The Arbitrary l-state Solutions of the Hellmann Potential by Feynman Path Integral Approach

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Author's contribution

The sole author designed, analysed, interpreted and prepared the manuscript.

Original Research Article

ABSTRACT

In this study, we used the Path integral method to obtain the bound state solutions of the Hellmann potential. Firstly we analytically derived the radial kernel expression of the Hellmann potential using the approximation of the centrifugal term and space-time transformations. Then we calculated the exact energy spectrum and the normalized eigenfunction from the poles of the Green function and their residues. We expressed normalized wave functions in terms of Jacobi polynoms and Hypergeometric functions.

1. INTRODUCTION

In recent years, numerous studies have been carried out to obtain the analytical full solutions of the wave equations of various potentials in relativistic and non-relativistic quantum mechanics. Many methods are used for this purpose: SUSYQM formalism the Nikiforov-Uvarov approach, Functional analysis approach, Factorization method, Path Integral, the power series expansion, the asymptotic iteration method [1–10].

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The Hellmann potential expressed as the sum of Yukawa and Coulomb potentials is:

$$V(r) = -\frac{A}{r} + B\frac{e^{-\alpha r}}{r} \quad . \tag{1}$$

Here A and B are the strengths of potentials and α is the screening parameter. A and B may also be positive and negative, assuming positive parameters α. The Hellmann potential, which has many applications in atomic physics and condensed physics, is used to represent electron-nuclei and electron-ion interactions [11-17]. It has been used as a model for potential alkaline hydride molecules and has been found to be an appropriate potential for studying inner shell ionization problems [18,19,20].

Feynman path integral is one of the methods of obtaining analytical solution used to describe the energy spectrum and wave functions of systems. This method is in complete agreement with the general formalism of quantum mechanics suggested by Schrödinger, Heisenberg and Dirac. It is based on the propagator containing quantum mechanical amplitude for a point particle at a position x_a at time t_a to reach a position x_b at time t_b integrate over all possible paths connecting by the classical action. Using path integral method, the kernel of the system and the Green function are obtained so that they can be derived with the help of the energy spectrum and the corresponding wave functions [21]. Although the path integral method is a powerful method, it is difficult to calculate the path integral for a number of quantum mechanical systems. Duru and Kleinert developed a method called Kustaanheimo-Stiefel (KS) transformation in order to apply this method to the H-atom problem in 1979 [5]. Then, relativistic and non-relativistic wave equations of various potentials were studied: the Morse oscillator, the Woods-Saxon potential, the Hulthen potential [6-10]. In spherical symmetric systems, the centrifugal barrier term appears, which plays an important role in the scattering problems of the physics. The Schrodinger equation with some exponential type potentials does not have analytical l-wave solutions. For such potentials, they must use approximation schemes because of the term centrifugal barrier. Several methods have been used to obtain exact or approximate solutions of the Schrödinger equation for exponential type potentials [12-17].

The object of this study is to evaluate energy spectrum and wave functions of the Hellmann potential via path integral method. The organization of this paper is as follows. In section 2.1 Kernel and energy dependent Green's function of Hellmann potential are derived using space-time transformation. In section 2.2 energy eigenvalues and the corresponding wave functions are obtained using Green's function.

2. MATERIALS AND METHODS

2.1 The Kernel of the Hellmann Potential

The kernel of spherical symmetric potential between the initial position r' at time $t' = 0$ and final position r'' at time t'' has the following form [22]:

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

where $P_l(cos\theta)$ is the Legendre Polynomial with the $\theta \equiv (r'', r')$ and $K_l(r'', t''; r', t')$ is the radial Kernel in the time interval Δt_j. Path integral express in terms of an integral over all paths in configuration space. Radial kernel is described as

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

Here S_j is partial action and $\Delta r_j = r_j - r_{j-1}$, $\varepsilon = t_j - t_{j-1}$, $t' = t_0 = t_a$, $t'' = t_N = t_b$. Partial action is

$$S_j = p_j(r_j - r_{j-1}) - \left[\frac{p_j^2}{2m} + \frac{\hbar^2 l(l+1)}{2\mu r^2} + V(r_j)\right]. \tag{4}$$

Using the term of the following approximation instead of the centrifugal term

$$\frac{1}{r^2} = \frac{\alpha^2}{(1-e^{-\alpha r})^2} \tag{5}$$

inserting the radial kernel Eq. (3) becomes

$$
K_l\left(r^{''},t^{''};r^{'},t^{'}\right) = \lim_{n\to\infty} \int_{-\infty}^{\infty} \prod_{j=1}^{n} dr_j \prod_{j=1}^{n+1} \frac{dp_j}{2\pi} \exp\left\{\frac{i}{\hbar}\sum_{j=1}^{n+1}[p_j(r_j - r_{j-1})\right.
$$
$$
\left. - \frac{p_j^2}{2\mu} - \frac{\hbar^2 l(l+1)}{2\mu}\left[\frac{\alpha^2}{(1 - e^{-\alpha r})^2}\right] - V(r_j)\right.
$$

(6)

Defining the new angular variable $\theta\epsilon(0,\pi)$ to transform the radial variable $r\epsilon(0,\infty)$

$$
r = -\frac{1}{\alpha}\ln(-cot^2\theta) \qquad p_r = \frac{\alpha}{2}sin\theta cos\theta p_\theta
$$

(7)

the kernel in Eq. (6) can be written as

$$
K_l\left(\theta^{''},\theta^{'};T\right) = \frac{\alpha}{2}sin\theta_b cos\theta_b \int D\theta Dp_\theta \exp\left\{i\int_0^T dt[p_\theta\dot{\theta}\right.
$$
$$
\left. - \frac{\alpha^2}{4}sin^2\theta cos^2\theta\frac{p_\theta^2}{2\mu} - \frac{\hbar^2 l(l+1)}{2\mu}\alpha^2 sin^4\theta + A\alpha sin^2\theta + B\alpha cos^2\theta]\right\}
$$

(8)

where $\alpha sin\theta_b cos\theta_b$ is the contribution to Jacobien because of the coordinate transformation in Eq. (7). When the factor $\alpha^2 sin^2\theta cos^2\theta$ in front of kinetic energy term is the eliminated by the time transformation [6-9]

$$
\frac{dt}{ds} = \frac{4}{\alpha^2 sin^2\theta cos^2\theta}
$$

(9)

the Fourier transform of the δ −function is added to the kernel as follows

$$
1 = \int ds \frac{4}{\alpha^2 sin^2\theta_b cos^2\theta_b}\delta\left(T - \int ds\frac{1}{\alpha^2 sin^2\theta cos^2\theta}\right)
$$
$$
= \int dS \int \frac{dE}{2\pi}\frac{4}{\alpha^2 sin^2\theta_b cos^2\theta_b}exp\left[i(ET - \int ds\frac{1}{\alpha^2 sin^2\theta cos^2\theta})\right].
$$

(10)

Then radial kernel becomes

$$
K_l\left(\theta^{''},\theta^{'};T\right) = \frac{1}{\alpha sin\theta_b cos\theta_b}\int_{-\infty}^{\infty}\frac{dE}{2\pi}e^{iET}\int_0^{\infty} dS\int D\theta Dp_\theta e^{i2\frac{\hbar^2 l(l+1)}{\mu}S}
$$

$$
\times \exp\left\{i\int_0^S ds\left[p_\theta\dot{\theta} - \frac{p_\theta^2}{2\mu} - \frac{1}{2\mu}\left(\frac{-\frac{8\mu B}{\alpha} + \frac{8\mu E}{\alpha^2}}{sin^2\theta} + \frac{4\hbar^2 l(l+1) - \frac{8\mu A}{\alpha} + \frac{8\mu E}{\alpha^2}}{cos^2\theta}\right)\right]\right\}
$$

(11)

We can symmetrize the contribution from Jacobien to coordinate transformation as follows

$$
\frac{1}{\alpha sin\,\theta_b\,cos\,\theta_b} = \frac{2}{\alpha\sqrt{sin\,2\,\theta_a\,sin\,2\,\theta_b}}exp\left(i\int_0^S ds(-i)\frac{cos\,2\,\theta}{sin\,2\,\theta}\dot{\theta}\right)
$$

(12)

Thus Eq. (11) takes

$$
K_l(r^{''},r^{'};E) = \int_0^{\infty} dS e^{i2\frac{\hbar^2 l(l+1)}{\mu}S}\int_{-\infty}^{\infty}\frac{dE}{2\pi}e^{iET}\frac{1}{\alpha\sqrt{sin\,2\theta_a\,sin\,2\theta_b}}K(\theta_b,\theta_a;S)
$$

(13)

where

$$K(\theta_b, \theta_a; S) = \int D\theta Dp_\theta \, exp\{i \int_0^S ds[p_\theta \dot{\theta} - \frac{p_\theta^2}{2\mu} - \frac{1}{2\mu}\left(\frac{\kappa(\kappa-1)}{sin^2 \theta} + \frac{\lambda(\lambda-1)}{cos^2 \theta}\right) - \frac{ip_\theta \cos 2\theta}{2 \sin 2\theta}]$$

(14)

and κ and λ are

$$\kappa = \frac{1}{2}\left[1 \pm \sqrt{1 + \frac{32}{\alpha}\left(\frac{\mu E}{\alpha} + \mu B\right)}\right]$$

$$\lambda = \frac{1}{2}\left[1 \pm \sqrt{1 + \frac{32}{\alpha}\left(-\mu A + \frac{\hbar^2}{2}l(l+1) + \frac{\mu E}{\alpha}\right)}\right]$$

(15)

The path integral solutions of the Trigonometric Pöschl-Teller potential are well known that the kernel in Eq. (14) can be reduced to the potential of this potential

$$K(\theta_b, \theta_a; S) = \int D\theta Dp_\theta \, exp\{i \int_0^S ds \, [p_\theta \dot{\theta} - \frac{p_\theta^2}{2} - \frac{1}{2}(\frac{\kappa(\kappa-1)}{sin^2 \theta} + \frac{\lambda(\lambda-1)}{cos^2 \theta})]$$

(16)

The expression of the kernel in Eq. (16) in relation to the wave functions is as follows

$$K(\theta_b, \theta_a; S) = \sum_{n=0}^{\infty} exp[-i(S/2)(\kappa + \lambda + 2n)^2] \, \psi_n(\theta_a)\psi^*_n(\theta_b)$$

(17)

Where

$$\psi_n(\theta) = \sqrt{2(\kappa + \lambda + 2n)}\sqrt{\frac{\Gamma(n+1)\Gamma(\kappa+\lambda+n)}{\Gamma(\lambda+n+1/2)\Gamma(\kappa+n+1/2)}}$$
$$\times (cos \, \theta)^\lambda (sin \, \theta)^\kappa P_n^{(\kappa-1/2, \lambda-1/2)}(1 - 2 \, sin^2 \, \theta)$$

(18)

and energy spectrum is $\varepsilon_n = \frac{1}{2}(\kappa + \lambda + 2n)^2$.

Using the kernel, we can obtain the Green's function. The Green's function for Hellmann potential is written as

$$G(x_b, x_a; E) = \frac{-4i}{\alpha\sqrt{sin \, 2\theta_a \cos 2\theta_b}}$$
$$\times \sum_{n=0}^{\infty} \int_{-\infty}^{\infty} \frac{dE}{2\pi} \frac{e^{iET}}{(\kappa + \lambda + 2n)^2 - 4\frac{\hbar^2}{\mu}l(l+1)} \psi_n(\theta_a)\psi^*_n(\theta_b)$$

(19)

2.2 Energy Eigenvalues and Wave Functions

Green's function and Kernel for the Hellmann potential was calculated in section (2.1) using Feynman Path integral method. Integrating over dE, the energy eigenvalues can be derived from the poles of the Green function as

$$E_n = -\frac{\alpha}{32\mu} - \alpha A + \frac{\hbar^2 \alpha^2 l(l+1)}{2\mu}$$

$$-\frac{\alpha^2}{2\mu}\left\{\frac{\frac{1}{4}[\sqrt{\frac{4\hbar^2 l(l+1)}{\mu}}-(2n+1)]^2-\hbar^2 l(l+1)-\frac{2\mu A}{\alpha}+\frac{2\mu B}{\alpha}}{\sqrt{\frac{4\hbar^2 l(l+1)}{\mu}}-(2n+1)}\right\}^2. \tag{20}$$

If Eq. (13) perform

$$K_l\left(r'',r';E\right)=\sum_{n=0}^{\infty}e^{-iE_{nl}T}\varphi_n(r_a)\varphi_n^*(r_b)$$

Here

$$\varphi_n(r)=2\sqrt{2}\sqrt{(\kappa_n+\lambda_n+2n)}\sqrt{\frac{\Gamma(n+1)\Gamma(\lambda_n+\kappa_n+n)}{\Gamma(\lambda_n+n+1/2)\Gamma(\kappa_n+n+1/2)}}$$
$$\times\frac{i(-e^{-\alpha r})^{\lambda_n-1/2}}{\alpha(1-e^{-\alpha r})^{\kappa_n+\lambda_n+2}(1+e^{-\alpha r})^{1/2}}P_n^{(K_n-1/2,\lambda_n-1/2)}\left(-\frac{1+e^{-\alpha r}}{1-e^{-\alpha r}}\right) \tag{21}$$

where we got

$$\lambda_n=$$
$$\frac{1}{2}\{1\pm\frac{\alpha}{[\sqrt{\frac{4\hbar^2 l(l+1)}{\mu}}-(2n+1)]}[(\sqrt{\frac{4\hbar^2 l(l+1)}{\mu}}-(2n+1))^2-\hbar^2 l(l+1)-\frac{2\mu A}{\alpha}+$$
$$\frac{2\mu B}{\alpha}]+\sqrt{-\frac{\alpha}{3}\frac{}{\mu}-\alpha A+\frac{\hbar^2\alpha^2 l(l+1)}{2\mu}}\}$$

$$\tag{22}$$

And

$$\kappa_n=\frac{1}{2}\{1\pm\frac{\alpha}{[\sqrt{\frac{4\hbar^2 l(l+1)}{\mu}}-(2n+1)]^2}[(\sqrt{\frac{4\hbar^2 l(l+1)}{\mu}}-(2n+1))^2-\hbar^2 l(l+1)-\frac{2\mu A}{\alpha}+\frac{2\mu B}{\alpha}]-$$
$$\sqrt{-\frac{\alpha}{3}\frac{}{\mu}-\alpha A+\frac{\hbar^2\alpha^2 l(l+1)}{2\mu}}\}.$$

Using the following equation

$$P_n^{(\alpha,\beta')}(z)=\frac{\Gamma(n+\alpha+1)}{n!\,\Gamma(\alpha+1)}F\left(-n,n+\alpha+\beta'+1,\beta'+1,\frac{1+z}{2}\right) \tag{21}$$

We can write the wave function in Eq. (21) with the terms of the hypergeometric functions as

$$\phi(x)=\sqrt{(\kappa_n+\lambda_n+2n)}\sqrt{\frac{\Gamma(n+1)\Gamma(\kappa_n+\lambda_n+n)\Gamma\left(n+\kappa_n+\frac{1}{2}\right)}{\Gamma\left(n+\lambda_n+\frac{1}{2}\right)}}$$
$$\times\frac{(-ie^{-\alpha r})^{\gamma-\frac{1}{2}}}{\alpha(1-e^{-\alpha r})^{\kappa_n+\lambda_n-2}(1-e^{-\alpha r})^{\frac{1}{2}}}$$
$$\times F\left(-n,\kappa_n+\lambda_n+n,\lambda_n+1/2,-\frac{e^{-\alpha r}}{1-e^{-\alpha r}}\right). \tag{24}$$

Therefore we evaluated energy spectrum and wave functions for the Hellmann potential.

3. CONCLUSIONS

In this work, we have investigated the Schrodinger Equation with the Hellmann potential for n, l quantum states. We used space-time transformation to obtain energy eigenvalues and corresponding wave functions. We expressed normalized wave functions in terms of Jacobi polynoms and Hypergeometric functions.

COMPETING INTERESTS

Author has declared that no competing interests exist.

REFERENCES

1. Gendenshtein L, Krive IV. Supersymmetry in quantum mechanics. Sov. Phys. USP. 1985;28:645.
2. Ikhdair SM, Sever R. Approximate analytical solutions of the generalized Woods-Saxon potentials including the spin-orbit coupling term and spin symmetry. Cent. Eur. J. Phys. 2010;8(4): 652.
3. Falaye BJ. The Klein-Gordon equation with ring-shaped potentials: Asymptotic iteration method. J. Math. Phys. 2012;53:082107.
4. Qiang WC, Dong SH. Analytical approximations to the solutions of the Manning–Rosen potential with centrifugal term. Phys. Lett. A. 2007;13:368.
5. Duru IH, Kleinert H. Solution of the path integral for the H-atom. Phys. Letters B. 1979;84:185.
6. Kandirmaz N, Sever R. Chinese J. Phys. 2009;47:47.
7. Kandirmaz N, Sever R. Acta Polytech. 2011;51.
8. Kandirmaz N. PT-/non-PT-symmetric and non-Hermitian generalized woods-saxon potential: Feynman path integral approach. Gazi Univ. Journal of Sci. 2017;30(1):133-138.
9. Kandirmaz N. Global Journal of Science Frontier Research: A. 2018;18(6).
10. Kandirmaz N. J. Math. Phys. 2018;59(6): 063510.
11. Hellmann H. A new approximation method in the problem of many electrons. J. Chem. Phys. 1935;3:61.
12. Qiang WC, Dong SH. Physics Letters A. 2007;368(1-2):13-17.
13. Adamowski J. Phys Rev. A. 1985;31:43.
14. Arda A, Sever R. Phys. Scr. 2014;89: 105204.
15. Sever R, Tezcan C. Bound state energy eigenvalues of generalized hellmann potential. Phys. Scr. 1995;51:13-15.
16. Onate CA, Onyeaju MC, Ikot AN, Ebomwonyi O. Eur Phys J Plus. 2017;132:462.
17. Ebomwonyi O, Onate CA, Onyeaju MC, Ikot AN. Karbala International Journal of Modern Science. 2017;3:56-98.
18. Hamzavi M, Thylwe KE, Rajabi A. Approximate bound states solution of the hellmann potential. A Com. Theo. Phys. 2013;60(1).
19. Varshni YP, Shukla RC. Rev. Mod. Phys. 1963;35:130.
20. Das JN, Chakraborty S. Phys. Rev. A. 1985;32:176.
21. Feynmann R, Hibbs A. Quantum mechanics and path integrals McGraw Hill, New York; 1965.
22. Khandekar DC, Lawande SV, Bhagmat KV. Path integral methods and their applications. World Scientific, Singapore; 1986.