Feynman integral treatement of the Hyperbolical potential with a centrifugal term approximation

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Abstract. We obtain an analytical expression for the energy eigenvalues of the Hyperbolical potential using an approximation of the centrifugal term. In order to obtain the l-states solutions, we use the the Feynman path integral approach to quantum mechanics. We show that by performing nonlinear space-time transformations in the radial path integral, we can derive a transformation formula that relates the original path integral to the Green function of a new quantum solvable system. The explicit expression of bound state energy is obtained and the eigenfunctions are given in terms of hypergeometric functions. The present results are consistent with those obtained by others methods.

1. Introduction

The calculation of exact solutions of the radial Schrödinger equation (rSe) in some physical potential models has been an important research area. Unfortunately, for an arbitrary l-state ($l \neq 0$), the radial Schrödinger equation (rSe) does not admit an exact solution. In this case, the rSe is solved numerically [1], or by approximation methods [2]. Different methods have been used in this sense such as the standard method [3] the asymptotic iteration method [4] and the exact quantization rule method [5]. An example of exponential-type potentials that we want to treat is the Hyperbolical potential, it has the form:

$$V^{Hyp}(r) = D\left[1 - \sigma_0 \coth(\alpha r)\right]^2 \tag{1}$$

Here D, α and σ_0 are positive parameters.

The purpose of this paper is to study l-states solution of the hyperbolical potential within the Feynman path integrals formalism in order to improve the previous results [6]. The method we propose consists of using the approximation [7] $\frac{1}{r^2} \approx \frac{1}{a^2}\left(C_0 + \frac{1}{e^{\frac{r}{a}}-1} + \frac{1}{(e^{\frac{r}{a}}-1)^2}\right)$, where C_0 is a dimensionless parameter, for the centrifugal term. This approximation is based on the expansion of the centrifugal term in a series of exponentials depending on the intermolecular distance r and keeping terms up to second order. The organization of the paper is as follows. In section 2, we calculate the l-wave eigensolutions for the Hyperbolical potential using the Duru-Kleinert method of path integral formalism. In section 3, we present our numerical results for certain values of the quantum numbers n and l. Conclusions are drawn in section 4.

2. The path integral for the Hyperbolical potential

The propagator related to the Hyperbolical potential, between two time-space points $(\vec{r}\,',t')$ and $\left(\vec{r}''\,,t''\right)$ is written [8]:

$$K(\vec{r}'',t'';\vec{r}',t') = \frac{1}{4\pi r'' r'} \sum_{l=0}^{\infty}(2l+1)K_l(r'',t'';r',t')P_l(\cos\theta). \tag{2}$$

$P_l(\cos\theta)$ is the Legendre polynomial with $\theta \equiv (\vec{r}'',\vec{r}')$ and

$$K_l(r'',t'';r',t') = \lim_{N\to\infty}\int \prod_{j=1}^{N}\exp\left[\frac{i}{\hbar}S_j\right]\prod_{j=1}^{N}\left[\frac{m}{2\pi i\hbar\varepsilon}\right]^{\frac{1}{2}}\prod_{j=1}^{N-1}dr_j. \tag{3}$$

with $S_j = \frac{m}{2\varepsilon}\left(\Delta r_j\right)^2 - \varepsilon V_{eff}(r_j)$ where

$$V_{eff}(r_j) = \frac{\hbar^2 l(l+1)}{2mr_j r_{j-1}} + D\left[1 - \sigma_0\coth(\alpha r_j)\right]^2 \tag{4}$$

$\Delta r_j = r_j - r_{j-1}$, $\varepsilon = t_j - t_{j-1}$, $t' = t_0$ and $t'' = t_N$,

To solve the above equation for non-zero angular momentum states, we need to apply the approximate scheme to the centrifugal term given by Ikhdair in ref [7]

$$\frac{1}{r^2} \approx 4\alpha^2\left[C_0 + \frac{e^{-2\alpha r}}{1-e^{-2\alpha r}} + \left(\frac{e^{-2\alpha r}}{1-e^{-2\alpha r}}\right)^2\right] \tag{5}$$

where the parameter $C_0 = 0.0823058167837972$ is a proper shift found by the expansion procedures. Therefore the equation (4) becomes

$$V_{eff}(r_j) = \frac{2\alpha^2\hbar^2 l(l+1)}{m}\left[C_0 + \frac{e^{-2\alpha r_j}}{1-e^{-2\alpha r_j}} + \left(\frac{e^{-2\alpha r_j}}{1-e^{-2\alpha r_j}}\right)^2\right]$$
$$+ D\left[1 - \sigma_0\coth(\alpha r_j)\right]^2 \tag{6}$$

we can also write :

$$V_{eff}(r_j) = -A\coth(\alpha r_j) + \frac{B}{\sinh^2(\alpha r_j)} + C, \tag{7}$$

where $A = 2D\sigma_0$, $B = \frac{\hbar^2}{8m}l(l+1)\left(2\alpha\right)^2 + D\sigma_0^2$ and $C = \frac{\hbar^2 l(l+1)C_0}{2m}\left(2\alpha\right)^2 + D\left(1+\sigma_0^2\right)$

In order to reach the expression of the space-time transformed propagator, we introduce the following space coordinate change

$$r = \left(\frac{1}{\alpha}\right)\text{arccoth}\left(2\text{coth}^2 q - 1\right). \tag{8}$$

The propagator expression becomes

$$\widehat{K}_l(q'',q';s'') = \exp\left[\frac{i}{\hbar}s''(E-C+A)(\frac{1}{\alpha})^2\right] \tag{9}$$

$$\times \int \mathcal{D}q(s)\exp\left[\frac{i}{\hbar}\int_0^{s''}\left(\frac{m}{2}\dot{q}^2 - \frac{\hbar^2}{2m}\left[\frac{\eta(\eta-1)}{\sinh^2 q} - \frac{\upsilon(\upsilon-1)}{\cosh^2 q}\right]\right)ds\right]$$

$$= \exp\left[\frac{i}{\hbar}s''(E-C+A)(\frac{1}{\alpha})^2\right]K_l^{MPT}(q'',q';s'') \tag{10}$$

with $\eta = \frac{1}{2} \pm \sqrt{1 + 8mB(\frac{1}{\alpha})^2/\hbar^2}$ and $\upsilon = \frac{1}{2} \pm \sqrt{-2m(\frac{1}{\alpha})^2(E - C - A)/\hbar^2}$ and K_l^{MPT} is the path integral of the modified Pöschl-Teller potential, which is a known solved problem [9].

The bound states and the wave functions are explicitly given by [10]:

$$\chi_{l,n}^{(k_1,k_2)}(q) = N_n^{(k_1,k_2)}(\sinh q)^{2k_2-1/2}(\cosh q)^{-2k_1+3/2} \tag{11}$$

$$\times {}_2F_1(-k_1 + k_2 + k, -k_1 + k_2 - k + 1; 2k_2; -\sinh^2 q) \tag{12}$$

and

$$E_n^{MPT} = -\frac{\hbar^2}{2m}\left[2(k_1 - k_2 - n) - 1\right]^2 \tag{13}$$

with $N_n^{(k_1,k_2)} = \frac{1}{\Gamma(2k_2)}\left(\frac{(2k-1)\Gamma(k_1+k_2-k)\Gamma(k_1+k_2+k-1)}{\Gamma(k_1-k_2+k)\Gamma(k_1-k_2-k+1)}\right)^{1/2}$, $k = k_1 - k_2 - n$.

The results (11) and (13) are used in the following section to determine the spectrum and wave functions of the Hyperbolical potential.

2.1. Energy spectrum and wave functions

Calculating $K_l(q'', q'; s'')$ allows us to obtain the Green function. Since this is known, the whole energy spectrum is obtained from its poles, and from the residues at the poles we obtain the corresponding wave functions.

Substituting (11) in (10), we get

$$\widehat{K}_l(q'', q'; s'') = \sum_{n=0}^{N_m} \exp\left\{\frac{i}{\hbar}s''\left[(E - C + A)(2a)^2 - E_n^{MPT}\right]\right\}\chi_{l,n}^{(k_1,k_2)}(q'')\chi_{l,n}^{*(k_1,k_2)}(q') \tag{14}$$

Then, by integrating this latter over the pseudo-time parameters s'', the Green function G is written as:

$$G_l(r'', r'; E) = \sum_{n=0}^{N_m} \frac{\chi_{l,n}^{MR(k_1,k_2)}(r'')\chi_{l,n}^{MR*(k_1,k_2)}(r')}{E_{n,l}^{MR} - E} \tag{15}$$

As in [11, 12], satisfying the boundary conditions for $r \to 0$ and $r \to \infty$ gives:

$$k_1 = \frac{1}{2}\left[(1 + \frac{1}{2}\left(s + 2n + 1\right)) + 2mA(\frac{1}{\alpha})^2/(\hbar^2(s + 2n + 1)))\right],$$
$$k_2 = \frac{1}{2}\left(1 + \sqrt{1 + 8mB(\frac{1}{\alpha})^2/\hbar^2}\right) \equiv \frac{1}{2}(1 + s).$$

Substituting these values of k_1, k_2 in (11) and (13), and by considering $u = \frac{1}{2}[1 + \tanh(2\alpha r)]$, we get

$$\chi_{l,n}^{Hyp(k_1,k_2)}(r) = \sqrt{\alpha}N_n^{(k_1,k_2)}(u - 1)^{(1/2)-k_1+n}u^{k_1-1-(1/2)s-n}{}_2F_1(-n, 2k_1 - n - 1; s + 1; \frac{1}{1-u}) \tag{16}$$

The energy spectrum is obtained from the poles,

$$E_{n,l}^{Hyp} = \alpha^2 E_n^{MPT} - A + C \tag{17}$$

$$= -\left[\frac{\hbar^2\alpha^2(s + 2n + 1)^2}{8m} + \frac{2mA^2}{\hbar^2\alpha^2(s + 2n + 1)^2}\right] + C \tag{18}$$

Table 1. Eigenvalues $-E_{n,l}$ of the Hyperbolical potential in atomic units ($\hbar = m = 1$) with $D = 10$ and $\sigma_0 = 0.1$.

States	α	Present	Ikhdair et al[7]	Lucha et al[1]
2p	0.1	2.61885	2.61874	2.61935
	0.15	3.90570	3.90544	3.90645
	0.2	5.00378	5.00331	5.00457
	0.25	5.88668	5.88594	5.88725
3p	0.1	4.73552	4.73540	4.73638
	0.15	6.04569	6.04543	6.04649
	0.2	6.91710	6.91663	6.91733
	0.25	7.48474	7.48400	7.48358
3d	0.1	3.62734	3.62699	3.62769
	0.15	5.29484	5.29404	5.29510
	0.2	6.47635	6.47492	6.47598
4p	0.1	6.00298	6.00287	6.00390
	0.15	7.11552	7.11526	7.11589
4d	0.1	5.33164	5.33129	5.33216
	0.15	6.73663	6.73583	6.73642
4f	0.1	4.69036	4.68965	4.69058
	0.15	7.43683	6.42992	6.43112

3. Results and discussions

With our method, the energy $E_{n,l}^{Hyp}$ of the Hyperbolical potential, for angular momentum ($l \neq 0$), has been calculated. Indeed, to show the accuracy of the approximation scheme, we calculate the energy eigenvalues for various n and l quantum numbers. Our main results for the Hyperbolical potential (Eq. (18)) are displayed in the Table 1 and compared with the numerical values of Lucha and Schöberl [1] and with the Numerov-Uvanov method [7]. It is found that our energy eigenvalues are in good agreement with those obtained numerically [1], and better than those obtained by using Numerov-Uvanov method [7].

4. Conclusion

In this paper, we have given analytic solutions for the Hyperbolical potential by using an approximation scheme for the centrifugal term potential. This approach enables us to find the l-dependent solutions and the corresponding energy eigenvalues for different screening parameters of the Hyperbolical potential.

Finally, the set of results we have ended with shows that the path integral approach constitutes a reliable alternative to the Schrödinger formalism for solving such problems.

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