Path integral solution for a deformed radial
Rosen-Morse potential

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Abstract

An exact path integral treatment of a particle in a deformed radial
Rosen-Morse potential is presented. For this problem with the Dirichlet
boundary conditions, the Green’s function is constructed in a closed form
by adding to \( V_q(r) \) a \( \delta \)-function perturbation and making its strength
infinitely repulsive. A transcendental equation for the energy levels \( E_n \)
and the wave functions of the bound states can then be deduced.

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1 Introduction

The so-called Rosen-Morse potential is a one-dimensional potential function
introduced by Rosen and Morse in 1932 to study the vibrational states of poly-
atomic molecules [1]. Since then, it has attracted a lot of interest due to its
numerous applications in several branches of physics [2, 3]. It has also been used
as an illustrative example in different methods such as the factorization method
[4, 5], the prepotential approach [6], the path integral technique [7, 8, 9, 10], the
supersymmetry in quantum mechanics and the shape invariance [11, 12] and the
Nikiforov-Uvarov method [13, 14, 15].

There is also the spherically symmetric Rosen-Morse potential which has
been discussed by many authors [16, 17, 18, 19, 20] in recent years without
distinguishing between the one-dimensional potential and the radial potential
problem. Consequently, the solutions which have been obtained until now are
not satisfactory.
The purpose of the present work is to re-examine and rederive, within the framework of path integrals, the correct solutions of the problem of the non-relativistic particle of mass $M$ moving in the $q$-deformed radial Rosen-Morse potential denoted by

$$V_q(r) = -\frac{V_1}{\cosh_q^2 \left( \frac{r}{a} \right)} + V_2 \tanh_q \left( \frac{r}{a} \right)$$

(1)

where $V_1, V_2, a$ and $q$ are four potential parameters. It is defined in terms of the $q$-deformed hyperbolic functions ($q > 0$)

$$\sinh_q x = \frac{e^x - qe^{-x}}{2}, \quad \cosh_q x = \frac{e^x + qe^{-x}}{2}, \quad \tanh_q x = \frac{\sinh_q x}{\cosh_q x}$$

(2)

which have been introduced for the first time by Arai [21]. The introduction of the parameter $q$ may be used as an additional parameter in the description of inter-atomic interactions, in particular, when the particle motion takes place in a half-space different from the half-space $r > 0$, i.e., the center of mass location of the molecule is not at the coordinate origin. In Fig. ?? the potential (1) is plotted for four different $q$ values.

Fig. ??: A plot of the Rosen-Morse potential (1) for different $q$ values. Here $V_2 = V_1/4$. The potential $V_q(r)$ is scaled in units of $V_1$, and the coordinate $r$ is scaled in units of $a$.

To do that, in section 2, the evaluation procedure of the Green’s function via the path integral approach for a potential with Dirichlet boundary conditions is used. We use a trick which consists in incorporating a $\delta$—function perturbation as an additional potential. After calculating the Green’s function in closed form, i.e., in a form that involves no summation, we shall make the strength of the $\delta$—function perturbation infinitely repulsive to obtain the Green’s function associated with the $s$ waves for the potential (1). Then in section 3, we derive a transcendental equation for the energy levels and the wave functions of the bound states. In section 4, the standard radial Rosen-Morse ($q = 1$) is considered as particular case. The section 5 will be a conclusion.
2 Green’s function

The propagator for a particle of mass \( M \) in the deformed radial Rosen-Morse potential is written in spherical coordinates as

\[
K^q\left( \vec{r}'' , \vec{r}' ; T \right) = \frac{1}{r'' r'} \sum_{l=0}^{\infty} \frac{2l + 1}{4\pi} K^q_l (r'' , r' ; T) P_l \left( \frac{r''}{r'} \right),
\]

(3)

where \( P_l \left( \frac{r''}{r'} \right) \) is the Legendre polynomial of degree \( l \) in \( \frac{r''}{r'} \). The radial propagator is given by the path integral representation

\[
K^q_l (r'' , r' ; T) = \lim_{N \to \infty} \prod_{j=1}^{N} \left[ \frac{M}{2i\pi\hbar} \right]^{\frac{1}{2}} N^{-1} \int dr \exp \left[ i \hbar \sum_{j=1}^{N} S(j , j - 1) \right],
\]

(4)

in which the action for each short-time interval is defined by

\[
S(j , j - 1) = \frac{M}{2\varepsilon} (\Delta r_j)^2 + \varepsilon \frac{l(l + 1)\hbar^2}{2Mr_j r_{j-1}} + \varepsilon \left( \frac{V_1}{\cosh^2 \left( \frac{r_j}{a} \right)} - V_2 \tanh \left( \frac{r_j}{a} \right) \right),
\]

(5)

with the usual notation \( r_j = r(t_j) \), \( \Delta r_j = r_j - r_{j-1} \), \( \varepsilon = t_j - t_{j-1} = T/N \), \( t' = t_0, t'' = t_N \) and \( T = t'' - t' \). By assuming that the system has only a discrete spectrum, expression (5) corresponds to the propagator expressed in spectral expansion as

\[
K^q_l (r'', r' ; T) = \sum_{n_r} \varphi^q_{n_r , l} (r) \varphi^q_{n_r , l} (r'') e^{\frac{i}{\hbar} E_{n_r} T}; \quad T > 0,
\]

(6)

where \( \varphi^q_{n_r , l} (r) \) is the reduced radial wave function, \( E_{n_r} \) are the energy eigenvalues and \( n_r \) denotes the number of the nodes of the radial wave functions.

Our aim is to find \( E_{n_r} \) and \( \varphi^q_{n_r} (r) \) for \( l = 0 \) by evaluating (4). Since the radial path integral (4) cannot directly be calculated, we consider the radial Green’s function (Fourier transform of the radial propagator):

\[
G^q_0 (r'', r' ; E) = \int_{0}^{\infty} dT \exp \left( \frac{i}{\hbar} ET \right) K^q_0 (r'', r' ; T).
\]

(7)

With the new variable \( u = \frac{E}{\varepsilon} = \ln \sqrt{q} \) and the new pseudo-time \( s = \frac{t'}{a} \), the radial Green’s function (7) becomes

\[
G^q_0 (r'', r' ; E) = a \tilde{G}_{\text{RM}} (u'' , u' ; E)
\]

(8)

and

\[
\tilde{G}_{\text{RM}} (u'' , u' ; E) = \int_{0}^{\infty} dS \exp \left( \frac{i}{\hbar} a^2 ES \right) K_0(u'' , u' ; S).
\]

(9)
where
\[
K_0(u'', u'; S) = \int Du(s) \exp \left\{ \frac{i}{\hbar} \int_0^S \left( \frac{M}{2} \dot{u}^2 - V(u) \right) ds \right\},
\]
(10)
with
\[
V(u) = a^2 \left( V_2 \tanh u - \frac{V_1}{q \cosh^2 u} \right); \quad u \geq - \ln \sqrt{q}.
\]
(11)
The propagator (10) has the same form as the path integral associated with the Rosen-Morse potential \( V_{RM}(u) \) for \( u \in \mathbb{R} \), but, in the present case, we have converted the path integral for the deformed radial potential (1) into a path integral for a Rosen-Morse potential type by means of the transformation \( r \rightarrow r(u) \), which maps \( \mathbb{R}^+ \rightarrow ]-\ln \sqrt{q}, +\infty[ \). This means that the motion of the particle takes place on the half line \( u \geq u_0 = - \ln \sqrt{q} \). As a direct path integration is not possible, the problem can be solved with the help of a trick which consists in adding an auxiliary \( \delta \)–function term to the action contained in Eq. (9) to form an impenetrable wall [23] at \( u = u_0 = - \ln \sqrt{q} \) by letting the strength of the \( \delta \)–function be infinitely repulsive. Then, in this case, the Green’s function is given by
\[
G^\delta_0 (u'', u'; E) = \int_0^{\infty} dS \exp \left( \frac{i}{\hbar} a^2 ES \right) K^\delta_0 (u'', u'; S)
\]
(12)
where
\[
K^\delta_0 (u'', u'; S) = \int Du(s) \exp \left\{ \frac{i}{\hbar} \int_0^S \left( \frac{M}{2} \dot{u}^2 - V^\delta(u) \right) ds \right\}
\]
(13)
is the propagator for a one-dimensional system bounded by a potential of the form:
\[
V^\delta(u) = V_{RM}(u) - \lambda \delta (u - u_0); \quad u \in \mathbb{R},
\]
(14)
in which \( V_{RM}(u) \) is the standard Rosen-Morse potential. As the path integration of (13) cannot directly be performed, we apply the perturbative approach by expanding \( \exp \left( \frac{i}{\hbar} \lambda \int_{u''}^{u'} \delta (u - u_0) ds \right) \) into the power series. This gives the following series expansion [24, 25, 26]:
\[
K^\delta_0 (u'', u'; S) = K_{RM}(u'', u'; S)
\]
\[\quad + \sum_{n=1}^{\infty} \frac{1}{n!} \left( \frac{i}{\hbar} \lambda \right)^n \int Du(s) \exp \left[ \frac{i}{\hbar} \int_0^S \left( \frac{M}{2} \dot{u}^2 - V_{RM}(u) \right) ds \right] \times \int_0^S \delta (u_1 - u_0) ds_1 \ldots \int_0^S \delta (u_n - u_0) ds_n \]
(15)
where \( K_{RM}(u'', u'; S) \) is the propagator for the standard Rosen-Morse potential. With the time-ordering \( s' = s_0 = 0 < s_1 < s_2 < ... < s_n < s'' = S \), the
propagator (15) can be rewritten as the Feynman-Dyson perturbation series

\[ K_0^\delta(u'', u'; S) = K_{RM}(u'', u'; S) \]

\[ + \sum_{n=1}^{\infty} \frac{1}{n!} \left( \frac{i}{\hbar} \lambda \right)^n \prod_{j=1}^{n} \int_{s_j}^{s_{j+1}} ds_j \int_{-\infty}^{+\infty} du_j \]

\[ \times K_{RM}(u_1, u'; s_1 - s') \delta(u_1 - u_0) K_{RM}(u_2, u_1; s_2 - s_1) \]

\[ \times \ldots \times \delta(u_{n-1} - u_{n-2}) K_{RM}(u_n, u_{n-1}; s_n - s_{n-1}) \]

\[ \times \delta(u_n - u_{n-1}) K_{RM}(u'', u_n; s'' - s_n) \]

\[ = K_{RM}(u'', u'; S) + \sum_{n=1}^{\infty} \frac{1}{n!} \left( \frac{i}{\hbar} \right)^n \int_{s'}^{s''} ds_n \]

\[ \times \int_{s_n}^{s_{n-1}} \ldots \int_{s_1}^{s_2} ds_1 K_{RM}(u_1, u'; s_1 - s') \]

\[ \times K_{RM}(u_2, u_1; s_2 - s_1) \times \ldots \times K_{RM}(u'', u_n; s'' - s_n), \]

(16)

In order to perform the successive integrations over the time variables \( t_j \) in (16), we insert (16) into (12), and making use the convolution theorem of the Fourier transformation, we arrive at

\[ G_{RM}(u'', u'; E) = G_{RM}(u'', u'; E) - \frac{G_{RM}(u'', u_0; E) G_{RM}(u_0, u'; E)}{G_{RM}(u_0, u_0; E) - \lambda}, \]

(17)

where \( G_{RM}(u'', u'; E) \) is the Green's function relative to the Rosen-Morse potential in the entire space \( \mathbb{R} \), and, as is known from the literature \([9, 10]\), its closed expression is given by

\[ G_{RM}(u'', u'; E) = \frac{-iM}{\hbar} \frac{\Gamma(M_1 - L\nu_q) \Gamma(L\nu_q + M_1 + 1)}{\Gamma(M_1 + M_2 + 1) \Gamma(M_1 - M_2 + 1)} \]

\[ \times \left( \frac{1 - \tanh u' - 1 - \tanh u''}{2} \right)^{\frac{M_1 + M_2}{2}} \]

\[ \times \left( \frac{1 + \tanh u' + 1 + \tanh u''}{2} \right)^{\frac{M_1 - M_2}{2}} \]

\[ \times {}_2F_1 \left( M_1 - L\nu_q, L\nu_q + M_1 + 1, M_1 - M_2 + 1; \frac{1}{2}(1 + \tanh u_>) \right) \]

\[ \times {}_2F_1 \left( M_1 - L\nu_q, L\nu_q + M_1 + 1, M_1 + M_2 + 1; \frac{1}{2}(1 - \tanh u_<) \right), \]

(18)
with the following abbreviations

\[
\begin{align*}
L_{\nu_q} &= \frac{1}{2} (\nu_q - 1), \\
\nu_q &= \sqrt{1 + \frac{8Ma^2V_1}{\hbar^2q}}, \\
M_{1,2} &= \sqrt{\frac{Ma^2}{2\hbar^2}} \left( \sqrt{V_2 - E} \pm \sqrt{-V_2 - E} \right).
\end{align*}
\] (19)

The \(2\)\(F\)\(1\)(\(\alpha, \beta, \gamma, u\)) are the hypergeometric functions. The symbols \(u>\) and \(u<\) denote \(\max(u'', u')\) and \(\min(u'', u')\), respectively.

Now, in the limit \(\lambda \to -\infty\), the physical system is forced to move in the potential \(V_{RM}(u)\) bounded by an infinitely repulsive barrier [23, 24] located at \(u = u_0\). In this case, the Green’s function is given by

\[
\tilde{G}_{RM}(u'', u'; E) = \lim_{\lambda \to -\infty} G_{\delta RM}(u'', u'; E)
= \frac{G_{RM}(u'', u_0; E)G_{RM}(u_0, u'; E)}{G_{RM}(u_0, u_0; E)}
\] (20)

### 3 Energy spectrum and wave functions of bound states

The energy spectrum for the bound states can be obtained from the poles of the Green’s function [20], i.e. by the equation \(G_{RM}(u_0, u_0; E) = 0\), or as well by the transcendental equation

\[
2\ F_1 \left( \frac{M_1(E_{n_r}) - L_{\nu_q} + M_1(E_{n_r}) + 1, M_1(E_{n_r}) + M_2(E_{n_r}) + 1; \frac{q}{q + 1}}{e^{2r/a} + q} \right) = 0.
\] (21)

The energies \(E_{n_r}\) of the bound states can be determined by solving numerically this equation and the wave functions satisfying the boundary conditions \(\varphi_{n_r}^q(0) = \varphi_{n_r}^q(\infty) = 0\) are given by.

\[
\varphi_{n_r}^q(r) = C \left( \frac{q}{e^{r/a} + q} \right)^{M_1(E_{n_r}) + M_2(E_{n_r})} \left( \frac{e^{2r/a}}{e^{r/a} + q} \right)^{M_1(E_{n_r}) - M_2(E_{n_r})}
\times \ F_1 \left( \frac{q}{e^{2r/a} + q} \right),
\] (22)

where \(C\) is a constant factor.

### 4 Radial Rosen-Morse potential

By setting \(q = 1\) in the expression [1], we obtain the so-called radial Rosen-Morse potential
\[ V(r) = -\frac{V_1}{\cosh^2 \left( \frac{r}{a} \right)} + V_2 \tanh \left( \frac{r}{a} \right). \] (23)

The \( L_{\nu_q} \) and \( \nu_q \) parameters defined by expressions (19) can be written
\[
\begin{cases}
L_{\nu_1} = \frac{1}{2} (\nu_1 - 1), \\
\nu_1 = \sqrt{1 + \frac{8m^2V_1}{\hbar^2}}.
\end{cases}
\] (24)

In this case, it follows from (21) and (22) that the transcendental quantization condition for the bound state energy levels \( E_{n_r} \) and the wave functions are
\[
_{2}F_{1} \left( M_1(E_{n_r}) - L_{\nu_1}, L_{\nu_1} + M_1(E_{n_r}) + 1, M_1(E_{n_r}) + M_2(E_{n_r}) + 1; \frac{1}{2} \right) = 0,
\] (25)

\[
_{2}F_{1} \left( M_1(E_{n_r}) - L_{\nu_1}, L_{\nu_1} + M_1(E_{n_r}) + 1, M_1(E_{n_r}) + M_2(E_{n_r}) + 1; \frac{1}{2} \frac{e^{2r/a}}{e^{2r/a} + 1} \right) = 0.
\] (26)

## 5 Conclusion

In this paper we have discussed the path integral problem for a deformed radial Rosen-Morse potential which is a potential with the Dirichlet boundary conditions. Our approach shows that the path integral in the present case is more rigorous in comparison to other methods. The derivation of the exact Green’s function for this potential problem contained in this study is obtained for the first time. The poles and the residues gave a transcendental quantization condition involving the hypergeometric function and the wave functions corresponding to the energy levels \( E_{n_r} \) of the \( s \)-states. The transcendental equation can be solved numerically.

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