset{|c_h| \to 0}{\simeq} -\frac{1}{2} + \left( 1 + \frac{1}{|c_h|} \right) \frac{\sqrt{2\mu \beta}}{\hbar^2}, \\
M_1 & \underset{|c_h| \to 0}{\simeq} \frac{\sqrt{2\mu \beta}}{\hbar^2} \sqrt{2 \mu (D-E)} + \frac{\sqrt{2\mu \beta}}{\hbar^2 |c_h|}, \\
M_2 & \underset{|c_h| \to 0}{\simeq} \frac{\sqrt{2\mu \beta}}{\hbar^2} \sqrt{2 \mu (D-E)} - \frac{\sqrt{2\mu \beta}}{\hbar^2 |c_h|}.
\end{align*}$$

(57)

On the other hand, taking into account the property of the hypergeometric function [28], it is easy to see that

$$\lim_{|c_h| \to 0} 2F_1 \left( M_1 - L_{E_0}, L_{E_0} + M_1 + 1, M_1 + M_2 + 1; \frac{|c_h|}{e^{-b_h r_e} + |c_h|} \right) = 1F_1 \left( \frac{1}{2} - \frac{\sqrt{2\mu D}}{\hbar^2}, \frac{\sqrt{2\mu (D-E)}}{\hbar^2}, \frac{\sqrt{2\mu (D-E)}}{\hbar^2}, \frac{2\sqrt{2\mu D}}{\hbar^2} e^{\beta r_e} \right) = 0.$$  

(58)

By considerations similar to those used in Refs. [29][30], it is easy to show that

$$\frac{1}{2} - \frac{\sqrt{2\mu D}}{\hbar^2} + \frac{1}{\hbar^2} \sqrt{2\mu (D-E)} = -n_r, \quad n_r = 0, 1, 2, ...$$

(59)

From where we find the well-known energy levels associated with the radial potential of Morse:
\[ E_{n_r} = -\frac{\hbar^2 \beta^2}{2\mu} \left[ \left( n_r + \frac{1}{2} \right)^2 - 2 \left( n_r + \frac{1}{2} \right) \frac{\sqrt{2\mu D}}{\hbar \beta} \right], \quad (60) \]

with \( n_{r_{\text{max}}} = \left\{ \sqrt{\frac{2\mu D}{\hbar \beta}} - \frac{1}{2} \right\}, \) and from the expression (55), passing to the limit where \( |c_h| \to 0, \) we will have for the corresponding wave functions:

\[
\chi_{n_r=0}^{|c_h|=0}(r) = C \exp \left[ \frac{\sqrt{2\mu D}}{\hbar \beta} e^{-\beta(r-r_e)} \right] \left( e^{-\beta(r-r_e)} \right)^{\frac{\sqrt{2\mu D}}{\hbar \beta} - n_r - \frac{1}{2}} 
\times \,_1F_1 \left( -n_r, -2n_r + 2 \frac{\sqrt{2\mu D}}{\hbar \beta}; \frac{2\sqrt{2\mu D}}{\hbar \beta} e^{-\beta(r-r_e)} \right), \quad (61) \]

where \( C \) is the normalization constant.

6 Conclusion

In this paper, we have seen that the problem of the Tietz-Wei potential is completely solved in the context of Feynman’s path integrals, contrary to the naive attempts of its treatment by various techniques [6, 7, 9–13] leading to partially acceptable results. It should be noted that a suitable study of this potential requires distinguishing three cases representing the standard Manning-Rosen potential for \( e^{-b_h r_e} \leq c_h < 1, \) the defined Manning-Rosen potential in a half-space when \( 0 < c_h < e^{-b_h r_e} \) and the Rosen-Morse potential for \(-1 < c_h < 0.\) Each case requires special handling. This proves that the optimization parameter \( c_h \) is an important parameter in the analysis of this problem. In particular, the analytical energy spectrum and the wave functions of the states \( l \) of certain diatomic molecules are obtained approximately for values of \( c_h \) greater than or equal to those contained in the table above. It should also be pointed out that the Pekeris approximation with dependent constants of \( c_h \) used in the works cited above applies very restrictively to diatomic molecules. In the last two cases, the perturbation expansion technique we did not repeat here is used to construct the Green’s function in a closed form. In each case, the poles of the Green’s function yield a transcendental equation involving the hypergeometric function that must be solved numerically to determine the bound state energy levels \( E_{n_r}.\)

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Fig. 1: A plot of the Tietz-Wei potential for $H_2(X^{1}\Sigma_g^+)$ with $r_e = 0.741(\text{Å})$, $\beta = 1.943319838 (\text{Å}^{-1})$ and $D = 47506.6564$ eV

Fig. 2: A plot of the Tietz-Wei potential for $I_2(X(O_g^+))$ with $r_e = 2.666 (\text{Å})$, $\beta = 1.858214554 (\text{Å}^{-1})$ and $D = 15555.7706$ eV

Fig. 3: A plot of the Tietz-Wei potential for $H_2(X^{1}\Sigma_g^+)$ with $r_e = 0.741 (\text{Å})$, $\beta = 1.943319838 (\text{Å}^{-1})$ and $D = 47506.6564$ eV

Fig. 4: A plot of the Tietz-Wei potential for $I_2(X(O_g^+))$ with $r_e = 2.666 (\text{Å})$, $\beta = 1.858214554 (\text{Å}^{-1})$ and $D = 15555.7706$ eV

Fig. 5: A plot of the Tietz-Wei potential for $H_2(X^{1}\Sigma_g^+)$ with $r_e = 0.741 (\text{Å})$, $\beta = 1.943319838 (\text{Å}^{-1})$ and $D = 47506.6564$ eV

Fig. 6: A plot of the Tietz-Wei potential for $I_2(X(O_g^+))$ with $r_e = 2.666 (\text{Å})$, $\beta = 1.858214554 (\text{Å}^{-1})$ and $D = 15555.7706$ eV