

ARBITRARY L-WAVE SOLUTION OF THE FEYNMAN PROPAGATOR FOR THE SCREEN COULOMB POTENTIAL

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Abstract: We present the l-states solutions of the Feynman propagator equation for the screen coulomb potential within the framework of the Duru-Kleinert transformation method. We show that the bound state energy eigen-values can be obtained for any n and l values without using an approximation of the centrifugal term required by other methods. Our results are compared with those obtained with other methods.

Index terms: Path integral, screen coulomb potential, l-states

I. INTRODUCTION

The search for exact solutions of the radial Schrödinger equation constitutes a very useful research area and is of general interest. There are only a few potentials that can be solved explicitly for all n and l but cannot be generalized to exponential type potentials. In this case, the radial Schrödinger equation as well as relativistic Dirac and Klein-Gordon equations are solved either numerically [1], or by approximation methods [2].

In this work, we study another exponential-type potential, namely an attractive screen Coulomb potential of the form:

$$U(r) = D \frac{e^{-\alpha r}}{r}, \quad (1)$$

where D represent the potential strength and α is the screening parameter. This potential is often used in atomic and molecular physics [3, 4]. This paper is organized as follows. In Sec. 2, we derive arbitrary l-states solutions of the screen Coulomb potential within the Feynman path integrals formalism by approximate method. In Sec.3, the numerical calculations are given to compare with those obtained by other method. The concluding remarks are given in Sec. 4.

II. PATH INTEGRAL METHOD

PATH INTEGRAL METHOD

The propagator for a particle of mass m in the spherically symmetric potential can be developed into a sum of partial waves of the form [5]:

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

$P_l(\cos(\theta))$ is the Legendre polynomial and

$$K(r'',t'';r',t') \lim_{n \rightarrow \infty} \left(\frac{\mu}{2\pi i \hbar \varepsilon} \right)^{\frac{n}{2}} \int \dots \int \exp \left\{ \frac{i}{\hbar} \sum_{j=1}^n S_j \right\} \prod_{j=1}^{n-1} dx_j \quad (3)$$

Here

$$S_j = \frac{\mu}{2\varepsilon} (r_j - r_{j-1})^2 - \varepsilon U_{eff}(r_j), \quad (4)$$

With

$$\Delta r_j = r_j - r_{j-1}, \quad \varepsilon = \Delta t_j = t_j - t_{j-1}, t' = t_0 \text{ and } t'' = t_n.$$

Where

$$U_{eff}(r_j) = U(r) + \frac{l(l+1)\hbar^2}{2\mu r^2} \quad (5)$$

To calculate the propagator K_l given by equation (3) for l- states, we apply the following approximate scheme to the centrifugal term [6]:

$$\frac{1}{r^2} \approx \frac{4\alpha^2 e^{-2\alpha r}}{(1-e^{-2\alpha r})^2} + \frac{\alpha^2}{3} \quad (6)$$

In addition, the term $1/r$ in the potential is replaced by [6]

$$\frac{1}{r} \approx \frac{2\alpha e^{-\alpha r}}{1-e^{-2\alpha r}}, \quad (7)$$

The potential (5), becomes

$$U_{eff}(r_j, \ell) = V_0 - V_1 \frac{e^{-2\alpha r}}{(1-e^{-2\alpha r})} + V_1 \left(\frac{e^{-2\alpha r}}{(1-e^{-2\alpha r})} \right)^2, \quad (8)$$

with

$$\begin{cases} V_0 = 2\alpha D \\ V_1 = \frac{2\ell(\ell+1)\alpha^2 \hbar^2}{m} \\ k = \frac{\ell(\ell+1)\alpha^2 \hbar^2}{6} \end{cases} \quad (9)$$

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

Putting

this gives

$$U_{eff}(r_j, \ell) = -A \coth(\alpha r) + \frac{B}{\sinh^2(\alpha r)} + C \quad (10)$$

With

$$\begin{cases} A = \frac{V_0 + V_1}{2} \\ B = \frac{V_1}{4} \\ C = k + \frac{V_0 + V_1}{2} \end{cases} \quad (11)$$

In the following, we study the potential (10) with the Duru-Kleinert method [7]. The path integral for the potential (7) is

$$K_1(r,t;r',t') = \int Dr(t) \exp \int_{t'}^t \left(\frac{m}{2} \dot{r}^2 - U_{eff}(r) \right) dt \quad (12)$$

By achieving the space-time transformations

$$\begin{cases} r = f(q) \\ dt = f'^2(q) ds \end{cases} \quad (13)$$

In our case, we choose

$$r = \frac{1}{\alpha} \operatorname{arccoth}(2 \coth^2 q - 1) \quad (14)$$

This transformation allows us to reformulate the problem of the potential to the modified Pöschl-Teller potential, which is a known solved problem.

A. Energy Spectrum

Calculating allows us to obtain the Green function G. Then, the whole energy spectrum is derived from the poles, and the corresponding wave functions from the residues at the poles.

The energy spectrum is given by

$$E_{n,l} = \left[\frac{\hbar^2 (s+2m+1)^2 \alpha^2}{32m} + \frac{8mA}{\hbar^2 (s+2m+1)^2} \right] + C, \quad (15)$$

with

$$s = \sqrt{1 + \frac{8mB}{\alpha^2 \hbar^2}}$$

III. NUMERICAL RESULTS

To show the accuracy of energy levels obtained in this work with the path integral method, we calculate the energy levels (15) for different quantum numbers n and l with two different values of parameter D. These results are compared to those exact results obtained by using a MATHEMATICA package programmed by Lucha and Schöberl [8] as shown in Tables 1 and 2. In addition, a comparison is made with the calculations of Dong et al. [6], who solved analytically the Schrödinger equation, but using the same approach for the centrifugal barrier. We remark that our results are almost indistinguishable from the numerical ones. Nevertheless, except in a few cases, we get results closer to the numerical estimates compared to the method of Dong [6]. This is due to our choice of the centrifugal barrier.

Table 1: Eigenvalues $E_{n,l}$ for the screen Coulomb potential in atomic units ($\hbar=m=1$) with $D=2.0$

state	α	D=5.0		
		Dong[6]	Present	Exact[8]
2p	0.025	-3.001042	-3.001040	-2.990105
	0.050	-2.879167	-2.879170	-2.869715
	0.075	-2.759375	-2.759380	-2.75225

3p	0.025	-1.266493	-1.266490	-1.262756
	0.050	-1.149306	-1.149310	-1.148927
	0.075	-1.037326	-1.037330	-1.041997
3d	0.025	-1.266076	-1.266080	-1.266778
	0.050	-1.147639	-1.147640	-1.151211
	0.075	-1.033576	-1.033580	-1.041558
4p	0.025	-0.661042	-0.661042	-0.660686
	0.050	-0.550417	-0.550417	-0.555443
4d	0.025	-0.660625	-0.660625	-0.662258
	0.050	-0.548750	-0.548750	-0.555393
4f	0.025	-0.660000	-0.660000	-0.661658
	0.050	-0.546250	-0.546250	-0.552427
5p	0.025	-0.382604	-0.382604	-0.384337
5d	0.025	-0.382188	-0.382188	-0.384921
5f	0.025	-0.381563	-0.381563	-0.384264
5g	0.025	-0.380729	-0.380729	-0.383204
6p	0.025	-0.233264	-0.233264	-0.236554
6d	0.025	-0.232847	-0.232847	-0.236689
6f	0.025	-0.232222	-0.232222	-0.236012
6g	0.025	-0.231389	-0.231389	-0.234998

CONCLUSION

In this paper, we have presented a path integral treatment for the screen Coulomb potential. By using an approximation scheme for the centrifugal term and a nonlinear space-time transformation in the radial path integral, we were able to derive explicit expression of the energy eigenvalues in function of the potential parameters.

The barrier approximation being fixed, we note that the Feynman integral method gives results closer to numerical one than solving the Schrödinger equation.

To conclude, our method is efficient in solving this type of potentials. We intend in a near future, to expand the path integral method to a more general form of potentials and relativistic cases.

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