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AID SALAH EDDINE

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Mr. M. Benarous	Professeur UHB-Chlef	Président
Mr. H. Boukabcha	M. C. A UDB-Khemis Miliana	Encadreur
Mr. M. Belabbas	Professeur UHB-Chlef	Co-encadreur
Mr. A. Hocine	M. C. A UHB-Chlef	Examinateur
Mr. K. Mohamed Elhadj	M. C. A UHB-Chlef	Examinateur
Mr. M. Douici	M. C. A UDB-Khemis Miliana	Examinateur

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Solving problems in the physics of the system of diatomic potentials via path integrals

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presented by

Aid Salah Eddine

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Supervisor: Dr. Boukabcha Hocine

Co-supervisor: Pr. M. Belabbas

Thesis committee:

President : Pr. M. Benarous

Examiners : Dr. A. Hocine
Dr. K. Mohamed Elhadj
Dr. M. Douici

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Dedication

To My father and my mother.

To my wife.

To my brothers and sisters.

To all my friends near and far without exception.

Acknowledgments

This thesis represents the culmination of several years of research. As an introduction, I would like to express my gratitude to God, the Almighty and Merciful, for granting me the strength and patience to complete this modest work.

Secondly, I would like to express my heartfelt gratitude to my supervisor, Dr H. Boukabcha, for initiating this work and providing me with invaluable guidance. His patience and unwavering support have been crucial in guiding me through challenges and helping me find solutions to advance my research.

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Finally, I would like to express my deepest gratitude to my family, loved ones, and all the friends who have accompanied, supported, and encouraged me throughout the process of completing this work.

الملخص

تُعنى هذه الأطروحة بدراسة بعض الأنظمة الكمومية من المنظورين النسبي وغير النسبي اعتمادا على طريقة تكامل المسار لفاينمان. لقد قدمنا لمحة موجزة عن طريقة تكامل المسار وطريقة Duru-Kleinert لتحويل الزمكان.

في الإطار غير النسبي تم معالجة ثلاث مسائل : كمون Pöschl-Teller المثلثي، كمون Pöschl-Teller المعدل وكمون يوكاوا التربيعي العكسي المعمم (GIQY). يتضمن نهجنا تجاه المشكلتين الأوليين توسيع حلول الحالات s المتاحة في المراجع باستخدام تقريب Greene-Aldrich لتعويض الحد المركزي $1/r^2$. ومن جهة أخرى، اعتمدت معالجة كمون يوكاوا التربيعي العكسي المعمم (GIQY) -بالإضافة إلى استعمال تقريب مناسب للحدين $1/r$ و$1/r^2$ على تحويل زمكاني ملائم سمح باختزال الناشر (propagator) إلى مشكلة كمون Pöschl-Teller المعدل. قمنا بمقارنة النتائج مع بعض الدراسات السابقة ووجدناها مرضية.

في الإطار النسبوي، تم أخذ مشكلتين في الاعتبار: قمنا بدراسة مسألة جسيم عديم اللف خاضع لكمون يوكاوا التربيعي العكسي المعمم. حيث أسسنا تمثيل تكاملات المسار لهذا الكمون ودالة Green الموافقة له باستخدام التحويل الزمكاني السابق. كما تم استنتاج نتائج بعض الحالات الخاصة لهذا الكمون ، مما جعل من الممكن إجراء مقارنة مع نتائج الدراسات الأخرى التي تم الحصول عليها بشكل مختلف. كمسألة نسبية ثانية، تعاملنا مع جسيم ذو لف 1/2 خاضع لكمون سلمي وآخر شعاعي من النوع GIQY. تم الأخذ في الاعتبار كل من حالتي التناظر السبيني وشبه السبيني (spin and pseudospin symmetries). حيث اشتققنا معادلتين شبيهتين بمعادلة شرودنغر انطلاقا من المعادلات التفاضلية الجزئية الأربعة المقترنة التي تتضمنها معادلة ديراك. بعدها كتبنا دالة غرين لكل معادلة. بفضل التحول الزمكاني، تمكنا من مكاملة دالة غرين واستنتاج مستويات الطاقة للطيف المنفصل والمركّبات العلوية والسفلية للدوال الموجية الموافقة. كما تم عرض النتائج العددية والحالات الخاصة في الجزء الأخير من هذا العمل.

Abstract

This thesis uses Feynman's path integrals formalism to explore quantum systems from both relativistic and non-relativistic perspectives. We have provided a brief overview of the path integral approach and the Duru-Kleinert space-time transformation. Three problems have been examined for the non-relativistic regime: the trigonometric Pöschl-Teller, the modified Pöschl-Teller and the Generalized Inverse Quadratic Yukawa (GIQY) Potentials. Our approach to the first two problems involves expanding the available s-states solutions using the Greene-Aldrich approximation scheme to compensate for the centrifugal term. However, in addition to approximating the 1/r and $1/\mathrm{r}^2$ terms, the Generalized Inverse Quadratic Yukawa Potential treatment relied on an appropriate space-time transformation that allowed the propagator to be reduced to that of a modified Pöschl-Teller problem. We have compared the results to some previous approaches and it was satisfactory. For the relativistic regime, two problems have been considered: we have investigated the problem of a spinless particle subjected to Generalized Inverse Quadratic Yukawa potential. Path integral representation and its corresponding Green's function has been derived with the help of the previous space-time transformation. Particular cases were also considered, which made it possible to make comparison with other results obtained differently. As a second relativistic problem we have dealt with a spin-1/2 particle in vector and scalar potentials of GIQY type. Both spin and pseudospin symmetries were taken into account. From the four coupled partial differential equations included in Dirac equation, two Schrödinger's like equations has been derived . For every equation, a Green's function has been evaluated. Thanks to a space-time transformation, we have been able to integrate the Green's function and deduce the discrete spectrum energy levels and the upper and lower components of corresponding wave functions. numerical results and special cases were also presented in the last of this work.

Résumé

Cette thèse utilize le formalisme des intégrales de chemin de Feynman pour explorer des systèmes quantiques d'un point de vue à la fois relativiste et non relativiste. Nous avons fourni un bref aperçu de l'approche intégrale de chemin et de la transformation spatio-temporel de Duru-Kleinert. Trois problèmes ont été examinés pour le régime non relativiste : le potentiel de Pöschl-Teller trigonométrique, le potentiel de Pöschl-Teller modifié et le potentiel de Yukawa quadratique inverse généralisé (GIQY). Notre approche des deux premiers problèmes implique d'élargir les solutions disponibles pour les états s en utilisant le schéma d'approximation de Greene-Aldrich pour compenser le terme centrifuge. Cependant, en plus d'approcher les termes 1/r et 1/r^2, le traitement du potentiel GIQY reposait sur une transformation spatio-temporel appropriée qui permettait de réduire le propagateur à celui d'un problème de Pöschl-Teller modifié. Nous avons comparé les résultats à certaines approches précédentes et cela s'est avéré satisfaisant. Pour le régime relativiste, deux problèmes ont été considérés : nous avons étudié le problème d'une particule sans spin soumise au potentiel de Yukawa quadratique inverse généralisé. La représentation des intégrales de chemin et la fonction de Green correspondante ont été dérivées à l'aide de la transformation spatio-temporel précédente. Des cas particuliers ont également été considérés, ce qui a permis de faire une comparaison avec d'autres résultats obtenus différemment. Comme deuxième problème relativiste nous avons traité d'une particule de spin-1/2 en potentiels vectoriels et scalaires de type GIQY. les symétries de spin et de pseudospin ont toutes deux été prises en compte. Deux équations de type Schrödinger ont été dérivées des quatre équations aux dérivées partielles couplées incluses dans l'équation de Dirac. Une fonction de Green a été évaluée pour chaque équation. Grâce à une transformation spatio-temporel, nous avons pu intégrer la fonction de Green et en déduire les niveaux d'énergie du spectre discret et les composantes supérieure et inférieure des fonctions d'onde correspondantes. des résultats numériques et des cas particuliers ont également été présentés dans la dernière partie de ce travail.

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Introduction

Due to its successful results in explaining a variety of phenomena in physics and chemistry, the wave formulation of quantum mechanics is very well known and frequently used among scientists. This formulation is based on resolving the Schrödinger equation, which is concerned with the Hamiltonian of the system under consideration. Since every physical quantity in classical mechanics corresponds to a Hermitian operator in quantum mechanics, the correspondence principle plays a crucial in constructing this formulation. As examples, we attach the momentum p to the Hermitian operator $-i\hbar\frac{\partial}{\partial r}$ and the total energy E to the Hamiltonian operator H. However, it is well known that classical mechanics can be formulated based on the principle of minimum action, which places the Lagrangian at the center of attention. At this point, an intriguing question arises for the observer: Is it possible to reformulate quantum mechanics by starting from the least action principle and the Lagrangian instead of the Hamiltonian?

The answer to this question is very important, especially for systems for which the Hamiltonian cannot be derived. A first attempt to deal with this problem was made by Dirac in an article that laid the foundations for a new formulation of quantum mechanics, later known as path integral theory [1]. Dirac had proposed the proportionality between the elementary transition amplitude and $\exp\left(\frac{iA(r)}{\hbar}\right)$ as follows

$$\langle r''(t+\epsilon)\,|r'(t)\rangle = \beta \exp\left(\frac{iA(r)}{\hbar}\right) \tag{1}$$

In 1942, Feynman, who had invested in this idea in his doctoral thesis [2], gave a formulation of quantum mechanics in terms of the Lagrangian and was able to demonstrate that the constant of proportionality β is nothing but $\sqrt{\frac{M}{2\pi i\hbar\varepsilon}}$.

Late due to the World War, Feynman's first public formulation was revealed in the 1948 article [3]. Then the picture began to become clearer until appeared complete and more pedagogical in 1965 in Feynman and Hibbs' book "Quantum Mechanics and Path Integrals" [4].

Physicists subsequently paid a lot of attention to this formulation and considered it a powerful mathematical tool, so it was used in a wide variety of fields, including: Quantum mechanics [5], Statistical mechanics [6], Quantum field theory [7], String theory[8], stochastic dynamics [9], quantum gravity theory [10], Condensed matter [11] and polymer physics [12].

Many problems have already been solved using the path integration method for $\ell-$states by employing an analytical approximation to the centrifugal term. In the non-relativistic framework, we mention, for example, the improved Tietz potential problem [13], the Manning-Rosen potential [14] and deformed radial Rosen-Morse potential [15]. As for the relativistic framework, a number of problems have been addressed for spin 0 and spin 1/2 particles. For example, the Generalized Hulthén potential was solved for a spin 0 particle [16] , and the deformed Hulthén potential was solved for a spin 1/2 particle [17].

The aim of this thesis is the determination, within the framework of Feynman's formalism, of the Energy spectrum associated with the bound and continuous states as well as the corresponding wave functions relating to different potentials that we have chosen as examples to demonstrate the effectiveness and importance of the path integration method in addressing physical issues in all relativistic and non-relativistic fields. This is evident by comparing the results obtained based on this Formulation with the results of some other methods such as Nikiforov's method and John's method.

This would be revealed by contrasting the outcomes of some other approaches, such John's and Nikiforov's, with the results derived from this formulation.

The work in this thesis is divided into four main chapters

1/ Theoretical introduction: This section aims to outline the key concepts in path integral formulation that will be used in later chapters.

2/ The examination of some physical potential problems from a nonrelativistic perspective is covered in the second chapter, where we discussed the solutions of the trigonometric Pöschl-Teller, modified Pöschl-Teller, and Generalized Inverse Quadratic Yukawa potentials

3/ Chapter Three: Here we address the problem of a spinless particle by solving the Klein-Gordon equation for the Generalized Inverse Quadratic Yukawa potential.

4/ Chapter Four: In which we study a spin 1/2 particle by solving the Dirac equation for the Generalized Inverse Quadratic Yukawa potential.

In the conclusion, we emphasize the significance of the findings and the future directions for research that might be pursued.

Chapter 1

An Overview of the Path Integral Method

This chapter aims to introduce in a simplified manner a set of basic concepts for path integration techniques that we will use later in discussing the problems we propose to address in this work.

1.1 Propagator

In non-relativistic quantum mechanics, the equation of motion that governs the motion of particles is the following Schrödinger equation

$$i\hbar \frac{d}{dt} |\psi(t)\rangle = H |\psi(t)\rangle \,, \tag{1.1}$$

which H is the Hamiltonian of the system, write:

$$H = \frac{P^2}{2M} + V(r), \tag{1.2}$$

which is the sum of operators corresponding to the kinetic and potential energies of a system

with $P = -i\hbar\nabla$ is the momentum operator, M is the mass of the particle and $V(r)$ is the potential energy operator.

Suppose now that we have a particle at position r at time t that moves later to position r' at time t'. From (1.1) it is possible to derive the evolution equation in the form

$$|\psi(t')\rangle = \exp -\frac{i}{\hbar} H \ (t'-t) \ |\psi(t)\rangle \,, \tag{1.3}$$

for systems whose Hamiltonians are independent of time. the quantity $\exp -\frac{i}{\hbar} H \ (t'-t)$ is known as time-evolution operator

$$U(t', t) = \exp(-\frac{i}{\hbar} H(t'-t)), \tag{1.4}$$

in the position representation eq. (1.3) becomes

$$\langle r' | \psi(t') \rangle = \langle r' | \exp(-\frac{i}{\hbar} H(t'-t)) \; |\psi(t)\rangle \,, \tag{1.5}$$

inserting a completeness relation $\int d^{\,3}r \; |r\rangle \langle r| = 1$

$$\langle r' | \psi(t') \rangle = \int d^{\,3}r \;\; \langle r' | \exp -\frac{i}{\hbar} H \; (t'-t) \, |r\rangle \, \langle r | \psi(t) \rangle \,, \tag{1.6}$$

which means

$$\psi(r', t') = \int d^{\,3}r \;\; \langle r' | \exp -\frac{i}{\hbar} H \; (t'-t) \, |r\rangle \;\; \psi(r,t), \tag{1.7}$$

The kernel $\langle r' | \exp -\frac{i}{\hbar} H \; (t'-t) \, |r\rangle$ in eq. (1.7) is called the **propagator**, denoted by $K(r', t'; r, t)$,

$$K(r', t'; r, t) = \langle r' | \exp -\frac{i}{\hbar} H(t'-t) \, |r\rangle \tag{1.8}$$

and it represents the transition amplitude for a particle to travel from point (r, t) to point (r', t')

$$\psi(r', t') = \int d^{\,3}r \; K(r', t'; r, t) \; \psi(r,t), \tag{1.9}$$

The advantage of this relation is that if one knows the propagator $K(r', t'; r, t)$ and the initial wave function $\psi(r, t)$ of the particle at position r and moment t, then one directly derives the final wave function $\psi(r', t')$.

It should be noted that the propagator is also a solution that satisfies the Schrödinger equation

$$i\hbar \frac{d}{dt} K(r', t'; r, t) = \left(\frac{P^2}{2M} + V(r) \right) K(r', t'; r, t), \tag{1.10}$$

1.1.1 Time sliced propagator

In this section we will focus on how to write the **propagator** as an integral over all possible paths connecting the two endpoints, and for that we will invest in an important property of the time-evolution operator called the fundamental composition law [12]. If we have $U(t', t)$, a time evolution operator that translates the system from state $|\psi(t)\rangle$ at moment t to state $|\psi(t')\rangle$ at moment t' where

$$|\psi(t')\rangle = U(t', t) \;\; |\psi(t)\rangle \,, \tag{1.11}$$

and if t_1 is a moment between t and t' then we can write

$$|\psi(t_1)\rangle = U(t_1, t) \;\; |\psi(t)\rangle \,, \tag{1.12}$$

and

$$|\psi(t')\rangle = U(t',t_1)\ |\psi(t_1)\rangle\,, \tag{1.13}$$

this means that we divided the transition from t to t' into two stages, a transition from t to t_1, and then a transition from t_1 to t', and this leads to

$$|\psi(t')\rangle = U(t',t_1)\ U(t_1,t)\ |\psi(t)\rangle\,, \tag{1.14}$$

therefore

$$U(t',t) = U(t',t_1)\ U(t_1,t), \tag{1.15}$$

Feynman noticed this feature and thought of dividing the propagator into a large (infinitely) number of parts. To illustrate the idea, let's divide the time domain between the two endpoints into $N+1$ parts $\varepsilon = \frac{t'-t}{N+1}$

$$U(t',t) = U(t',t_N)U(t_N,t_{N-1})\ ....U(t_1,t), \tag{1.16}$$

and thus the propagator takes the form

$$\langle r'|\, U(t',t)\, |r\rangle = \langle r'|\, U(t',t_N)U(t_N,t_{N-1})\ ....U(t_1,t)\, |r\rangle \tag{1.17}$$

setting $t' = t_{N+1}$, $t = t_0$, $r' = r_{N+1}$, $r = r_0$ and inserting N completeness relation between each successive operator $U(t_n,t_{n-1})$

$$\int_{-\infty}^{+\infty} d^{\,3}r_n\, |r_n\rangle\, \langle r_n| = 1, \qquad\qquad n = 1,2,3,...,N \tag{1.18}$$

one can find the product

$$\langle r'|\, U(t',t)\, |r\rangle = \prod_{n=1}^{N}\left[\int_{-\infty}^{+\infty} d^{\,3}r_n\right]\prod_{n=1}^{N+1}\langle r_n|\, U(t_n,t_{n-1})\, |r_{n-1}\rangle \tag{1.19}$$

We calculate the propagator with the infinitesimal time, let it be

$$\langle r_n|\, U(t_n,t_{n-1})\, |r_{n-1}\rangle = \langle r_n|\exp\left(-\frac{i}{\hbar}H\ \varepsilon\right)|r_{n-1}\rangle \tag{1.20}$$

$$\langle r_n|\, U(t_n,t_{n-1})\, |r_{n-1}\rangle = \int_{-\infty}^{+\infty} d^{\,3}p_n\ \ \langle r_n|\ p_n\rangle\, \langle p_n|\exp\left(-\frac{i}{\hbar}H\ \varepsilon\right)|r_{n-1}\rangle \tag{1.21}$$

$$\langle r_n|\, U(t_n,t_{n-1})\, |r_{n-1}\rangle = \int_{-\infty}^{+\infty}\frac{d^{\,3}p_n}{2\pi\hbar}\ \ \exp\frac{i}{\hbar}\left(p_n(r_n-r_{n-1}) - H\ \varepsilon\right) \tag{1.22}$$

returning to eq. (1.19) we find

$$\langle r'| U(t',t) |r\rangle = \prod_{n=1}^{N}\left[\int_{-\infty}^{+\infty} d^{\,3}r_n\right]\prod_{n=1}^{N+1}\int_{-\infty}^{+\infty}\frac{d^{\,3}p_n}{2\pi\hbar}$$
$$\exp\frac{i}{\hbar}\sum_{n=1}^{N+1}\left(p_n(r_n-r_{n-1})-H\ \varepsilon\right) \tag{1.23}$$

The integral (1.23) over the momentum can be done using Gaussian integral formula which gives

$$\langle r'| U(t',t) |r\rangle = \lim_{N\to\infty}\left(\sqrt{\frac{M}{2\pi i\hbar\varepsilon}}\right)^{3(N+1)}\prod_{n=1}^{N}\left[\int_{-\infty}^{+\infty} d^{\,3}r_n\right]$$
$$\exp\frac{i}{\hbar}\sum_{n=1}^{N+1}\varepsilon\left(\frac{M(r_n-r_{n-1})^2}{2\varepsilon^2}-V(r_n)\right) \tag{1.24}$$

When N tends to infinity ∞, the integral (1.24) becomes inclusive of all possible intermediate positions between r' and r , and it can be said, then, that this is an integral over all possible paths linking between the two endpoints, and we write

$$\langle r'| U(t',t) |r\rangle = \int Dr(t)\ \exp\left(\frac{i}{\hbar}A\left(r\left(t\right)\right)\right) \tag{1.25}$$

where $A\left(r(t)\right)=\int Ldt$ is the Action defined in terms of the Lagrangian

$$L=\frac{M}{2}\dot{r}^{2}-V(r). \tag{1.26}$$

$Dr(t)$ is path integral measure.

Eq. (1.25) is the original Feynman's expression of the probability amplitude.

1.1.2 The spectral representation of the propagator

The importance of the propagator lies in the fact that it carries the necessary information related to the studied system, such as the energy spectrum and wave functions, and this can be summarized as follows:

Let us assume that we know the complete solutions of the time-independent Schrödinger equation

$$H\ \left|\varphi_n\right\rangle = E_n\left|\varphi_n\right\rangle, \tag{1.27}$$

which means that we know all states $\left|\varphi_n\right\rangle$, that achieve the relation

$$\sum_n \left|\varphi_n\right\rangle\left\langle\varphi_n\right| = 1, \tag{1.28}$$

inserting this relation into Eq. (1.8)

$$K(r',t';r,t) = \sum_n \langle r' | \, \varphi_n \rangle \, \langle \varphi_n \, | r \rangle \exp\left(-\frac{i}{\hbar} E_n (t'-t) \right), \tag{1.29}$$

thus

$$K(r',t';r,t) = \sum_n \varphi_n(r') \varphi_n^*(r) \exp\left(-\frac{i}{\hbar} E_n (t'-t) \right), \tag{1.30}$$

where $\langle r' | \, \varphi_n \rangle = \varphi_n(r')$ and $\langle \varphi_n \, | r \rangle = \varphi_n^*(r)$ are the wave functions corresponding to the eigenstates $|\varphi_n\rangle$ and $\langle \varphi_n|$, respectively.

1.2 Green's function

Green's function or the **fixed-energy amplitude** is the Fourier-transform of the propagator [18]

$$G(r',r;E) = \int_0^\infty e^{\frac{iE}{\hbar}T} K(r',r;T) dT \tag{1.31}$$

with $T = t' - t$,

At this point, it is desirable for the sake of simplicity to introduce the new quantity

$$P(r',r;T) = e^{\frac{iE}{\hbar}T} K(r',r;T) \tag{1.32}$$

which is called the **promotor [19],** in the discrete form we have

$$P(r',r;T) = \int Dr(t) \, \exp\left(\frac{i}{\hbar} A^E \right) \tag{1.33}$$

with the new action A^E defined by

$$A^E = \int_0^T dt \left(\frac{M}{2} \dot{r}^2 - V(r) + E \right). \tag{1.34}$$

therefore

$$G(r',r;E) = \int_0^\infty P(r',r;T) dT \tag{1.35}$$

For the spectral representation of the Green's function one can use eq. (1.30) in eq. (1.31) and find

$$G(r',r;E) = \sum_n \varphi_n(r') \varphi_n^*(r) \int_0^\infty dT \, \exp\left(\frac{i \; (E-E_n)}{\hbar} T \right), \tag{1.36}$$

performing the integral on dT gives

$$G(r', r; E) = \sum_n \varphi_n(r')\varphi_n^*(r)\frac{i\,\hbar}{E - E_n + i\eta}, \tag{1.37}$$

where η is an infinitesimal positive number.

Thinking about this expression (1.37) gives the impression that Green's function carries as much information as the propagator's, with regard to energy eigen values and corresponding wave functions. However, extracting the relations of these latter is easier when dealing with Green's function, where we see that the energy eigen values represent the poles of the Green's function and the wavefunctions represent its residues.

1.3 Path Integrals in Spherical Coordinates

In physics, there are many systems that have spherical symmetry and do not change with rotation. Therefore, it is very appropriate to study this type of system in spherical coordinates, which is easy to deal with and solve, and even simplifies it to a one-dimensional issue. In this section, we will derive the propagator expression's in spherical coordinates, to be used later in solving a number of issues intended by this thesis.

The spherical coordinates are defined by:

$$\begin{cases} x = r\sin\theta\cos\varphi, \\ y = r\sin\theta\sin\varphi, \\ z = r\cos\theta, \end{cases} \tag{1.38}$$

with $r \in [0, \infty[$, $\theta \in [0, \pi]$ and $\varphi \in [0, 2\pi[$,

the volume element in spherical coordinates is written as follows

$$d\overrightarrow{r} = r^2 \sin\theta dr d\theta d\varphi, \tag{1.39}$$

taking these considerations into account when writing the propagator, we find

$$\begin{aligned} K(r', t'; r, t) \quad &= \quad \lim_{N\to\infty}\left(\sqrt{\frac{M}{2\pi i\hbar\varepsilon}}\right)^{3(N+1)} \prod_{n=1}^{N}\left[\int_0^{+\infty}\int_0^{\pi}\int_0^{2\pi} r^2\sin\theta dr_n d\theta_n d\varphi_n\right] \\ &\exp\frac{i}{\hbar}\sum_{n=1}^{N+1}\varepsilon\left(\frac{M(r_n^2 + r_{n-1}^2 - 2r_n r_{n-1}\cos\Theta_{n,n-1})}{2\varepsilon^2} - V(r_n)\right), \end{aligned} \tag{1.40}$$

where

$$\begin{aligned} \Theta_{n,n-1} \quad &= \quad (\overrightarrow{r_n}, \overrightarrow{r_{n-1}}) \\ &= \quad \cos\theta_n\cos\theta_{n-1} + \sin\theta_n\sin\theta_{n-1}\cos\Delta\varphi_n \end{aligned} \tag{1.41}$$

with

$$\Delta\varphi_n = \varphi_n - \varphi_{n-1}. \tag{1.42}$$

Using the formula

$$e^{a\cos\phi} = \sqrt{\frac{\pi}{2a}}\sum_{l=0}^{+\infty}(2\ell+1)I_{l+1/2}(a)P_\ell(\cos\phi), \tag{1.43}$$

where $I_{l+1/2}(a)$ are the modified Bessel functions and $P_l(\cos\phi)$ are the Legendre polynomials of argument ϕ, we can write

$$\begin{aligned}\exp\left[-\frac{iMr_nr_{n-1}}{\varepsilon\hbar}\cos\Theta_{n,n-1}\right] &= \sqrt{\frac{i\varepsilon\hbar\pi}{2Mr_nr_{n-1}}}\\ &\sum_{\ell=0}^{+\infty}(2\ell+1)I_{\ell+1/2}\left(-\frac{iMr_nr_{n-1}}{\varepsilon\hbar}\right)\\ &P_\ell(\cos\Theta_{n,n-1}).\end{aligned} \tag{1.44}$$

The spherical harmonic addition theorem is

$$P_\ell(\cos\Theta_{n,n-1}) = \frac{4\pi}{2\ell+1}\sum_{m=-\ell}^{\ell}Y_{\ell,m}(\theta_n,\varphi_n)Y^*_{\ell,m}(\theta_{n-1},\varphi_{n-1}), \tag{1.45}$$

with the spherical harmonics defined by

$$Y_{\ell,m}(\theta_n,\varphi_n) = (-1)^m\sqrt{\frac{2\ell+1}{4\pi}\frac{(\ell+m)!}{(\ell-m)!}}P_\ell^m(\cos\theta)e^{im\varphi} \tag{1.46}$$

$$\begin{aligned}K(r',t';r,t) &= \lim_{N\to\infty}\left(\sqrt{\frac{M}{2\pi i\hbar\varepsilon}}\right)^{3(N+1)}\prod_{n=1}^{N}\left[\int_0^{+\infty}\int_0^{\pi}\int_0^{2\pi}r^2\sin\theta dr_nd\theta_nd\varphi_n\right]\\ &\exp\frac{i}{\hbar}\sum_{n=1}^{N+1}\varepsilon\left(\frac{M(r_n^2+r_{n-1}^2)}{2\varepsilon^2}-V(r_n)\right)\\ &\prod_{n=1}^{N+1}\sqrt{\frac{i\varepsilon\hbar\pi}{2Mr_nr_{n-1}}}\sum_{\ell=0}^{+\infty}(2\ell+1)I_{\ell+1/2}\left(-\frac{iMr_nr_{n-1}}{\varepsilon\hbar}\right)\frac{4\pi}{2\ell+1}\\ &\sum_{m=-\ell}^{\ell}Y_{\ell,m}(\theta_n,\varphi_n)Y^*_{\ell,m}(\theta_{n-1},\varphi_{n-1}),\end{aligned} \tag{1.47}$$

Now, if one uses the expansion

$$\int_0^{2\pi}\int_0^{\pi}Y^*_{\ell,m}(\theta,\varphi)Y_{\ell',m'}(\theta,\varphi)\sin\theta d\theta d\varphi = \delta_{\ell\ell'}\delta_{mm'}, \tag{1.48}$$

and the asymptotic behavior of modified Bessel functions

$$I_\delta\left(\frac{z}{\varepsilon}\right) \underset{\varepsilon\to 0}{\rightarrow} \left(\frac{\varepsilon}{2\pi z}\right)^{\frac{1}{2}} \exp\left(\frac{z}{\varepsilon} - \frac{1}{2}\frac{\varepsilon}{z}\left(\delta^2 - \frac{1}{4}\right)\right), \tag{1.49}$$

and thus

$$I_{\ell+1/2}\left(\frac{Mr_n r_{n-1}}{i\varepsilon\hbar}\right) \underset{\varepsilon\to 0}{\rightarrow} \left(\frac{i\varepsilon\hbar}{2\pi M r_n r_{n-1}}\right)^{\frac{1}{2}} \exp\left(\frac{Mr_n r_{n-1}}{i\varepsilon\hbar} - \frac{1}{2}\frac{i\varepsilon\hbar}{Mr_n r_{n-1}}\ell\left(\ell+1\right)\right), \tag{1.50}$$

then it is possible to obtain the statement

$$\begin{aligned} K(r',t';r,t) &= \lim_{N\to\infty}\left(\frac{M}{i\hbar\varepsilon}\right)^{(N+1)}\left(\frac{1}{\sqrt{r'r}}\right)\prod_{n=1}^{N}\left[\int_0^{+\infty} r_n dr_n\right] \\ &\quad \sum_{\ell=0}^{+\infty}\frac{(2\ell+1)}{4\pi}\prod_{n=1}^{N+1} I_{\ell+1/2}\left(-\frac{iMr_n r_{n-1}}{\varepsilon\hbar}\right) \\ &\quad \prod_{n=1}^{N+1}\left[\exp\left\{\frac{i}{\hbar}\left(\frac{M(r_n^2+r_{n-1}^2)}{2\varepsilon} - \varepsilon V(r_n)\right)\right\}\right] P_\ell(\cos\Theta_{i,f}), \end{aligned} \tag{1.51}$$

and therefore

$$\begin{aligned} K(r',t';r,t) &= \lim_{N\to\infty}\left(\frac{M}{2\pi i\hbar\varepsilon}\right)^{\frac{1}{2}(N+1)}\left(\frac{1}{r'r}\right)\prod_{n=1}^{N}\left[\int_0^{+\infty} r_n dr_n\right]\sum_{\ell=0}^{+\infty}\frac{(2\ell+1)}{4\pi} \\ &\quad \exp\frac{i}{\hbar}\sum_{n=1}^{N+1}\left(\frac{M(r_n^2+r_{n-1}^2)}{2\varepsilon} - \varepsilon V(r_n) - \frac{\ell(\ell+1)\varepsilon\hbar^2}{2Mr_n r_{n-1}}\right) \\ &\quad P_\ell(\cos\Theta_{i,f}), \end{aligned} \tag{1.52}$$

in which the separation between the radial and angular parts is achieved, so we can now write

$$K(r',t';r,t) = \sum_{\ell=0}^{+\infty}\frac{(2\ell+1)}{4\pi}K_\ell(r',t';r,t)\ P_\ell(\cos\Theta_{i,f}), \tag{1.53}$$

with the radial propagator $K_\ell(r',t';r,t)$ introduced in the form

$$\begin{aligned} K_\ell(r',t';r,t) &= \lim_{N\to\infty}\left(\frac{M}{2\pi i\hbar\varepsilon}\right)^{\frac{1}{2}(N+1)}\left(\frac{1}{r'r}\right)\prod_{n=1}^{N}\left[\int_0^{+\infty} r_n dr_n\right] \\ &\quad \exp\frac{i}{\hbar}\sum_{n=1}^{N+1}\left(\frac{M(r_n^2+r_{n-1}^2)}{2\varepsilon} - \varepsilon V(r_n) - \frac{\ell(\ell+1)\varepsilon\hbar^2}{2Mr_n r_{n-1}}\right) \end{aligned} \tag{1.54}$$

in an integral form

$$K_\ell(r',t';r,t) = \int Dr(s)\ \exp\frac{i}{\hbar}\int_0^T \left(\frac{M}{2\varepsilon}\dot{r}^2 - \varepsilon V_{eff}(r)\right)dt \tag{1.55}$$

with

$$V_{eff}(r) = V(r) + \frac{\ell(\ell+1)\hbar^2}{2Mr^2} \tag{1.56}$$

is a new effective potential

1.4 Space-Time transformation

Many physicists view the Duru-Kleinert method as a revolutionary turning point in the history of path integral theory. In 1979, Duru and Kleinert derived the full Feynman path integral for the most important problem in quantum mechanics, the hydrogen atom. The idea is to link the original system to another solvable system by means of an appropriate spatial transformation accompanied by a path-dependent time transformation.

To further illustrate let us assume a system with the following Lagrangian

$$L = \frac{M}{2}\dot{r}^2 - V(r), \tag{1.57}$$

First, we start with a spatial transformation that changes the variable r to y, it can be defined as

$$r = g(y) \tag{1.58}$$

this leads to the new transformed Lagrangian

$$L(y,\dot{y},t) = \frac{M}{2}\left[g'(y)\right]^2\dot{y}^2 - V(y), \tag{1.59}$$

where $g'(y)$ is the derivative of $g(y)$ according to y.

The elementary action corresponding to the Lagrangian (1.57) reads

$$A\left(r(t)\right) = \int L dt = \sum_{n=1}^{N+1}\left(\frac{M(r_n - r_{n-1})^2}{2\varepsilon} - \varepsilon V(r_n)\right), \tag{1.60}$$

where $\frac{M(r_n - r_{n-1})^2}{2\varepsilon}$ is simply the kinetic term,

the energy-dependent action related to the promoter (1.33) is then

$$A^E\left(r(t)\right) = \int L dt = \sum_{n=1}^{N+1}\left(\frac{M(r_n - r_{n-1})^2}{2\varepsilon} - \varepsilon\left[V(r_n) - E\right]\right), \tag{1.61}$$

with

$$\begin{cases} r_n = g(y_n) \\ r_{n-1} = g(y_{n-1}) \end{cases} \tag{1.62}$$

we now perform a Taylor series expansion of $g(y_n)$ and $g(y_{n-1})$

$$g(y_n) = g(\widetilde{y_n} + \frac{\Delta y_n}{2}) = g(\widetilde{y_n}) + \frac{\Delta y_n}{2} g'(\widetilde{y_n}) + \frac{(\Delta y_n)^2}{8} g''(\widetilde{y_n}) + \frac{(\Delta y_n)^3}{48} g^{(3)}(\widetilde{y_n}) + ..., \tag{1.63}$$

$$g(y_{n-1}) = g(\widetilde{y_n} - \frac{\Delta y_n}{2}) = g(\widetilde{y_n}) - \frac{\Delta y_n}{2} g'(\widetilde{y_n}) + \frac{(\Delta y_n)^2}{8} g''(\widetilde{y_n}) - \frac{(\Delta y_n)^3}{48} g^{(3)}(\widetilde{y_n}) + ..., \tag{1.64}$$

with the help of the midpoint concept

$$\widetilde{y_n} = \frac{y_n + y_{n-1}}{2}, \tag{1.65}$$

and therefore

$$\begin{cases} y_n = \widetilde{y_n} + \frac{\Delta y_n}{2}, \\ y_{n-1} = \widetilde{y_n} - \frac{\Delta y_n}{2}, \end{cases} \tag{1.66}$$

where

$$\Delta y_n = y_n - y_{n-1} \tag{1.67}$$

we find for the interval $\Delta r = r_n - r_{n-1}$ the expansion up to the third order

$$\Delta r_n = g(y_n) - g(y_{n-1}) = \Delta y_n g'(\widetilde{y_n}) + \frac{(\Delta y_n)^3}{24} g^{(3)}(\widetilde{y_n}) + ... \tag{1.68}$$

consequently, the kinetic term becomes

$$\begin{aligned} \varepsilon T &= \frac{M(r_n - r_{n-1})^2}{2\varepsilon} \approx \frac{M(\Delta y_n g'(\widetilde{y_n}) + \frac{(\Delta y_n)^3}{24} g^{(3)}(\widetilde{y_n}))^2}{2\varepsilon} \\ &\approx \frac{M(\Delta y_n g'(\widetilde{y_n}) + \frac{(\Delta y_n)^3}{12} g^{(3)}(\widetilde{y_n}))}{2\varepsilon} \\ &= \frac{M}{2\varepsilon} \Delta y_n g'(\widetilde{y_n}) \left(1 + \frac{(\Delta y_n)^2}{12} \frac{g^{(3)}(\widetilde{y_n})}{g'(\widetilde{y_n})} \right). \end{aligned} \tag{1.69}$$

For the potential term of the action (1.60), we have

$$\begin{aligned} \varepsilon V(r_n) &= \varepsilon V(g(y_n)) = \varepsilon V(g(\widetilde{y_n} + \frac{\Delta y_n}{2})) \\ &= \varepsilon \left\{ \begin{array}{c} V(g(\widetilde{y_n})) + \frac{\Delta y_n}{2} g'(\widetilde{y_n}) V'(g(\widetilde{y_n})) \\ + \frac{(\Delta y_n)^2}{8} \left[g''(\widetilde{y_n}) V'(g(\widetilde{y_n})) + g'(\widetilde{y_n})^2 V''(g(\widetilde{y_n})) \right] \end{array} \right\} \\ &= \varepsilon V(g(\widetilde{y_n})) + O(\varepsilon^2). \end{aligned} \tag{1.70}$$

therefore

$$\varepsilon\left[V(r_n)-E\right]=\varepsilon\left[V(g(\widetilde{y_n}))-E\right] \tag{1.71}$$

After inserting (1.69) and (1.70) into (1.60) we find the action

$$A^E=\sum_{n=1}^{N+1}\left(\frac{M}{2\varepsilon}\Delta y_n g'(\widetilde{y_n})\left(1+\frac{(\Delta y_n)^2}{12}\frac{g^{(3)}(\widetilde{y_n})}{g'(\widetilde{y_n})}\right)-\varepsilon\left[V(g(\widetilde{y_n}))-E\right]\right) \tag{1.72}$$

We now turn to the second transformation. The path-dependent time transformation connect time t to a new pseudotime s by

$$dt=\left[g'(y(s))\right]^2 ds \tag{1.73}$$

which means that

$$\varepsilon=g'(y_n)g'(y_{n-1})\varepsilon_s \tag{1.74}$$

with ε_s is the infinitesimal parameter corresponding to s.

in the same way as the expansions (1.63) and (1.64), one can expand $g'(y_n)$ and $g'(y_{n-1})$ in the following series

$$g'(y_n)=g'(\widetilde{y_n}+\frac{\Delta y_n}{2})=g'(\widetilde{y_n})+\frac{\Delta y_n}{2}g''(\widetilde{y_n})+\frac{(\Delta y_n)^2}{8}g^{(3)}(\widetilde{y_n})+...,\tag{1.75}$$

$$g'(y_{n-1})=g'(\widetilde{y_n}-\frac{\Delta y_n}{2})=g'(\widetilde{y_n})-\frac{\Delta y_n}{2}g''(\widetilde{y_n})+\frac{(\Delta y_n)^2}{8}g^{(3)}(\widetilde{y_n})+...,\tag{1.76}$$

with these, equation (1.74) becomes

$$\varepsilon\approx\left[g'(\widetilde{y_n})\right]^2\left[1+\frac{1}{4}(\Delta y_n)^2\left(\frac{g^{(3)}(\widetilde{y_n})}{g'(\widetilde{y_n})}-\left[\frac{g''(\widetilde{y_n})}{g'(\widetilde{y_n})}\right]^2\right)\right]\varepsilon_s \tag{1.77}$$

inserting this in the kinetic term (1.69) gives the relation

$$\varepsilon T=\frac{M}{2\varepsilon_s}\Delta y_n\frac{\left(1+\frac{(\Delta y_n)^2}{12}\frac{g^{(3)}(\widetilde{y_n})}{g'(\widetilde{y_n})}\right)}{g'(\widetilde{y_n})\left[1+\frac{1}{4}(\Delta y_n)^2\left(\frac{g^{(3)}(\widetilde{y_n})}{g'(\widetilde{y_n})}-\left[\frac{g''(\widetilde{y_n})}{g'(\widetilde{y_n})}\right]^2\right)\right]} \tag{1.78}$$

and hence

$$\varepsilon T=\frac{M}{2\varepsilon_s}(\Delta y_n)^2+\frac{M}{8\varepsilon_s}(\Delta y_n)^4\left[\left(\frac{g''(\widetilde{y_n})}{g'(\widetilde{y_n})}\right)^2-\frac{2}{3}\frac{g^{(3)}(\widetilde{y_n})}{g'(\widetilde{y_n})}\right]+... \tag{1.79}$$

For the potential term, we write

$$\varepsilon\left[V(g(\widetilde{y_n}))-E\right]\approx\varepsilon_s\left[g'(\widetilde{y_n})\right]^2\left[V(g(\widetilde{y_n}))-E\right] \tag{1.80}$$

Inserting this and (1.79) back into (1.72) renders the action

$$A^E=\sum_{n=1}^{N+1}\left(\begin{array}{c}\frac{M}{2\varepsilon_s}\left(\Delta y_n\right)^2+\frac{M}{8\varepsilon_s}\left(\Delta y_n\right)^4\left[\left(\frac{g''(\widetilde{y_n})}{g'(\widetilde{y_n})}\right)^2-\frac{2}{3}\frac{g^{(3)}(\widetilde{y_n})}{g'(\widetilde{y_n})}\right]\\ -\varepsilon\left[V(g(\widetilde{y_n}))-E\right]\end{array}\right). \tag{1.81}$$

For the measure of path integration (1.24)

$$\prod_{n=1}^{N}dr_n=\prod_{n=1}^{N}g'(y_n)dy_n. \tag{1.82}$$

Noting that

$$\prod_{n=1}^{N}g'(y_n)=\frac{1}{\sqrt{g'(y_0)g'(y_N)}}\prod_{n=1}^{N+1}\sqrt{g'(y_n)g'(y_{n-1})} \tag{1.83}$$

equation (1.82) becomes

$$\prod_{n=1}^{N}dr_n=\frac{1}{\sqrt{g'(y_0)g'(y_N)}}\prod_{n=1}^{N+1}\sqrt{g'(y_n)g'(y_{n-1})}\prod_{n=1}^{N}dy_n \tag{1.84}$$

and according to the relation

$$\prod_{n=1}^{N}dy_n=\prod_{n=1}^{N+1}d\left(\Delta y_n\right) \tag{1.85}$$

we have

$$\prod_{n=1}^{N}dr_n=\frac{1}{\sqrt{g'(y_0)g'(y_N)}}\prod_{n=1}^{N+1}\sqrt{g'(y_n)g'(y_{n-1})}d\left(\Delta y_n\right). \tag{1.86}$$

The promotor (1.33) becomes then

$$\begin{aligned}P_\ell(y',y;S) &= \lim_{N\to\infty}\left(\sqrt{\frac{M}{2\pi i\hbar\varepsilon}}\right)^{(N+1)}\frac{1}{\sqrt{g'(y_0)g'(y_N)}}\\ &\quad \prod_{n=1}^{N+1}\left[\int_{-\infty}^{+\infty}\sqrt{g'(y_n)g'(y_{n-1})}d\left(\Delta y_n\right)\right]\exp\frac{i}{\hbar}\sum_{n=1}^{N+1}A_n^E\end{aligned} \tag{1.87}$$

with

$$A_n^E=\left(\begin{array}{c}\frac{M}{2\varepsilon_s}\left(\Delta y_n\right)^2+\frac{M}{8\varepsilon_s}\left(\Delta y_n\right)^4\left[\left(\frac{g''(\widetilde{y_n})}{g'(\widetilde{y_n})}\right)^2-\frac{2}{3}\frac{g^{(3)}(\widetilde{y_n})}{g'(\widetilde{y_n})}\right]\\ -\varepsilon_s\left[g'(\widetilde{y_n})\right]^2\left[V(g(\widetilde{y_n}))-E\right]\end{array}\right). \tag{1.88}$$

Using the integral formula valid for large a[20]

$$\int_{-\infty}^{+\infty} dx \exp(-ax^2 - bx^4) = \int_{-\infty}^{+\infty} dx \exp(-ax^2 - \frac{3b}{4a^2}) + O(1/a^3), \tag{1.89}$$

in (1.87), one find

$$\begin{aligned} P_\ell(y', y; S) &= \lim_{N\to\infty} \left(\sqrt{\frac{M}{2\pi i\hbar\varepsilon_s}}\right)^{(N+1)} [g'(y)g'(y')]^{-\frac{1}{2}} \\ &\prod_{n=1}^{N} \left[\int_{-\infty}^{+\infty} dy_n\right] \exp\frac{i}{\hbar}\sum_{n=1}^{N+1} A_n, \end{aligned} \tag{1.90}$$

with

$$A_n^E = \left(\frac{M}{2\varepsilon_s}(\Delta y_n)^2 - \varepsilon_s [g'(\widetilde{y_n})]^2 [V(g(\widetilde{y_n}) - E] - \varepsilon_s \Delta V\right), \tag{1.91}$$

where is defined as

$$\Delta V = \frac{3\hbar^2}{8M}\left[\left(\frac{g''}{g'}\right)^2 - \frac{2}{3}\frac{g^{(3)}}{g'}\right] \tag{1.92}$$

in order to obtain the transformed Green's function, we insert (1.90) with the transformation $dT = g'(y)g'(y')dS$ in Forrier transformation (1.35), this gives

$$G(r', r; E) = \sqrt{g'(y)g'(y')}\int_0^{\infty} P_\ell(y', y; S)dS \tag{1.93}$$

This expression will play an important role in solving the problems that we will see in the next chapters.

Chapter 2

Non Relativistic Particle in Diatomic Potential

2.1 Introduction

For a very long time, physicists have attempted to model nuclear, atomic, and even molecular interactions by suggesting theoretical potential functions in terms of experimentally determined parameters. As a result, many proposed potentials have come to the scientific surface , including those of Morse [21], Rosen-Morse [22], Manning Rosen [23], Pöschl-Teller [24], Deng-Fan [25], Tietz[26], Schiöberg [27], Wei [28], modified Rosen–Morse[29], Scarf II [30], second Pöschl-Teller like [31] and Coulomb plus scalar potential [32] and others. These potentials have undergone numerous generalizations over time in an effort to create a universal potential function that can explain and describe the greatest number of nuclear, atomic, and molecular phenomena. They have also undergone improvements over time to fit empirical potential energy curves of certain systems.

Solving the Schrödinger equation for one of those potential functions is an issue of great importance in various fields in physics and chemistry. It provides complete information about the studied system. That's why physicists' efforts directed early towards looking for analytical and numerical solutions. These attempts resulted in a number of developed methods include, for example: Nikiforov Uvarov (NU) method [33, 34, 35, 36, 37], super-symmetric quantum mechanics method (SUSY) [38, 39, 40, 41], asymptotic iteration method (AIM)[42, 43, 44, 45], factorization method [46, 47, 48], exact and proper quantization method [49, 50, 51, 52] and others.

In this chapter, we will test path integral method in solving the Schrödinger equation for three types of physical potentials: The trigonometric Pöschl-Teller, the modified Pöschl-Teller and the Generalized Inverse Quadratic Yukawa Potentials

2.2 The trigonometric and the modified Pöschl-Teller Potentials

2.2.1 Introduction

Despite the critical importance of the Schrödinger equation and the years of work that have gone into solving it, its exact solutions are still restricted to a small subset of potentials, including the trigonometric and the modified Pöschl-Teller potentials. The latter's solutions are only accessible for s-states. In this chapter, we intend to provide a non-relativistic treatment of the trigonometric and the modified Pöschl-Teller potentials problems, these treatments rests on two pillars:

- The centrifugal term $1/r^2$ is approximated using suitable methods, which allows the s-states solutions to be extended to include ℓ-states.
- The use of path integral technique of R. Feynman as an analytical method for addressing.

2.2.2 The trigonometric Pöschl-Teller potential

Pöschl and Teller [24] introduced the trigonometric Pöschl-Teller potential (tPT) in 1933, it is also known as the first Pöschl-Teller potential and has been used to describe diatomic molecular vibration ever since. This potential can be expressed as

$$V_{tPT}(r) = \frac{V_1}{\sin^2(\alpha r)} + \frac{V_2}{\cos^2(\alpha r)}, \tag{2.1}$$

where the parameters V_1 and V_2 represent the potential's characteristics and the parameter α relates to its range [53].

The importance of this molecular potential appears through the attention it received from researchers, for example. With this potential, Liu et al. [53] performed a fermionic analysis, for instance. In the relativistic regime, the bound state solutions have also been tested by Falaye et al [54], Hamzavi [55], Candemir [56] and Chen [57]. The Nikiforov-Uvarov approach was used by Hamzavi et al [58] to study the s-wave solutions of the Schrödinger equation for this potential. The Nikiforov-Uvarov method was also used by the authors of ref [59] to derive the approximate solutions of the rotating trigonometric PT potential's radial Schrödinger equation. For any given ℓ-state. Recently, within the framework of the Functional Analysis Approach, analytical solutions of the Schrödinger equation for a generalized form of the trigonometric Pöschl-Teller potential by utilizing an adequate approximation to the centrifugal term have been investigated by Edet et al [60].

The work we present in this section falls within this same context, as we will discuss non-relativistic solutions to the trigonometric Pöschl-Teller potential problem for any ℓ-state, where we will consider an approximate formula for the centrifugal term similar to

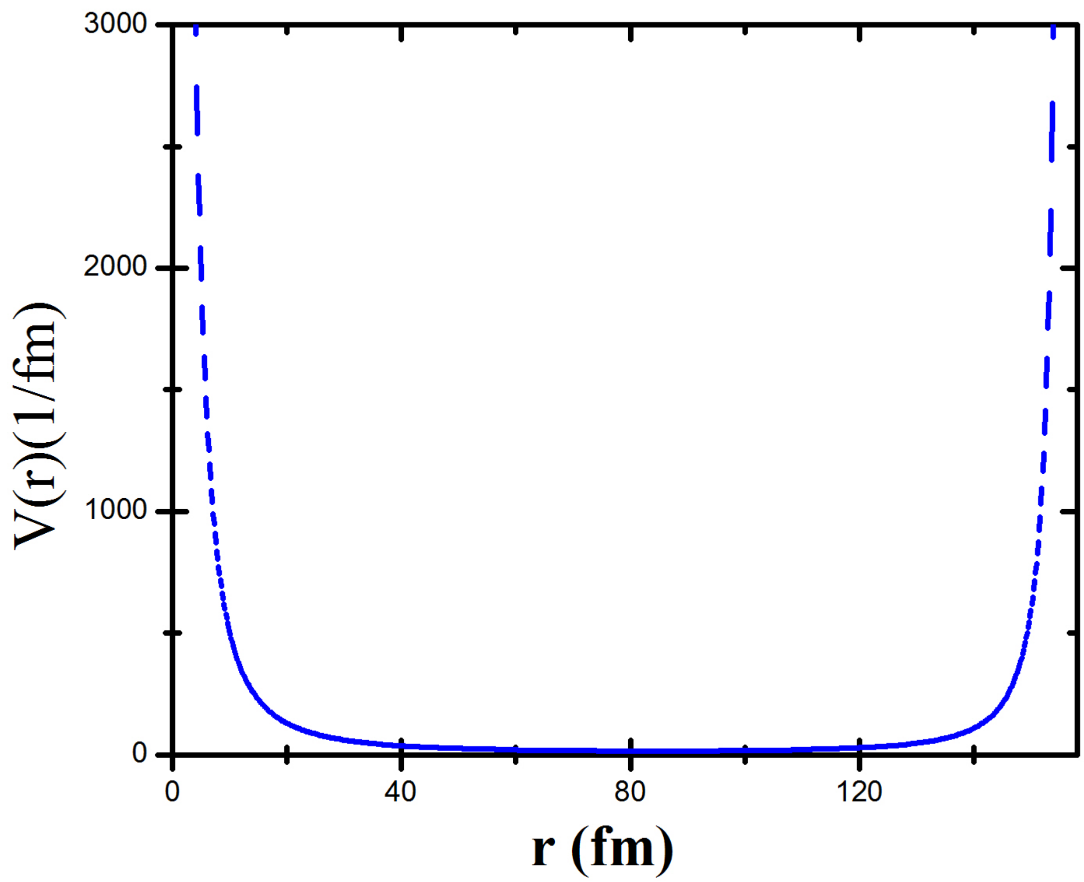

Figure 2.1: Represent the shape of the trigonometric Pöschl-Teller potential against the interatomic distance ($\alpha = 0.01$).

the improved Greene-Aldrich approximation scheme. Feynman's formulation of quantum mechanics will be adapted as an analytical approach which culminated in the energy eigenvalues and eigenfunctions expressions.

The effective potential takes the form

$$V_{eff}(r) = \frac{\hbar^2 \ell(\ell+1)}{2mr^2} + V_{tPT}(r), \tag{2.2}$$

therefore

$$V_{eff}(r) = \frac{\hbar^2 \ell(\ell+1)}{2Mr^2} + \frac{V_1}{\sin^2(\alpha r)} + \frac{V_2}{\cos^2(\alpha r)}, \tag{2.3}$$

In order to bypass the centrifugal term problem, we suggest using the following approximation [59]

$$\frac{1}{r^2} \approx \lim_{\alpha \to 0} \alpha^2 \left(\frac{1}{12} + \frac{1}{\sin^2(\alpha r)} \right), \tag{2.4}$$

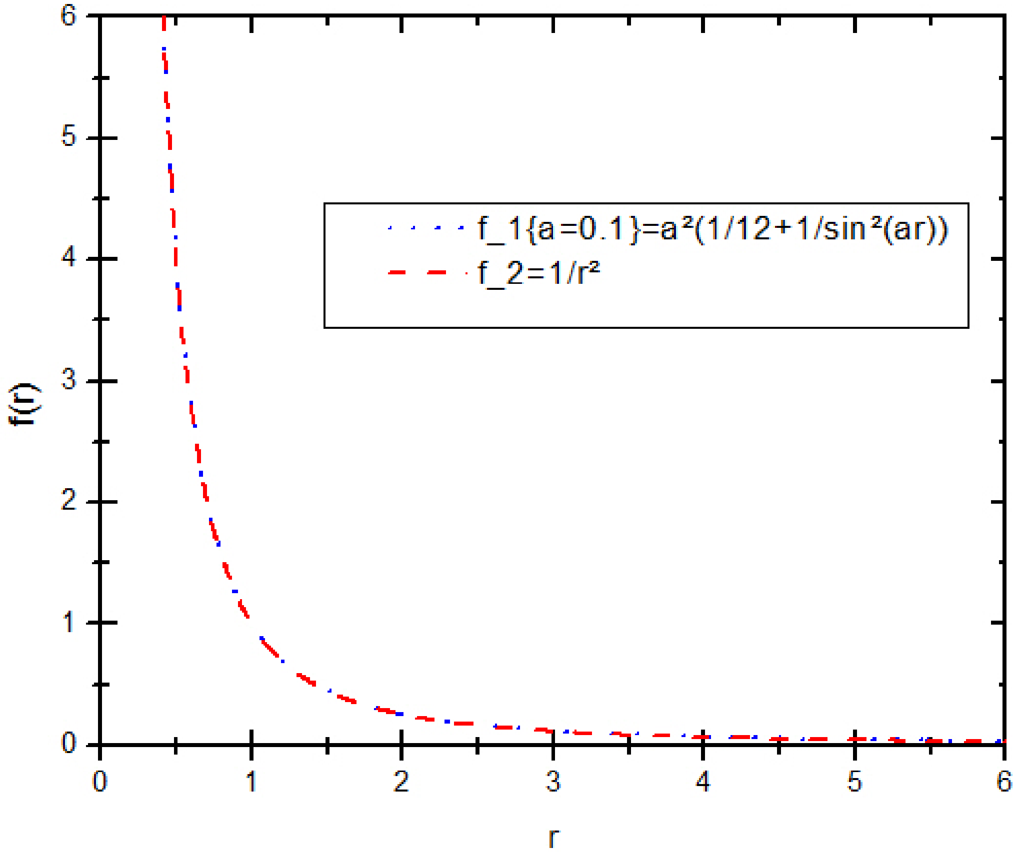

Figure 2.2: The term $1/r^2$ and its approximation for $\alpha = 0.1$.

which has a structure very similar to the Greene-Aldrich approximation, therefore

$$V_{eff}(r) \approx \frac{\hbar^2 \alpha^2 l(l+1)}{2M} \left(\frac{1}{12} + \frac{1}{\sin^2(\alpha r)} \right) + \frac{V_1}{\sin^2(\alpha r)} + \frac{V_2}{\cos^2(\alpha r)}, \tag{2.5}$$

and then

$$V_{eff}(r) \approx \frac{\hbar^2 \alpha^2 \ell(\ell+1)}{2m} \frac{1}{12} + \frac{\hbar^2 \alpha^2 \ell(\ell+1)}{2m} \frac{1}{\sin^2(\alpha r)} + \frac{V_1}{\sin^2(\alpha r)} + \frac{V_2}{\cos^2(\alpha r)}, \tag{2.6}$$

2.2. The trigonometric and the modified Pöschl-Teller Potentials

consequently

$$V_{eff}(r) \approx \frac{\hbar^2\alpha^2\ell(\ell+1)}{2m}\frac{1}{12} + \left(\frac{\left(\frac{\hbar^2\alpha^2\ell(\ell+1)}{2m} + V_1\right)}{\sin^2(\alpha r)} + \frac{V_2}{\cos^2(\alpha r)}\right), \tag{2.7}$$

Green's function

The radial promotor corresponding to the trigonometric Pöschl-Teller potential is

$$P_l(r_b, t_b; r_a, t_a) = \int Dr(t) \exp\left[\frac{i}{\hbar}A_n\right], \tag{2.8}$$

hence

$$P_l(r_b, t_b; r_a, t_a) = \left(\frac{1}{r_a r_b}\right) \lim_{N\to\infty} \left(\frac{M}{2\pi i\hbar\varepsilon}\right)^{\frac{1}{2}(N+1)} \times \left[\prod_{j=1}^{N}\int_0^\infty dr_j\right] \exp\left(\frac{i}{\hbar}A_n\right), \tag{2.9}$$

where

$$t_b = t_{N+1}; t_a = t_0, \tag{2.10}$$
$$r_b = r_{N+1}; r_a = r_0, \tag{2.11}$$

with the action A_n depended on energy E

$$A_n = \sum_{j=1}^{N+1}\left[\frac{M}{2\varepsilon}(\Delta r_j)^2 - \varepsilon(V_{eff}(r_j) - E)\right], \tag{2.12}$$

by inserting Eq. (2.7) in Eq. (2.12), we obtain

$$A_n = \sum_{j=1}^{N+1}\left[\frac{M}{2\varepsilon}(\Delta r_j)^2 - \varepsilon\left\{\left(\frac{\left(\frac{\hbar^2\alpha^2\ell(\ell+1)}{2m} + V_1\right)}{\sin^2(\alpha r)} + \frac{V_2}{\cos^2(\alpha r)}\right) + \frac{\hbar^2\alpha^2\ell(\ell+1)}{2m}\frac{1}{12} - E\right\}\right], \tag{2.13}$$

and then, by introducing the new parameters

$$D = E - \frac{\hbar^2\alpha^2\ell(\ell+1)}{2m}\frac{1}{12}, \tag{2.14}$$

we can write the action as

$$A_n = \sum_{j=1}^{N+1}\left[\frac{M}{2\varepsilon}(\Delta r_j)^2 - \varepsilon\left\{\frac{\left(\frac{\hbar^2\alpha^2\ell(\ell+1)}{2m} + V_1\right)}{\sin^2(\alpha r)} + \frac{V_2}{\cos^2(\alpha r)} - D\right\}\right], \tag{2.15}$$

Now, substitution of the latter in the promotor (2.9)

$$P_\ell(r_b,r_a;T) = \int_{r_a}^{r_b} Dr(t)\exp\left[\frac{i}{\hbar}\int_{t_a}^{t_b}\left\{\frac{M}{2}\dot{r}^2-\left(\frac{\left(\frac{\hbar^2\alpha^2\ell(\ell+1)}{2m}+V_1\right)}{\sin^2(\alpha r)}+\frac{V_2}{\cos^2(\alpha r)}\right)\right\}dt\right] \times \exp\frac{i}{\hbar}DT, \tag{2.16}$$

with
$T = t_b - t_a$,
performing the Fourier transformation gives the Green's function associated with this system

$$G_\ell(r_b,r_a;E) = \int_0^\infty P_\ell(r_b,r_a;T)dT, \tag{2.17}$$

which leads to

$$G_\ell(r_b,r_a;D) = \int_0^\infty dT e^{\frac{i}{\hbar}DT}\int_{r_a}^{r_b} Dr(t) \exp\left[\frac{i}{\hbar}\int_{t_a}^{t_b}\left\{\frac{M}{2}\dot{r}^2-\left(\frac{\left(\frac{\hbar^2\alpha^2\ell(\ell+1)}{2m}+V_1\right)}{\sin^2(\alpha r)}+\frac{V_2}{\cos^2(\alpha r)}\right)\right\}dt\right], \tag{2.18}$$

changing variables $y = \alpha r$ and $dt = \alpha^{-2}ds$ gives

$$G_\ell(r_b,r_a;D) = \alpha^{-1}G'_\ell(y_b,y_a;\frac{D}{\alpha^2}) = \alpha^{-1}\int_0^\infty ds e^{\frac{i}{\hbar}\frac{D}{\alpha^2}s}\int_{y_a}^{y_b} Dy(s) \exp\left[\frac{i}{\hbar}\int_{s_a}^{s_b}\left\{\frac{M}{2}\dot{y}^2-\left(\frac{\left(\frac{\hbar^2\ell(\ell+1)}{2M}+\frac{V_1}{\alpha^2}\right)}{\sin^2(\alpha r)}+\frac{\frac{V_2}{\alpha^2}}{\cos^2(\alpha r)}\right)\right\}ds\right], \tag{2.19}$$

It is preferable to use the new variables λ and β defined by

$$\begin{cases} \lambda = \sqrt{\ell(\ell+1)+\frac{2M}{\hbar^2\alpha^2}V_1+\frac{1}{4}} \\ \beta = \sqrt{\frac{2M}{\hbar^2\alpha^2}V_2+\frac{1}{4}} \end{cases} \tag{2.20}$$

to re-express the Green's function

$$G'_\ell(y_b, y_a; \frac{D}{\alpha^2}) = \int_0^\infty ds e^{\frac{i}{\hbar}\frac{D}{\alpha^2}s} \int_{y_a}^{y_b} Dy(s)$$
$$\exp\left[\frac{i}{\hbar}\int_{s_a}^{s_b}\left\{\frac{M}{2}\dot{y}^2 - \frac{\hbar^2}{2M}\left(\frac{(\lambda^2-\frac{1}{4})}{\sin^2(y)} + \frac{(\beta^2-\frac{1}{4})}{\cos^2(y)}\right)\right\}ds\right] \quad (2.21)$$

This last Green function is similar to that associated with the trigonometric Pöschl-Teller potential in s-states which is an exact solvable problem. Its solution is available in different previous references[59, 61].

$$\begin{aligned} G'_\ell(r_b, r_a; \frac{D}{\alpha^2}) &= \frac{M}{2\hbar^2}\sqrt{\sin 2\alpha r_a \sin 2\alpha r_b}\frac{\Gamma(m_1 - L_E)\Gamma(m_1 + L_E + 1)}{\Gamma(m_1 + m_2 + 1)\Gamma(m_1 - m_2 + 1)} \\ &\times(\sin\alpha r_a \sin\alpha r_b)^{(m_1 - m_2)}(\cos\alpha r_a \cos\alpha r_b)^{m_1 + m_2} \\ &\times {}_2F_1(m_1 - L_E, m_1 + L_\beta + 1; m_1 - m_2 + 1; \sin^2\alpha r_\leq) \\ &\times {}_2F_1(m_1 - L_E, m_1 + L_E + 1; m_1 + m_2 + 1; \cos^2\alpha r_\geq), \end{aligned} \quad (2.22)$$

with the notation

$$\begin{cases} m_{1,2} = \frac{1}{2}(\beta \pm \lambda), \\ L_E = -\frac{1}{2} + \frac{1}{2}\sqrt{\frac{2MD}{\hbar^2\alpha^2}}. \end{cases} \quad (2.23)$$

Energy spectrum and wavefunctions

It is possible to extract the energy eigenvalues by calculating the poles of the Green's function (2.22). The poles of the Green's function are contained in the gamma function $\Gamma(m_1 - L_E)$.

$$m_1 - L_E = -n_r. \quad (2.24)$$

Substitution of m_1 and L_E relations in Eq. (2.24) gives

$$\frac{1}{2}(\beta + \lambda) + \frac{1}{2} - \frac{1}{2}\sqrt{\frac{2MD}{\hbar^2\alpha^2}} = -n_r, \quad (2.25)$$

leading to

$$D = \frac{\hbar^2\alpha^2}{2M}(2n_r + \lambda + \beta + 1)^2, \quad (2.26)$$

thus

$$E_{n,\ell} = \frac{\hbar^2\alpha^2}{2M}(2n_r + \lambda + \beta + 1)^2 + \frac{\hbar^2\alpha^2\ell(\ell+1)}{2M}\frac{1}{12}, \quad (2.27)$$

therefore

$$E_{n,\ell} = \frac{\hbar^2\alpha^2}{2M}\left[(2n_r+\lambda+\beta+1)^2 + \frac{\ell(\ell+1)}{12}\right], \tag{2.28}$$

by using Eq. (2.20), one finally find the energy eigenvalues

$$E_{n,\ell} = \frac{\hbar^2\alpha^2}{2M}\left[(2n_r+\sqrt{\ell(\ell+1)+\frac{2M}{\hbar^2\alpha^2}V_1+\frac{1}{4}}+\sqrt{\frac{2M}{\hbar^2\alpha^2}V_2+\frac{1}{4}}+1)^2+\frac{\ell(\ell+1)}{12}\right], \tag{2.29}$$

This result is completely consistent with results shown in Equation (17) of Ref. [60] which adopts the Functional Analysis method and in Equation (19) of Ref. [59] obtained by using the Nikiforov–Uvarov method.

the associated wavefunctions

$$\begin{aligned}\psi_n^{(\lambda,\beta)}(r) \;&=\; \left[\frac{2(\beta+\lambda+1+2n)n!\Gamma(n+1+\lambda+\beta)}{\Gamma(\lambda+n+1)\Gamma(n+1+\beta)}\right]^{1/2} \\ &\times(\sinh(\alpha r))^{\lambda+\frac{1}{2}}(\cosh(\alpha r))^{\beta+\frac{1}{2}}P_n^{(\lambda,\beta)}(\cos 2\alpha r)\end{aligned} \tag{2.30}$$

state	n	ℓ	$E_{n,\ell}$(N-U)[59]	$E_{n,\ell}$(F-A)[60]	$E_{n,\ell}$(present)
1s	1	0	15.85264289	15.85264290	15.85264289
2s	2	0	15.92394680	15.92394680	15.92394680
2p	2	1	15.92402151	15.92402152	15.92402152
3s	3	0	15.99541071	15.99541072	15.99541072
3p	3	1	15.99548559	15.99548559	15.99548560
3d	3	2	15.99563534	15.99563535	15.99563535
4s	4	0	16.06703463	16.06703462	16.06703463
4p	4	1	16.06710967	16.06710967	16.06710966
4d	4	2	16.06725974	16.06725975	16.06725974
4f	4	3	16.06748486	16.06748486	16.06748485

Table 2.1: Energy eigenvalues (in $1/fm$) of tPT potential for different values of n, ℓ and for $\hbar = 1$. We put $\alpha = 0.01$, $V_1 = 5.0$ and $V_2 = 3.0$, $M = 10.0$.

In Table 2.1 with parameters $V_1 = 5fm^{-1}$, $V_2 = 3fm^{-1}$, $\alpha = 0.02$ and $M = 10fm^{-1}$, we compute the energy eigenvalues using Eq. (2.29) for various quantum numbers n and ℓ. Our main results are compared with the numerical values of the Nikiforov–Uvarov method and with the Functional Analysis method. It is found that our energy eigenvalues are in good agreement with the other results.

2.2. The trigonometric and the modified Pöschl-Teller Potentials

It is also observed that for increasing orbital angular momentum, at a fixed value of the principal quantum number, the energy increases

2.2.3 The modified Pöschl-Teller Potential

The modified Pöschl-Teller potential (also known as the second Pöschl-Teller potential) is a potential function that has taken a great deal of researchers' interests in recent years due to its physical importance. It was proposed early in 1933 by Pöschl and Teller [24] to model diatomic interactions and explain spectrum vibration. It is defined in the following form [61]

$$V_{mPT}(r) = \frac{\hbar^2\alpha^2}{2M}\left(\frac{\eta^2 - \frac{1}{4}}{\sinh^2(\alpha r)} + \frac{\upsilon^2 - \frac{1}{4}}{\cosh^2(\alpha r)}\right), \tag{2.31}$$

with α relates to the range of the potential, η and υ are adjustable real parameters, M is the reduced mass of a diatomic molecule and r is the interatomic distance.

This potential is relevant in a variety of fields, including semiconductor physics [62] astronomy and astrophysics [63], condensed matter [64], molecular chemistry and physics [65, 66, 67] and photonics physics [68, 69].

Accordingly, the effective potential of the radial propagator (1.56) can be written as follows

$$V_{eff}(r) = V_{mPT}(r) + \frac{\ell(\ell+1)\hbar^2}{2Mr^2} \tag{2.32}$$

which means that

$$V_{eff}(r) = \frac{\hbar^2\alpha^2}{2M}\left(\frac{\eta^2 - \frac{1}{4}}{\sinh^2(\alpha r)} + \frac{\upsilon^2 - \frac{1}{4}}{\cosh^2(\alpha r)}\right) + \frac{\ell(\ell+1)\hbar^2}{2Mr^2}, \tag{2.33}$$

The Greene-Aldrich approximation

The centrifugal term $1/r^2$ poses a significant challenge to researchers seeking ℓ-wave solutions for most physical problems because it frequently makes analytical problem solving extremely difficult. As a result, exact solutions are only available for a limited number of physical potentials. Physicists utilize one of two approaches to get around this barrier: either they employ a numerical method to address the problem or they employ an approximation scheme for the centrifugal term that aligns with the general shape of the potential that is being studied. Here, we'll use the second approach to treat the modified Pöschl-Teller potential and recommend applying the Greene-Aldrich approximation [59, 70], which is described as follows

$$\frac{1}{r^2} \approx \alpha^2\left(\frac{1}{12} + \frac{1}{\sinh^2(\alpha r)}\right) \tag{2.34}$$

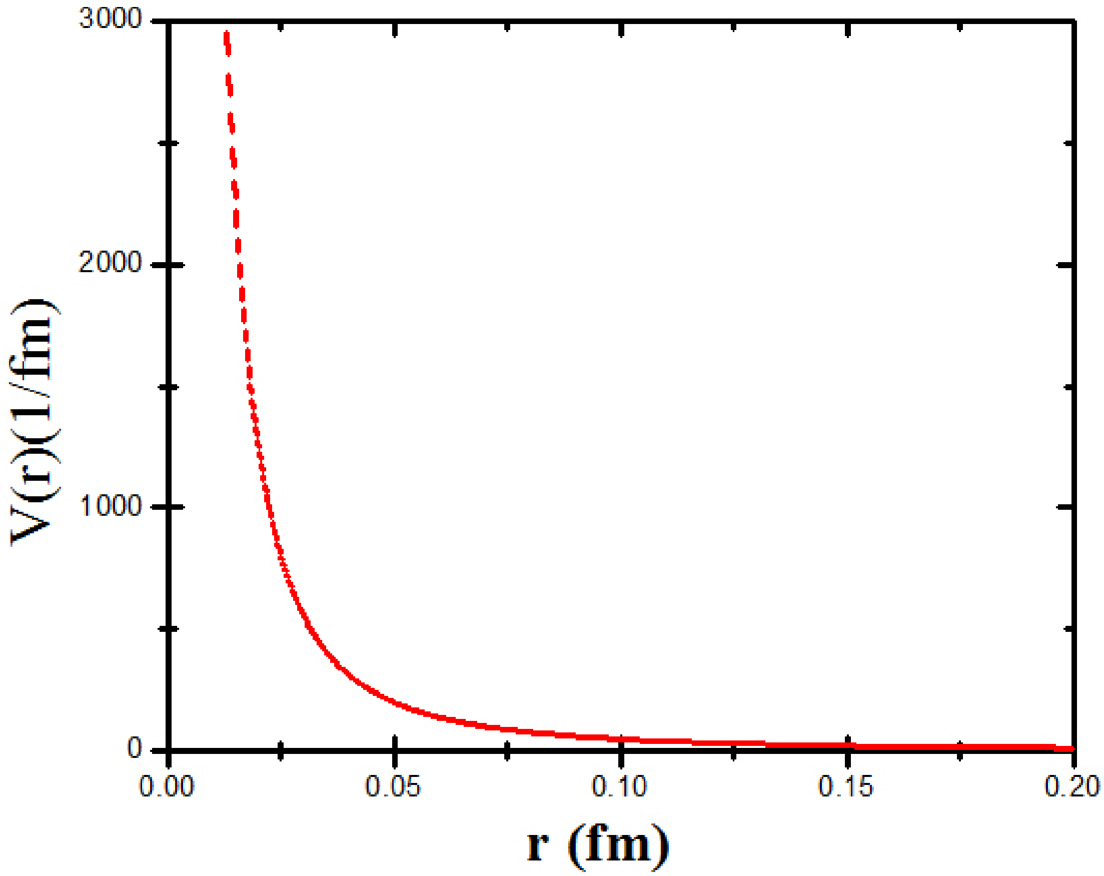

Figure 2.3: Represent the shape of the modified Pöschl-Teller potential against the interatomic distance ($\alpha = 0.01$, $\eta = 2$, $\upsilon = 1.5$).

In Figure 2.4, we present the variations of Greene-Aldrich's approximation for $\alpha = 0.01$ and $\alpha = 0.9$, which are compared with the variations of the $1/r^2$ term. From this comparison, it is evident that the accuracy of Greene-Aldrich's approximation improves as the value of α decreases.

therefore, substituting the centrifugal term by this approximation scheme on the effective potential expression give us

$$V_{eff}(r) = \frac{\hbar^2\alpha^2}{2M}\left(\frac{\eta^2 - \frac{1}{4}}{\sinh^2(\alpha r)} - \frac{\upsilon^2 - \frac{1}{4}}{\cosh^2(\alpha r)}\right) + \frac{\ell(\ell+1)\hbar^2\alpha^2}{2M}\left(\frac{1}{12} + \frac{1}{\sinh^2(\alpha r)}\right), \quad (2.35)$$

which can be written in a more appropriate way

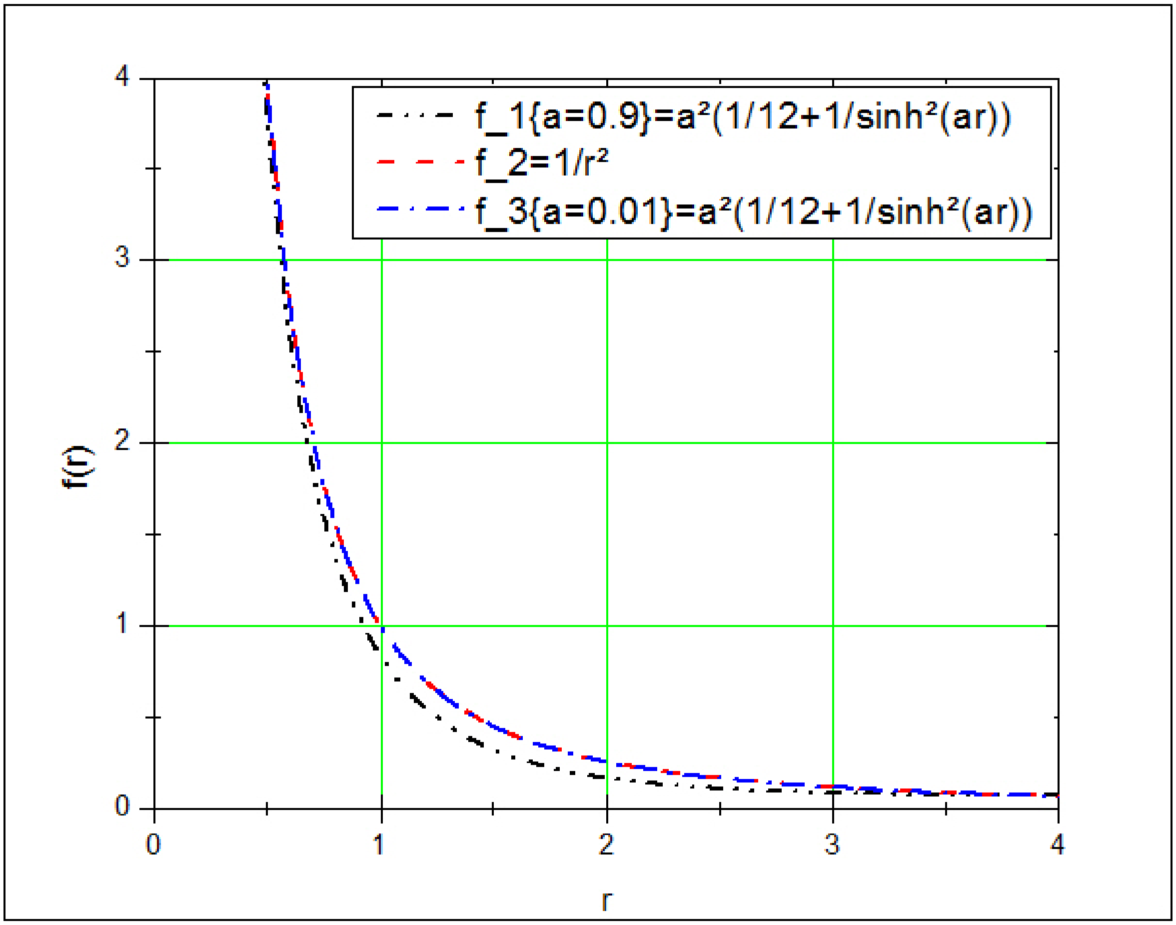

Figure 2.4: The term $1/r^2$ (red) and its Greene-Aldrich approximation for $\alpha = 0.01$ in blue and $\alpha = 0.5$ in black .

$$V_{eff}(r) = \frac{\hbar^2\alpha^2}{2M}\left(\frac{\ell(\ell+1)+\eta^2-\frac{1}{4}}{\sinh^2(\alpha r)} - \frac{\upsilon^2-\frac{1}{4}}{\cosh^2(\alpha r)}\right) + \frac{\hbar^2}{2M}\frac{\alpha^2\ell(\ell+1)}{12}, \tag{2.36}$$

for computational purposes, we now prefer to propose a new parameter

$$\lambda = \sqrt{\ell(\ell+1)+\eta^2}, \tag{2.37}$$

further, the effective potential will take the following most familiar form

$$V_{eff}(r) = \frac{\hbar^2\alpha^2}{2M}\left(\frac{\lambda^2-\frac{1}{4}}{\sinh^2(\alpha r)} - \frac{\upsilon^2-\frac{1}{4}}{\cosh^2(\alpha r)}\right) + \frac{\hbar^2}{2M}\frac{\alpha^2\ell(\ell+1)}{12}, \tag{2.38}$$

This completes the preparation of the effective potential expression for next stages.

Green's function

Just as we have done in presenting relation (1.35). It is simple to demonstrate that radial Green's function fulfills

$$G_\ell(r',r;E)=\int_0^\infty P_\ell(r',r;T)dT \tag{2.39}$$

by using spherical coordinates equation of the propagator (1.53).
The kernel $P_\ell(r',r;T)$ is the radial part of the promotor (1.33)

$$P_\ell(r',r;T)=\int Dr(t)\ \exp\left(\frac{i}{\hbar}A^E\right) \tag{2.40}$$

with the new action A^E reads

$$A^E=\int_0^T dt\left(\frac{M}{2}\dot{r}^2-V_{eff}(r)+E\right). \tag{2.41}$$

thus

$$A^E=\int_0^T dt\left(\frac{M}{2}\dot{r}^2-\left(\frac{\hbar^2\alpha^2}{2M}\left(\frac{\lambda^2-\frac{1}{4}}{\sinh^2(\alpha r)}-\frac{\upsilon^2-\frac{1}{4}}{\cosh^2(\alpha r)}\right)+\frac{\hbar^2}{2M}\frac{\alpha^2\ell(\ell+1)}{12}-E\right)\right). \tag{2.42}$$

and by identification we introduce a new entity

$$D=E-\frac{\hbar^2}{2M}\frac{\alpha^2\ell(\ell+1)}{12} \tag{2.43}$$

These considerations makes the radial Green's function (2.39)

$$\begin{aligned}G_\ell(r',r;D) &= \int_0^\infty dT\ e^{\frac{i}{\hbar}TD}\int Dr(t)\\ &\exp\left(\frac{i}{\hbar}\int_0^T dt\left(\frac{M}{2}\dot{r}^2-\frac{\hbar^2\alpha^2}{2M}\left(\frac{\lambda^2-\frac{1}{4}}{\sinh^2(\alpha r)}-\frac{\upsilon^2-\frac{1}{4}}{\cosh^2(\alpha r)}\right)\right)\right).\end{aligned} \tag{2.44}$$

Now in order to write $G_\ell(r',r;E)$ in a solvable way, we need to change the variables $r=\frac{y}{\alpha}$ and $dt=\alpha^{-2}ds$, which gives

$$\begin{aligned}G_\ell(r',r;D) &= \alpha^{-1}G'_\ell(y',y;\frac{D}{\alpha^2})=\int_0^\infty dS\ e^{\frac{i}{\hbar}\frac{D}{\alpha^2}S}\int Dy(s)\\ &\exp\left(\frac{i}{\hbar}\int_0^S ds\left(\frac{M}{2}\dot{y}^2-\frac{\hbar^2}{2M}\left(\frac{\lambda^2-\frac{1}{4}}{\sinh^2(y)}-\frac{\upsilon^2-\frac{1}{4}}{\cosh^2(y)}\right)\right)\right).\end{aligned} \tag{2.45}$$

This last transformed Green's function $G'_\ell(y',y;\frac{D}{\alpha^2})$ is similar to that associated with modified Pöschl-Teller potential in s states which is exactly solved in several references [61]

2.2. The trigonometric and the modified Pöschl-Teller Potentials

$$
\begin{aligned}
G_l(y', y; \frac{D}{\alpha^2}) \quad = \quad & \frac{M}{\hbar^2} \frac{\Gamma(m_1 - L_\upsilon)\Gamma(m_1 + L_\upsilon + 1)}{\Gamma(m_1 + m_2 + 1)\Gamma(m_1 - m_2 + 1)} \\
& \times (\cosh y \cosh y')^{-(m_1 - m_2)} (\tanh y \tanh y')^{m_1 + m_2 + 1/2} \\
& \times {}_2F_1(m_1 - L_\upsilon, m_1 + L_\upsilon + 1; m_1 - m_2 + 1; \cosh^{-2} y_\leq) \\
& \times {}_2F_1(m_1 - L_\upsilon, m_1 + L_\upsilon + 1; m_1 + m_2 + 1; \tanh^2 y_\geq),
\end{aligned} \tag{2.46}
$$

consequently

$$
\begin{aligned}
G_l(r', r; \frac{D}{\alpha^2}) \quad = \quad & \frac{M}{\alpha\hbar^2} \frac{\Gamma(m_1 - L_\upsilon)\Gamma(m_1 + L_\upsilon + 1)}{\Gamma(m_1 + m_2 + 1)\Gamma(m_1 - m_2 + 1)} \\
& \times (\cosh \alpha r \cosh \alpha r')^{-(m_1 - m_2)} (\tanh \alpha r \tanh \alpha r')^{m_1 + m_2 + 1/2} \\
& \times {}_2F_1(m_1 - L_\upsilon, m_1 + L_\upsilon + 1; m_1 - m_2 + 1; \cosh^{-2} \alpha r_\leq) \\
& \times {}_2F_1(m_1 - L_\upsilon, m_1 + L_\upsilon + 1; m_1 + m_2 + 1; \tanh^2 \alpha r_\geq),
\end{aligned} \tag{2.47}
$$

with parameters

$$
\begin{cases}
m_{1,2} = \frac{1}{2}(\lambda \pm \sqrt{-\frac{2MD}{\hbar^2\alpha^2}}); \\
L_\upsilon = \frac{1}{2}(\upsilon - 1).
\end{cases} \tag{2.48}
$$

Energy spectrum and wavefunctions

The energy spectrum is obtained from the poles of the Green's function that are in fact all contained in the gamma function $\Gamma(m_1 - L_\beta)$. They are given by

$$
m_1 - L_\upsilon = -n_r, \tag{2.49}
$$

therefore

$$
D = -\frac{\hbar^2\alpha^2}{2M}(2n_r + 1 - \upsilon + \lambda)^2, \tag{2.50}
$$

leading to

$$
E = \frac{\hbar^2\alpha^2}{2M} \frac{\ell(\ell+1)}{12} - \frac{\hbar^2\alpha^2}{2M} (2n_r + 1 - \upsilon + \lambda)^2 , \tag{2.51}
$$

which means that

$$
E = \frac{\hbar^2\alpha^2}{2M} \frac{\ell(\ell+1)}{12} - \frac{\hbar^2\alpha^2}{2M} \left(2n_r + 1 - \upsilon + \sqrt{\ell(\ell+1) + \eta^2}\right)^2 , \tag{2.52}
$$

the associated wavefunctions

$$\begin{aligned}\psi_{n,\,\ell}^{(\lambda,\,\upsilon)}(r) &= \frac{1}{\Gamma(\lambda+1)}\left[\frac{2(\upsilon-\lambda-2n-1)\Gamma(n+1+\lambda)\Gamma(\upsilon-n)}{\Gamma(\upsilon-\lambda-n)}\right]^{1/2} \\ &\times(\sinh\alpha r)^{\lambda+\frac{1}{2}}(\cosh\alpha r)^{n-\upsilon+\frac{1}{2}} \\ &\times{}_2F_1(-n,\upsilon-n;\lambda+1;\tanh^2(\alpha r)), \end{aligned} \tag{2.53}$$

state	n	ℓ	$E_{n,\ell}(\alpha=1.2)$ present	$E_{n,\ell}(\alpha=0.4)$ present	$E_{n,\ell}(\alpha=0.02)$ present	$E_{n,\ell}(\alpha=0.02)$ Fuchsian differential equations approach[71]
1s	1	0	-0.8820000000	-0.09800000000	-0.0002450000000	-0.0002450000000
2s	2	0	-2.178000000	-0.2420000000	-0.0006050000000	-0.0006050000000
2p	2	1	-2.536542830	-0.2818380923	-0.0007045952307	-0.0007079285640
3s	3	0	-4.050000000	-0.4500000000	-0.001125000000	-0.001125000000
3p	3	1	-4.537995876	-0.5042217642	-0.001260554411	-0.001263887744
3d	3	2	-5.366523905	-0.5962804340	-0.001490701085	-0.001500701085
4s	4	0	-6.498000000	-0.7220000000	-0.001805000000	-0.001805000000
4p	4	1	-7.115448920	-0.7906054352	-0.001976513589	-0.001979846922
4d	4	2	-8.149259875	-0.9054733190	-0.002263683298	-0.002273683298
4f	4	3	-9.450000000	-1.050000000	-0.002625000000	-0.002645000000

Table 2.2: The energy eigenvalues (in $1/fm$) of the mPT potential for various values of n,ℓ and for $\hbar=1$. We set $\upsilon=1.5$, $\eta=2.0$ and $M=10.0$.

Table (2.2) represents numerical results of energy eigenvalues using Eq. (2.52) for different quantum numbers n and ℓ with parameters $\upsilon=1.5fm^{-1}$, $\eta=2.0fm^{-1}$, and $M=10.0fm^{-1}$.

We parallel our findings with the outcomes of the Fuchsian differential equations method [71]. The outcomes of the two approaches seem to be extremely comparable.

2.2.4 Conclusion

As you have seen, we have dealt with the problems of the trigonometric and modified Pöschl-Teller potentials in the non-relativistic framework using Feynman's formulation of quantum mechanics. the studies we have done were comprehensive for the ℓ states where we used the Greene-Aldrich approximations for the centrifugal term. Finally, we established Green's functions related to the system and were able to solve it, based on which we extracted the energy spectrum and wavefunctions of this problem.

2.3 Motion of a particle in the Generalized Inverse Quadratic Yukawa potential

2.3.1 Introduction

In 1934, Yukawa proposed a potential function to describe nucleon-nucleon interactions in the nucleus [72].

$$V_Y(r) = -\delta\, \frac{\exp(-\alpha r)}{r} \tag{2.54}$$

where α is the screening parameter, and δ is the coupling strength.

However, this potential has been applied recently in many areas, such as solid state [73], quantum field theory [74, 75], plasma physics [76, 77], and even modeling systems of colloidal particles in electrolytes [78]. A new potential formula was introduced in 2012 by Hamzavi et al named Inversely Quadratic Yukawa (IQY) potential [79]

$$V_{IQY}(r) = -\lambda\, \frac{\exp(-2\alpha r)}{r^2} \tag{2.55}$$

and then Ikhdaira et all also presented the so-called Generalized Inverse Quadratic Yukawa potential (GIQY) [80], which can be said to be more like a combinations of the IQY potential and Yukawa potential, this last potential takes the form

$$\begin{aligned} V_{GIQY}(r) &= -V_0\left(1+\frac{\exp(-\alpha r)}{r}\right)^2 \\ &= -V_0 - 2V_0\frac{\exp(-\alpha r)}{r} - V_0\frac{\exp(-2\alpha r)}{r^2}, \end{aligned} \tag{2.56}$$

where V_0 is the potential strength.

Actually, a dimensional problem has been raised against this formula (2.56) [81]. The amount in parentheses is the sum of an inverse length quantity ($\frac{\exp(-\alpha r)}{r}$) and a dimensionless quantity (the unity). Thus, it is preferable to use the form

$$V(r) = -a - \delta\, \frac{e^{-\alpha r}}{r} - \lambda\, \frac{e^{-2\alpha r}}{r^2}, \tag{2.57}$$

to express the GIQY potential which is more grounded, where a, δ and λ are different parameters.

In Figure 2.5 we present a comparative plot of the shapes of GIQY, Yukawa potential and the IQY potential in order to clarify and understand the system we are studying.

The aim of this section is to treat the problem of a particle subjected to the Generalized Inverse Quadratic Yukawa potential in a non-relativistic framework using path integral method, we will write the radial green's function in a path integration form and use a suggested space-time transformation in order to pass to an already solved

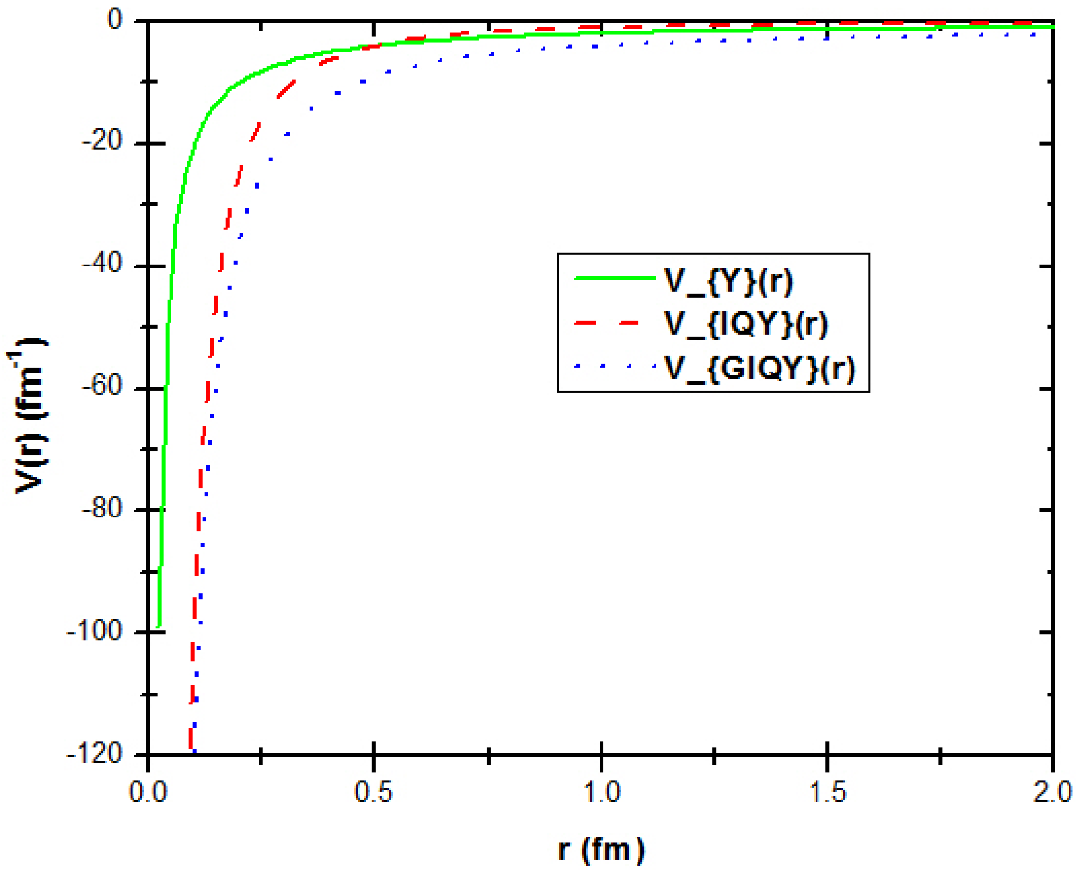

Figure 2.5: The shape of the GIQY potential compared with the Yukawa potential and the IQY potential for parameter values: $a = 1.0$, $\delta = 2.0$, $\lambda = 1.0$ and $\alpha = 0.01$.

problem which is modified Pöschl-Teller (PT) potential problem, which leads (as it will be clear later) to the wave functions and the related energies. Yukawa potential, inversely quadratic Yukawa potential and Coulomb potential problems will be discussed last as special cases.

2.3.2 Green's function

Path integral quantum mechanics researchers usually concentrate on writing the system's propagator because it is exactly equivalent to the Schrödinger equation, which represents the equation of motion in the wave formulation of non-relativistic quantum mechanics and completely describes the evolution of the particle under study.

The propagator is a probability amplitude for a particle traveling from coordinates

(r', t') to (r'', t'') which can be defined as a sum of the contributions of all paths that connect the two endpoints

$$K(\overrightarrow{r''}, t''; \overrightarrow{r'}, t') = \langle r'', t'' | r', t' \rangle = \int_{r'}^{r''} Dr \ \exp(\frac{i}{\hbar}\hat{A}(r)), \tag{2.58}$$

where $\hat{A}(r)$ is the action.

Since the spherical symmetry of most potentials modeling atomic or diatomic systems including GIQY potential, it is preferable to write the propagator in spherical coordinates

$$K(\overrightarrow{r''}, t''; \overrightarrow{r'}, t') = \frac{1}{r''r'} \sum_{\ell=0}^{\infty} \frac{2\ell+1}{4\pi} K_\ell(r'', t''; r', t') P_\ell(\cos\Theta), \tag{2.59}$$

where the radial propagator associated with a Generalized Inverse Quadratic Yukawa potential is [2]

$$\begin{aligned} & K_\ell(r'', t''; r', t') \\ = \ & \lim_{N\to\infty} \left(\frac{M}{2i\pi\hbar\varepsilon}\right)^{(N+1)/2} \left(\prod_{j=1}^{N} \left[\int_0^\infty dr_j\right]\right) \times \exp\left(\frac{i}{\hbar} A_N\right) \end{aligned} \tag{2.60}$$

with the action A_j given by

$$A_N = \sum_{l=1}^{N+1} \left(\frac{M}{2\varepsilon}(\Delta r_j)^2 - \varepsilon V_{eff}\right). \tag{2.61}$$

where the effective potential V_{eff} is given by

$$V_{eff} = V_{GIQY}(r) + \frac{\hbar^2 \ell(\ell+1)}{r^2}. \tag{2.62}$$

where $V_{GIQY}(r)$ is the potential under consideration in this study.

The general form of Generalized Inverse Quadratic Yukawa Potential is:

$$V(r) = -a - \delta \ \frac{e^{-\alpha r}}{r} - \lambda \ \frac{e^{-2\alpha r}}{r^2},$$

which means that the effective potential becomes

$$V_{eff}(r) = -a - \delta \ \frac{e^{-\alpha r}}{r} - \lambda \ \frac{e^{-2\alpha r}}{r^2} + \frac{\hbar^2 \ell(\ell+1)}{2r^2}. \tag{2.63}$$

2.3.3 Approximations

Since the singular terms $1/r$ and $1/r^2$ in the effective potential (2.63) create obstacles to the search for precise solutions to the problem, we thought about using the following approximation formula [70, 82].

$$\frac{1}{r} \approx F_1 = \frac{2\alpha e^{-\alpha r}}{1 - e^{-2\alpha r}}, \tag{2.64}$$

and consequently

$$\frac{1}{r^2} \approx F_2 = \frac{4\alpha^2 e^{-2\alpha r}}{(1 - e^{-2\alpha r})^2}, \tag{2.65}$$

To check how the value of alpha affects the approximation we plot in figures (2.6, 2.7) the curves of $y = 1$, $y = r * F_1$ and $y = r^2 * F_2$ for different values of alpha.

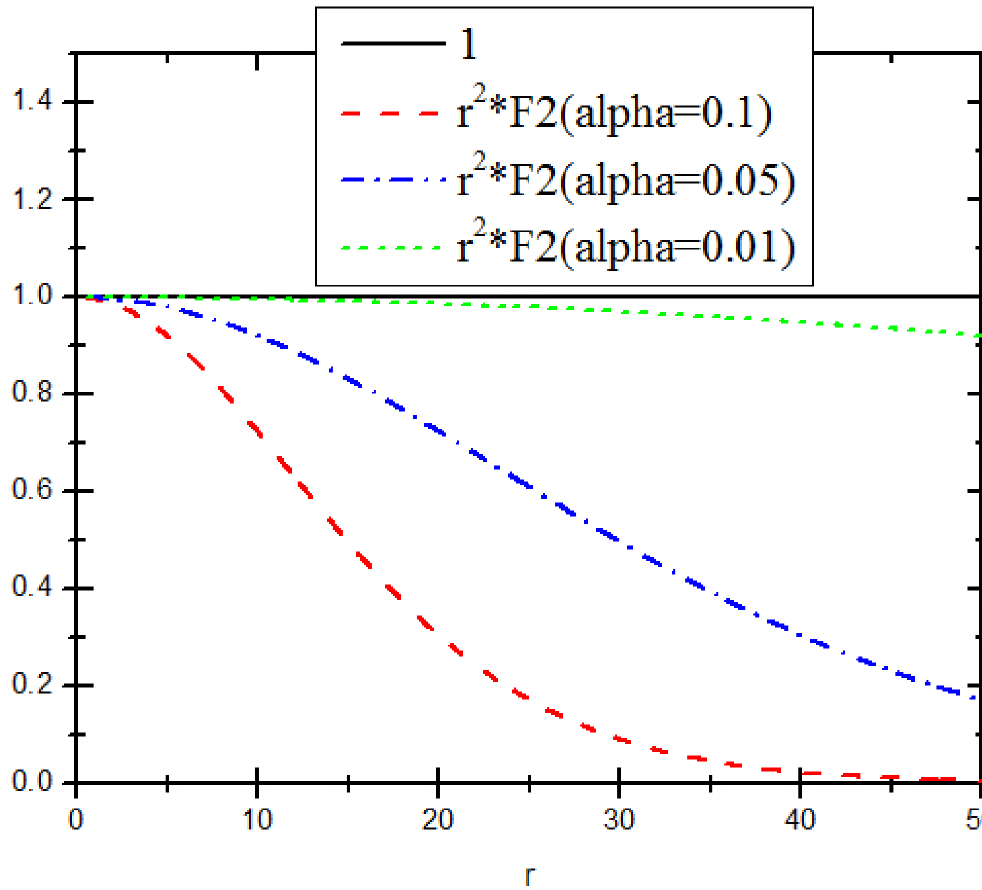

Figure 2.6: The effect of the α value on the approximation (2.65)

From these perspectives, we see that the approximations are more effective the lower the alpha.

putting these considerations together we find the following

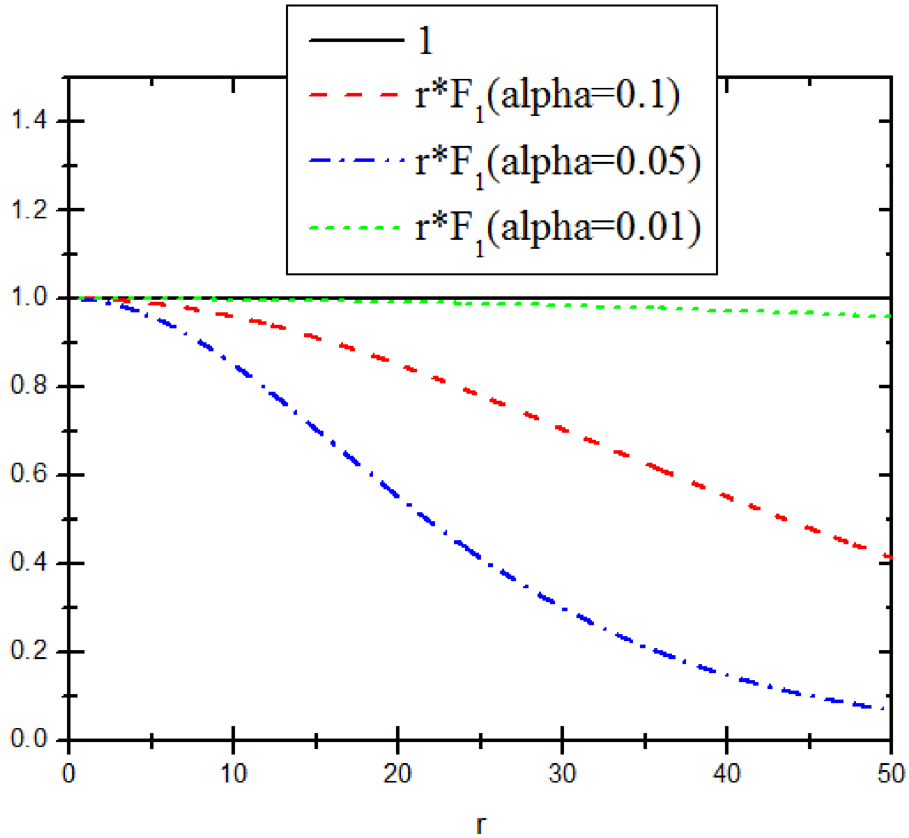

Figure 2.7: The effect of the α value on the approximation (2.64)

$$V_{eff}(r) \approx -\delta \frac{2\alpha e^{-2\alpha r}}{1-e^{-2\alpha r}} - \lambda \frac{4\alpha^2 e^{-4\alpha r}}{(1-e^{-2\alpha r})^2} + \frac{\hbar^2 \ell(\ell+1)}{2} \frac{4\alpha^2 e^{-2\alpha r}}{(1-e^{-2\alpha r})^2} - a, \tag{2.66}$$

for mathematical reason,$V_{eff}(r)$ can be then reformulated as

$$V_{eff}(r) = A\coth(\alpha r) + \frac{B}{\sinh^2(\alpha r)} + C, \tag{2.67}$$

with

$$\begin{cases} A = \alpha(2c\alpha - \delta); \\ B = \alpha^2(\frac{\hbar^2}{2M}\ell(\ell+1) - \lambda); \\ C = -2\lambda\alpha^2 + \delta\alpha - a. \end{cases} \tag{2.68}$$

It should be noted here that the Green's function that we will use to extract the eigenfunction and energy spectrum is nothing but the Fourier transformation of the radial propagator [12], which means that:

$$G_\ell(r_b, r_a; E) = \int_0^\infty e^{\frac{iE}{\hbar}T} K_\ell(r_b, r_a; T)dT = \int_0^\infty P_\ell(r_b, r_a; T)dT, \tag{2.69}$$

where the radial promotor $P_\ell(r_b, r_a; T)$ is given by:

$$P_\ell(r_b, r_a; T) = \lim_{N\to\infty} \left(\frac{M}{2i\pi\hbar\varepsilon}\right)^{1/2(N+1)} \left(\prod_{j=1}^{N}\left[\int_0^\infty dr_j\right]\right) \times \exp\left(\frac{i}{\hbar}A_N^E\right), \tag{2.70}$$

with the modified action

$$A_N^E = \int_0^T \left[\frac{M}{2}\dot{r}^2 - V_{eff}(r) + E\right] dT, \tag{2.71}$$

2.3.4 Space-time transformation

Since the difficulties of doing the integration (2.69) straightforwardly, we perform a space-time transformation depending on Duru-Kleinert method [83, 12], so we do a non-trivial change of variable ($r \to q$) followed by time local transformation ($t \to s$) [14]

$$\begin{cases} r = h(q) = \frac{1}{\alpha} \arg\coth(2\coth^2(q) - 1); \\ t \to s \Leftrightarrow dt = [h'(q(s))]^2 ds. \end{cases} \tag{2.72}$$

Putting this considerations together we find the new Green's function

$$G_\ell(q_b, q_a; E) = \frac{i}{\hbar}\left[h'(q_a)h'(q_b)\right]^{\frac{1}{2}} \int_0^\infty P_\ell(q_b, q_a; S)dS, \tag{2.73}$$

where h' is the derivative of h according to q, $S = s_b - s_a$ and the new form of the promoter is

$$P_\ell(q_b, q_a; s) = \int Dq(s) \exp\left[\frac{i}{\hbar}\int_0^S \left\{\frac{M}{2}\dot{q}^2 - h'^2(V_{eff}(q) - E) - \Delta V(q)\right\} ds\right], \tag{2.74}$$

the quantum correction $\Delta V(q)$[12] is given by(1.92)

$$\Delta V(q) = \frac{\hbar^2}{8M}\left(3\frac{h''^2}{h'^2} - 2\frac{h'''}{h'}\right) = \frac{\hbar^2}{8M}\left(\frac{1}{\cosh^2(q)} + \frac{1}{\sinh^2(q)}\right), \tag{2.75}$$

and the transformed effective potential is

$$V_{eff}(q) = A(2\coth^2(q) - 1) + 2B(2\coth^2(q) - 2)\coth^2(q) + C, \tag{2.76}$$

therefore

$$\begin{aligned} h'^2(V_{eff}(q)-E)+\Delta V(q) &= -\frac{1}{\alpha^2}(E-A-C)+ \\ &\frac{\hbar^2}{2M}\left(\frac{\frac{8MB}{\alpha^2\hbar^2}+\frac{3}{4}}{\sinh^2(q)}+\frac{\frac{2M}{\alpha^2\hbar^2}(E+A-C)+\frac{1}{4}}{\cosh^2(q)}\right). \end{aligned} \tag{2.77}$$

And by using the following abbreviations

$$\begin{cases} D=\frac{1}{\alpha^2}(E-A-C); \\ \eta=\sqrt{1+\frac{8MB}{\alpha^2\hbar^2}}; \\ \upsilon=\sqrt{-\frac{2M}{\alpha^2\hbar^2}(E+A-C)}, \end{cases} \tag{2.78}$$

eq. (2.77) becomes

$$\begin{aligned} h'^2(V_{eff}(q)-E)+\Delta V(q) &= -D+ \\ &\frac{\hbar^2}{2M}\left(\frac{\eta^2-\frac{1}{4}}{\sinh^2(q)}-\frac{\upsilon^2-\frac{1}{4}}{\cosh^2(q)}\right). \end{aligned} \tag{2.79}$$

hence the promotor (2.74) can be rewritten as follows

$$\begin{aligned} P_\ell(q_b,q_a;S) &= \exp\left[\frac{i}{\hbar}DS\right]\times\int Dq(s) \\ &\exp\left[\frac{i}{\hbar}\int_0^S\left\{\frac{M}{2}\dot{q}^2-\frac{\hbar^2}{2M}\left(\frac{\eta^2-\frac{1}{4}}{\sinh^2(q)}-\frac{\upsilon^2-\frac{1}{4}}{\cosh^2(q)}\right)\right\}ds\right], \end{aligned} \tag{2.80}$$

this is nothing but a promotor formula corresponding to a system with modified Pöschl-Teller potential and energy D [85], and accordingly, the integration over time S enables us to obtain directly the radial Green's function related to this system

$$G_\ell(q_b,q_a;D)=\int_0^\infty P_\ell(q_b,q_a;S)dS, \tag{2.81}$$

thus

$$\begin{aligned} G_\ell(q_b,q_a;D) &= \int_0^\infty \exp\left[\frac{i}{\hbar}DS\right]\int Dq(s) \\ &\exp\left[\frac{i}{\hbar}\int_0^S\left\{\frac{M}{2}\dot{q}^2-\frac{\hbar^2}{2M}\left(\frac{\eta^2-\frac{1}{4}}{\sinh^2(q)}-\frac{\upsilon^2-\frac{1}{4}}{\cosh^2(q)}\right)\right\}ds\right]dS, \end{aligned} \tag{2.82}$$

and as you can see in Reference [86] and other literature, the problem of modified Pöschl-Teller potential is a previously solved problem, therefore, integrating equation (2.82) gives us the following expression

$$\begin{aligned} G_\ell(q_b, q_a; D) &= \frac{M}{\hbar^2}\frac{\Gamma(m_1 - L\upsilon)\Gamma(m_1 + L\upsilon + 1)}{\Gamma(m_1 + m_2 + 1)\Gamma(m_1 - m_2 + 1)} \\ &\times(\cosh q_a \cosh q_b)^{-(m_1-m_2)}(\tanh q_a \tanh q_b)^{m_1+m_2+1/2} \\ &\times{}_2F_1(m_1 - L\upsilon, m_1 + L\upsilon + 1; m_1 - m_2 + 1; \cosh^{-2} q_\leq) \\ &\times{}_2F_1(m_1 - L\upsilon, m_1 + L\upsilon + 1; m_1 + m_2 + 1; \tanh^2 q_\geq), \end{aligned} \tag{2.83}$$

with the notation

$$\begin{cases} m_{1,2} = \frac{1}{2}(\eta \pm \sqrt{-2MD}/\hbar); \\ L\upsilon = \frac{1}{2}(\upsilon - 1). \end{cases} \tag{2.84}$$

2.3.5 Energy spectrum and wavefunctions

The energy spectrum is obtained from the poles of the Green's function that are in fact all contained in the gamma function $\Gamma(m_1 - L\upsilon)$. They are given by

$$m_1 - L\upsilon = -n_r, \tag{2.85}$$

by inserting the values of m_1 and $L\upsilon$ in (2.85), we obtain

$$D = -\frac{\hbar^2}{2M}(2n_r + \eta - \upsilon + 1)^2, \tag{2.86}$$

inserting the value of D leads to

$$\frac{1}{\alpha^2}(E - A - C) = -\frac{\hbar^2}{2M}\left(2n_r + \sqrt{1 + \frac{8MB}{\alpha^2\hbar^2}} - \sqrt{-\frac{2M}{\alpha^2\hbar^2}(E + A - C) + 1}\right)^2, \tag{2.87}$$

and therefore

$$\begin{aligned} E_n &= -\frac{\hbar^2\alpha^2}{8M}\left(2n_r + 1 + \sqrt{1 + \frac{8MB}{\alpha^2\hbar^2}}\right)^2 \\ &-\frac{2A^2}{\frac{\hbar^2\alpha^2}{M}\left(2n_r + 1 + \sqrt{1 + \frac{8MB}{\alpha^2\hbar^2}}\right)^2} + C, \end{aligned} \tag{2.88}$$

finally, energy eigen values of a non relativistic particle moving in the Generalized Inverse Quadratic Yukawa potential [87] are

$$\begin{aligned} E_n &= -\frac{\hbar^2\alpha^2}{8M}\left(2n_r+1+\sqrt{1+4\ell(\ell+1)-\frac{8M}{\hbar^2}\lambda}\right)^2 \\ &\quad -\frac{2(2\lambda\alpha-\delta)^2}{\frac{\hbar^2}{M}\left(2n_r+1+\sqrt{1+4\ell(\ell+1)-\frac{8M}{\hbar^2}\lambda}\right)^2}-2\lambda\alpha^2+\delta\alpha-a, \end{aligned} \tag{2.89}$$

this equation is fully consistent with the results obtained in Ref. [81] which is a comment and correction of Ref. [86] that depend on the proper quantization rule and formula method, respectively (PQRF).

On the other hand, the associated wavefunctions can be extracted from residues of the radial Green's function (2.83)

$$\begin{aligned} \psi_{n_r}(r) &= \left[\left(\alpha-\frac{4MA}{\alpha\hbar^2(\eta+2n_r+1)^2}\right)\frac{(2k_1-2n_r-\eta-2)n!\Gamma(2k_1-n_r-1)}{\Gamma(n_r+\eta+1)\Gamma(2k_1-\eta-n_r-1)}\right]^{1/2} \\ &\quad\times(1-\exp(-2\alpha r))^{\frac{\eta+1}{2}}\exp(k_1-\eta/2-n_r-1) \\ &\quad\times P_n^{(2k_1-2n_r-\eta-2,\eta)}(1-2\exp(-2\alpha r)), \end{aligned} \tag{2.90}$$

where $P_n^{(2k_1-2n_r-\eta-2,\eta)}$ are Jacobi polynomials with the notations

$$\begin{cases} k_1=\frac{1}{2}\left(1+\frac{1}{2}(\eta+2n_r+1)-\frac{2MA}{\alpha^2\hbar^2(\eta+2n_r+1)}\right); \\ k_2=\frac{1}{2}(1+\eta), \end{cases} \tag{2.91}$$

2.3.6 Discussion

Using eq. (2.89), we calculate in Table (2.3) the energy eigenvalues (in fm^{-1}) of GIQY potential for various values of n, ℓ and for $\hbar=M=1$. We set $\alpha=0.01$, $a=\lambda=1.0$ and $\delta=2.0$. for comparison with the outcomes of [86].

It is found that our results and the results of the proper quantization rule and formula method are identical.

An increase in angular momentum quantum ℓ, leads to an increase in the energy spectrum as the principal quantum number n increases.

Special cases that are implicit in the GIQY potential can be obtained by adjusting the alpha parameter.

Modified Screened Coulomb Plus Inversely Quadratic Yukawa Potential

For $a=0$, the GIQY potential reduces to Modified Screened Coulomb Plus Inversely Quadratic Yukawa potential (MSC-IQY) of the form

n	ℓ	$E_{n,\ell}$ (our results)	$E_{n,\ell}$ [86]
0	1	-2.940450000	-2.940450000
0	2	-1.279268339	-1.279268339
0	3	-1.123949058	-1.123949058
1	1	-1.470450000	-1.470450000
1	2	-1.135367365	-1.135367365
1	3	-1.069983263	-1.069983262
2	1	-1.198450000	-1.198450000
2	2	-1.075445609	-1.075445609
2	3	-1.042124745	-1.042124745
3	1	-1.103512500	-1.103512500
3	2	-1.045120125	-1.045120125
3	3	-1.026091933	-1.026091933
4	1	-1.059858000	-1.059858000
4	2	-1.027881596	-1.027881596
4	3	-1.016213517	-1.016213517
5	1	-1.036450000	-1.036450000
5	2	-1.017341821	-1.017341821
5	3	-1.009874302	-1.009874302

Table 2.3: The nonrelativistic energy eigenvalues (in $1/fm$) of GIQY potential for various values of n, ℓ and for $\hbar = M = 1$. We set $\alpha = 0.01$, $a = \lambda = 1.0$ and $\delta = 2.0$.

$$V(r) = -\delta\frac{e^{-\alpha r}}{r} - \lambda\frac{e^{-2\alpha r}}{r^2}, \tag{2.92}$$

and the energy eigenvalues associated with it are obtained as

$$\begin{aligned} E_n &= -\frac{\hbar^2\alpha^2}{8M}\left(2n_r + 1 + \sqrt{1 + 4\ell(\ell+1) - \frac{8M}{\hbar^2}\lambda}\right)^2 \\ &\quad -\frac{2(2c\alpha - \delta)^2}{\frac{\hbar^2}{M}\left(2n_r + 1 + \sqrt{1 + 4\ell(\ell+1) - \frac{8M}{\hbar^2}c}\right)^2} - 2\lambda\alpha^2 + \delta\alpha. \end{aligned} \tag{2.93}$$

Kratzer Potential

For $\alpha = 0$, $a = 0, \delta = 2D_e r_e$ and $\lambda = D_e r_e^2$, the GIQY potential reduces to the Kratzer Potential of the form

$$V_k(r) = -2D_e\left(\frac{r_e}{r} - \frac{1}{2}\frac{r_e^2}{r^2}\right), \tag{2.94}$$

where r_e is the equilibrium bond length, D_e is the dissociation energy.
Energy eigenvalues of the Kratzer Potential are obtained as

$$E_n = -\frac{\delta^2}{\frac{\hbar^2}{2M}\left(2n_r + 1 + \sqrt{1 + 4\ell(\ell+1) - \frac{8M}{\hbar^2}\lambda}\right)^2}, \tag{2.95}$$

thus

$$E_n = -\frac{(2D_e r_e)^2}{\frac{\hbar^2}{2M}\left(2n_r + 1 + \sqrt{1 + 4\ell(\ell+1) - \frac{8M}{\hbar^2}D_e r_e^2}\right)^2}. \tag{2.96}$$

this relation is in complete agreement with equation (18) of ref. [88] and eq. (46) of ref. [89].

modified Kratzer potential

For $\alpha = 0$, $a = -D_e, b = 2D_e r_e$ and $c = -D_e r_e^2$, the GIQY potential reduces to the modified Kratzer Potential of the form

$$V_k(r) = D_e\left(\frac{r - r_e}{r}\right)^2, \tag{2.97}$$

The energy eigenvalues of the Kratzer Potential are obtained as

$$E_{n_r,\ell} = D_e - \frac{(2D_e r_e)^2}{\frac{\hbar^2}{2M}\left(2n_r + 1 + \sqrt{1 + 4\ell(\ell+1) + \frac{8M}{\hbar^2}D_e r_e^2}\right)^2}. \tag{2.98}$$

Equation (15) is in excellent agreement with the result presented in eq. (61) of Ref. [90], eq. (15) of Ref. [91] and eq. (39) of Ref. [92]

Yukawa Potential

Setting $a = 0$ and $\lambda = 0$, eq. (2.57) takes the form

$$V(r) = -\delta\frac{e^{-\alpha r}}{r}, \tag{2.99}$$

which is known as Yukawa potential or screened Coulomb potential, its corresponding energy eigenvalues achieve

$$\begin{aligned} E_n &= -\frac{\hbar^2\alpha^2}{8M}\left(2n_r+1+\sqrt{1+4\ell(\ell+1)}\right)^2 \\ &\quad -\frac{2\delta^2}{\frac{\hbar^2}{M}\left(2n_r+1+\sqrt{1+4\ell(\ell+1)}\right)^2}+\delta\alpha, \end{aligned} \tag{2.100}$$

therefore

$$E_n = -\frac{\hbar^2\alpha^2}{2M}\left(n_r+1+\ell\right)^2 - \frac{\delta^2}{\frac{\hbar^2}{M}2\left(n_r+1+\ell\right)^2}+\delta\alpha, \tag{2.101}$$

which is consistent with equation (19) of ref. [93]

Inversely Quadratic Yukawa Potential

As $a=0$ and $\delta=0$, eq. (2.57) reduces to the Inversely Quadratic Yukawa potential (IQY)[94] of the form

$$V(r) = -\lambda\frac{e^{-2\alpha r}}{r^2}, \tag{2.102}$$

the energy eigenvalues equation becomes

$$\begin{aligned} E_n &= -\frac{\hbar^2\alpha^2}{8M}\left(2n_r+1+\sqrt{1+4\ell(\ell+1)-\frac{8M}{\hbar^2}\lambda}\right)^2 \\ &\quad -\frac{2(2\lambda\alpha)^2}{\frac{\hbar^2}{M}\left(2n_r+1+\sqrt{1+4\ell(\ell+1)-\frac{8M}{\hbar^2}\lambda}\right)^2}-2\lambda\alpha^2, \end{aligned} \tag{2.103}$$

Coulomb potential

When $a=0$, $\alpha=0$ and $\lambda=0$, eq. (2.57) reduces to the Coulomb potential of the form

$$V(r) = -\frac{\delta}{r}, \tag{2.104}$$

the energy eigenvalues of the coulomb Potential are obtained as

$$E_n = -\frac{\delta^2}{\frac{\hbar^2}{2M}\left(2n_r+1+\sqrt{1+4\ell(\ell+1)}\right)^2}, \tag{2.105}$$

hence

$$E_n = -\frac{2M}{\hbar^2}\frac{\delta^2}{2\left(n_r+\ell+1\right)^2}, \tag{2.106}$$

this relation is consistent with the results in eq. (50) of Ref. [89] and eq. (7.14) of Ref. [95]

2.3. Motion of a particle in the Generalized Inverse Quadratic Yukawa potential

2.3.7 Conclusion

In this work, the Schrödinger solutions of Generalized Inverse Quadratic Yukawa potential problem was obtained approximately using Feynman path integral formulation of quantum mechanics, an appropriate space-time transformation was applied to the Green's function associated with the problem, which made it an integrable function.

Energy levels and the corresponding wave functions have been extracted easily from the poles and residues of the integrated Green's function. In the last special cases and numerical data for the energy spectrum were discussed for various values of n and ℓ.

Chapter 3

A Klein Gordon Particle in GIQY Potential

3.1 Introduction

The Klein Gordon equation is the first attempt to construct a quantum mechanics that takes into account Einstein's special theory of relativity, so that the Schrödinger equation does not achieve this because it is built on the non-relativistic relationship between energy and linear momentum $E = \frac{P^2}{2M}$. The Klein Gordon equation starts from the relative relationship between these two $E^2 = p^2c^2 + m^2c^4$.

In fact, Klein-Gordon equation describes the behavior of spinless relativistic particles and has a wide range of applications in current physics.

For the first time, we will use the path integrals approach to treat a Klein-Gordon particle moving in a vector and scalar Generalized Inverse Quadratic Yukuwa (GIQY) potential in this chapter. First, we derive the Green's function for a Klein Gordon particle traveling in a scalar and vector potential. Second, we handle the Green's function of the GIQY potential in a manner akin to the Duru-Kleinert method, in which we reformulate the real challenging problem in terms of the non-relativistic modified Pöschl-Teller (mPT), a well-known and previously solved problem, by performing a non trivial space-time transformation.

The associated eigenfunctions and energy eigenvalues are obtained. In the final section, special cases pertaining to other works such as the Coulomb potential, inversely quadratic Yukawa potential, Kratzer potential, and Yukawa potential are also covered.

3.1.1 Path integral formulation for the Klein-Gordon equation

Path integral technique relies on building the system's propagator or it's Green's function because they contain all of the information associated with the quantum system, including the energy spectrum and the wave function.

Since the spherical symmetry of the considered potential, it is preferable to express

Green's function in spherical coordinates

$$G(\overrightarrow{r''},t'';\overrightarrow{r'},t')=\frac{1}{r''r'}\sum_{l=0}^{\infty}\frac{2\ell+1}{4\pi}G_{\ell}(r'',t'';r',t')P_{\ell}(\cos\Theta), \tag{3.1}$$

where the radial Green's function associated with a Klein-Gordon particle is [96]

$$\begin{aligned} G_{\ell}(r'',t'';r',t') &= \frac{1}{2i}\times \\ &\int_0^{\infty} d\Lambda \left\langle r'',t'' \middle| \exp\left\{\frac{i}{2}\left(\begin{array}{c} -P_r^2+(P_0-V)^2 \\ -\frac{\ell(\ell+1)}{r^2}-(M+S)^2 \end{array}\right)\Lambda\right\} \middle| r',t'\right\rangle, \end{aligned} \tag{3.2}$$

in Feynman formulation

$$G_{\ell}(r'',t'';r',t')=\frac{1}{2i}\int_0^{\infty}d\Lambda P_{\ell}(r'',t'',r',t';\Lambda), \tag{3.3}$$

where $P_{\ell}(r'',t'',r',t';\Lambda)$ is the promotor defined as

$$\begin{aligned} P_{\ell}(r'',t'',r',t';\Lambda) &= \lim_{N\to\infty}\prod_{j=1}^{N}\left[\int_0^{\infty}dr_j dt_j\right]\prod_{j=1}^{N+1}\left[\int_0^{\infty}\frac{d(P_r)_j d(P_0)_j}{(2\pi)^2}\right] \\ &\quad\times\exp\left(i\sum_{j=1}^{N+1}A_j\right), \end{aligned} \tag{3.4}$$

using the A_j action provided by

$$\begin{aligned} A_j &= -(P_r)_j\Delta r_j+(P_0)_j\Delta t_j \\ &\quad+\frac{\varepsilon_{\Lambda}}{2}\left(-(P_r)_j^2+((P_0)_j-V(r_j))^2-\frac{\ell(\ell+1)}{r_j^2}-(M+S(r_j))^2\right). \end{aligned} \tag{3.5}$$

The path integrals (3.4) can be performed in two steps as follows. First we do the integrals over times t_j taking into account that

$$\frac{1}{2\pi}\int_{-\infty}^{\infty}dt_j\ \exp\left[-i\ t_j\ \left((P_0)_j-(P_0)_{j+1}\right)\right]=\delta\left((P_0)_j-(P_0)_{j+1}\right), \tag{3.6}$$

we obtain N Dirac distributions $\delta\left((P_0)_j-(P_0)_{j+1}\right)$.

In a second step we integrate the result on variables $(P_0)_j$, the process that enforce all $(P_0)_j$ to be equal to each other, i.e.,

$$(P_0)_1=(P_0)_2=...=(P_0)_{N+1}\equiv E. \tag{3.7}$$

It is an equation that expresses the energy conservation law.

The final result can be written as

$$\begin{aligned} P_{\ell}(r'',t'',r',t';\Lambda) &= \frac{1}{2\pi}\lim_{N\to\infty}\int\limits_{-\infty}^{\infty} dE\exp\left[-iE\left(t''-t'\right)\right]\prod_{j=1}^{N}\left[\int dr_j\right] \\ &\times\prod_{j=1}^{N+1}\left[\int\frac{d(P_r)_j}{2\pi}\right]\times\exp\left(i\sum_{j=1}^{N+1}A'_j\right), \end{aligned} \tag{3.8}$$

with a new action of the form

$$A'_j = -(P_r)_j\Delta r_j + \frac{\varepsilon_\Lambda}{2}\left(-\left(P_r\right)_j^2 + (E-V(r_j))^2 - \frac{\ell(\ell+1)}{r_j^2} - (M+S(r_j))^2\right). \tag{3.9}$$

Putting

$$P_\ell(r'',r';\Lambda) = \lim_{N\to\infty}\prod_{j=1}^{N}\left[\int dr_j\right]\prod_{j=1}^{N+1}\left[\int\frac{d(P_r)_j}{2\pi}\right]\exp\left(i\sum_{j=1}^{N+1}A'_j\right), \tag{3.10}$$

This is just a promotor image of a non-relativistic particle traveling from r' to r'' over a time interval of Λ, with P_r momentum.

Thus,

$$P_\ell(r'',t'',r',t';\Lambda) = \frac{1}{2\pi}\lim_{N\to\infty}\int\limits_{-\infty}^{\infty} dE\exp\left[-iE\left(t''-t'\right)\right]P_l(r'',r';\Lambda). \tag{3.11}$$

Performing the integrations over $(P_r)_j$ variables, as is commonly used in non-relativistic situations, results in

$$P_\ell(r'',r';\Lambda) = \lim_{N\to\infty}\left(\frac{1}{2i\pi\varepsilon_\Lambda}\right)^{\frac{N+1}{2}}\left[\prod_{j=1}^{N}\int_0^\infty dr_j\right]\exp\left(i\sum_{j=1}^{N+1}A''_j\right), \tag{3.12}$$

with a new form of the action

$$A''_j = \frac{\left(\Delta r_j\right)^2}{2\varepsilon_\Lambda} - \frac{\varepsilon_\Lambda}{2}\left((M+S(r_j))^2 - (E-V(r_j))^2 + \frac{\ell(\ell+1)}{r_j^2}\right), \tag{3.13}$$

therefore

$$\begin{aligned} P_\ell(r'',r';\Lambda) &= \lim_{N\to\infty}\left(\frac{1}{2i\pi\varepsilon_\Lambda}\right)^{\frac{N+1}{2}}\left[\prod_{j=1}^{N}\int dr_j\right]\exp\left(i\frac{E^2-M^2}{2}\Lambda\right) \\ &\exp\left(i\sum_{j=1}^{N+1}\left[\frac{\left(\Delta r_j\right)^2}{2\varepsilon_\Lambda} - \frac{\varepsilon_\Lambda}{2}\left(\begin{array}{c}(S(r_j))^2-(V(r_j))^2+ \\ 2\left(MS(r)+EV(r)\right)+\frac{\ell(\ell+1)}{r_j^2}\end{array}\right)\right]\right), \end{aligned} \tag{3.14}$$

in a short form

$$P_\ell(r'',r';\Lambda)=\lim_{N\to\infty}\left(\frac{1}{2i\pi\varepsilon_\Lambda}\right)^{\frac{N+1}{2}}\left[\prod_{j=1}^{N}\int dr_j\right]\exp\left(i\widetilde{E}^2\Lambda\right)\exp\left(i\sum_{j=1}^{N+1}A_j'''\right),\qquad(3.15)$$

where we used the abbreviation

$$A_j'''=\left[\frac{(\Delta r_j)^2}{2\varepsilon_\Lambda}-\frac{\varepsilon_\Lambda}{2}\left((S(r_j))^2-(V(r_j))^2+2\left(MS(r)+EV(r)\right)+\frac{\ell(\ell+1)}{r_j^2}\right)\right],\qquad(3.16)$$

and

$$\widetilde{E}^2=\frac{E^2-M^2}{2}.\qquad(3.17)$$

Based on (3.8) and (3.10), we rebuild the Green's function (3.3) as follow

$$G_\ell(r'',t'';r',t')=\frac{1}{2\pi}\int_{-\infty}^{+\infty}dE\exp\left[-iE\left(t''-t'\right)\right]\frac{1}{2i}\int_0^{\infty}d\Lambda P_\ell(r'',r';\Lambda),\qquad(3.18)$$

thus

$$G_\ell(r'',t'';r',t')=\frac{1}{2\pi}\int_{-\infty}^{+\infty}dE\exp\left[-iE\left(t''-t'\right)\right]G_\ell(r'',r'),\qquad(3.19)$$

where

$$G_\ell(r'',r')=\frac{1}{2i}\int_0^{\infty}d\Lambda P_\ell(r'',r';\Lambda)=\frac{1}{2i}\int_0^{\infty}d\Lambda\exp\left(i\widetilde{E}^2\Lambda\right)K_\ell(r'',r';\Lambda),\qquad(3.20)$$

with the propagator $K_\ell(r'',r';\Lambda)$ given by

$$\begin{aligned}K_\ell(r'',r';\Lambda)\;&=\;\lim_{N\to\infty}\left(\frac{1}{2i\pi\varepsilon_\Lambda}\right)^{\frac{N+1}{2}}\left[\prod_{j=1}^{N}\int_0^{\infty}dr_j\right]\\&\quad\times\exp\left(i\sum_{j=1}^{N+1}\left[\frac{(\Delta r_j)^2}{2\varepsilon_\Lambda}-\varepsilon_\Lambda V_{eff}(r_j)\right]\right),\end{aligned}\qquad(3.21)$$

where the effective potential $V_{eff}(r_j)$ can be defined as

$$V_{eff}(r_j)=\frac{(S(r_j))^2-(V(r_j))^2}{2}+\left(MS(r)+EV(r)\right)+\frac{\ell(\ell+1)}{2r_j^2}.\qquad(3.22)$$

In this work, our study is restricted to the case of vector and scalar potential equality, i.e. $S(r) = V(r)$.

Accordingly

$$V_{eff}(r_j) = \left((M+E)\, V(r_j) + \frac{\ell(\ell+1)}{2r_j^2} \right), \tag{3.23}$$

where $V(r_j)$ represents the potential under consideration in our study.

3.2 Applying the formulation to the GIQY Potential

In this section we want to apply the path integral formulation for the radial Klein-Gordon equation on the Generalized Inverse Quadratic Yukawa Potential (2.57),

this leads to the effective potential

$$V_{eff}(r) = \frac{\ell(\ell+1)}{2r^2} - (M+E) \left(a + \delta \frac{e^{-\alpha r}}{r} + \lambda \frac{e^{-2\alpha r}}{r^2} \right). \tag{3.24}$$

Initially, we employ the same approximation as in the non-relativistic case (2.64) to handle the centrifugal terms.

$$\frac{1}{r} \approx \frac{2\alpha e^{-\alpha r}}{1 - e^{-2\alpha r}}, \tag{3.25}$$

and then

$$\frac{1}{r^2} \approx \frac{4\alpha^2 e^{-2\alpha r}}{(1 - e^{-2\alpha r})^2}, \tag{3.26}$$

It should be mentioned that these approximations are more reliable the smaller the α. [97, 98]

Together, these considerations lead to the following

$$V_{eff}(r) = \frac{\ell(\ell+1)}{2} \frac{4\alpha^2 e^{-2\alpha r}}{(1 - e^{-2\alpha r})^2} - (M+E) \left(a + \delta \frac{2\alpha e^{-2\alpha r}}{1 - e^{-2\alpha r}} + \lambda \frac{4\alpha^2 e^{-4\alpha r}}{(1 - e^{-2\alpha r})^2} \right), \tag{3.27}$$

after some algebraic operations this can be simplified to

$$V_{eff}(r_j) = A \coth(\alpha r) + \frac{B}{\sinh^2(\alpha r)} + C, \tag{3.28}$$

with

$$\begin{cases} A = (E+M)\alpha(2\lambda\alpha - \delta); \\ B = \alpha^2(\frac{1}{2}\ell(\ell+1) - (E+M)\lambda); \\ C = -(E+M)(2\lambda\alpha^2 - \delta\alpha + a). \end{cases} \tag{3.29}$$

3.3 Space-Time transformation

The propagator calculation problem is made simpler by applying the Duru-Kleinert method [83, 12], which reformulates the considered problem in terms of a well-known, solved one.

By suggesting the following suitable space-time transformation (2.72)

$$r = h(q) = \frac{1}{\alpha} \arg\coth(2\coth^2(q) - 1), \Lambda \to s \Leftrightarrow d\Lambda = \left[h'(q(s))\right]^2 ds. \tag{3.30}$$

In combination with Duru-Kleinert relation (1.93) this leads to a transformed Green's function

$$\begin{aligned} G_\ell(q_b, q_a; \widetilde{E}^2) &= i\left[h'(q_a)h'(q_b)\right]^{1/2} \int_0^\infty dS \times \\ & \int Dq(s) \exp\left[i \int_0^S \left\{ \frac{1}{2}\dot{q}^2 - h'^2(V_{eff}(q) - \widetilde{E}^2) - \Delta V(q) \right\} ds \right] \end{aligned} \tag{3.31}$$

where the quantum correction $\Delta V(q)$ [12] results from the prior variable changes.

$$\Delta V(q) = \frac{1}{2}\left(3\frac{h''^2}{h'^2} - 2\frac{h'''}{h'}\right) = \frac{1}{2}\left(\frac{1}{\cosh^2(q)} + \frac{1}{\sinh^2(q)}\right), \tag{3.32}$$

together with (3.28), the effective potential takes the form

$$V_{eff}(q) = A(2\coth^2(q) - 1) + 2B(2\coth^2(q) - 2)\coth^2(q) + C, \tag{3.33}$$

therefore

$$\begin{aligned} h'^2(V_{eff}(q) - \widetilde{E}^2) + \Delta V(q) &= \frac{1}{2}\left(\frac{\frac{8B}{\alpha^2} + \frac{3}{4}}{\sinh^2(q)} + \frac{\frac{2}{\alpha^2}(\widetilde{E}^2 + A - C) + \frac{1}{4}}{\cosh^2(q)} \right) \\ & -\frac{1}{\alpha^2}(\widetilde{E}^2 - A - C), \end{aligned} \tag{3.34}$$

with the identifications

$$\begin{cases} \eta = \frac{1}{2} + \sqrt{1 + \frac{8B}{\alpha^2}}; \\ \upsilon = \frac{1}{2} + \sqrt{-\frac{2}{\alpha^2}(\widetilde{E}^2 + A - C)}, \end{cases} \tag{3.35}$$

and therefore

$$\begin{cases} \eta(\eta - 1) = \frac{8B}{\alpha^2} + \frac{3}{4}; \\ \upsilon(\upsilon - 1) = -\frac{2}{\alpha^2}(\widetilde{E}^2 + A - C) - \frac{1}{4}, \end{cases} \tag{3.36}$$

the transformed promotor (1.90, 2.74) goes over into

$$P_\ell(q_b, q_a; s) = \int Dq(s) \exp\left[\frac{i}{\hbar}\int_0^S \left\{\frac{1}{2}\dot{q}^2 - \frac{1}{2}\left(\frac{\eta(\eta-1)}{\sinh^2(q)} + \frac{\upsilon(\upsilon-1)}{\cosh^2(q)}\right)\right\} ds\right] \times \exp\left[i\frac{1}{\alpha^2}(\widetilde{E}^2 - A - C)s\right]. \tag{3.37}$$

This expression can be better displayed as follows

$$P_\ell(q_b, q_a; s) = K_\ell^{MPT} \times \exp\left[i\frac{1}{\alpha^2}(\widetilde{E}^2 - A - C)s\right], \tag{3.38}$$

where K_ℓ^{MPT} is the propagator of the so-called modified Pöschl-Teller potential [99]

$$K_\ell^{MPT} = \int Dq(s) \exp\left[i\int_0^s \left\{\frac{M}{2}\dot{q}^2 - \frac{1}{2}\left(\frac{\eta(\eta-1)}{\sinh^2(q)} - \frac{\upsilon(\upsilon-1)}{\cosh^2(q)}\right)\right\} ds\right], \tag{3.39}$$

which is an issue with a known solution.

$$K_\ell^{MPT} = \sum_{n=0}^{N_m} \exp(-isE_n^{MPT})\chi_{\ell,n}^{(k_1,k_2)}(q_b)\chi_{\ell,n}^{*(k_1,k_2)}(q_a), \tag{3.40}$$

where the associated wave functions [99]

$$\begin{aligned}
\chi_{\ell,n}^{(k_1,k_2)}(q) &= N_n^{(k_1,k_2)}(\sinh(q))^{2k_2-1/2}(\cosh(q))^{-2k_2+3/2} \\
&\quad \times 2F_1(-k_1+k_2+k, -k_1+k_2-k; 2k_2; -\sinh^2(q)) \\
&= \left[\frac{2n!(2k_1-1)\Gamma(2k_1-n-1)}{\Gamma(2k_2+n)\Gamma(2k_1-2k_2-n)}\right]^{1/2} \\
&\quad \times(\sinh(q))^{2k_2-1/2}(\cosh(q))^{2n-2k_1+3/2} \\
&\quad \times P_n^{(2k_2-1, 2(k_1-k_2-n)-1)}\left(\frac{1-\sinh^2(q)}{\cosh^2(q)}\right),
\end{aligned} \tag{3.41}$$

and the energy eigenvalues

$$E_n^{MPT} = -\frac{1}{2M}\left[2(k_1-k_2-n)-1\right]^2. \tag{3.42}$$

According to ref [61, 100] the quantities k_1 and k_2 are given by

$$\begin{cases} k_1 = \frac{1}{2}\left(1 + \frac{1}{2}(s+2n+1) - \frac{2A}{\alpha^2(s+2n+1)}\right); \\ k_2 = \frac{1}{2}\left(1 + \sqrt{1+\frac{8B}{\alpha^2}}\right) \equiv \frac{1}{2}(1+s), \end{cases} \tag{3.43}$$

with

$$s = \sqrt{1 + \frac{8B}{\alpha^2}}. \tag{3.44}$$

In light of this, the promotor linked to GIQY potential is going to be:

$$\begin{aligned} P_\ell(q_b, s_b; q_a, s_a) &= \sum_{n=0}^{Nm} \exp\left(is \left[\frac{(\widetilde{E}^2 - A - C)}{\alpha^2} - E_n^{MPT} \right] \right) \\ &\quad \times \chi_{\ell,n}^{(k_1,k_2)}(q_b) \chi_{\ell,n}^{*(k_1,k_2)}(q_a), \end{aligned} \tag{3.45}$$

As we've already seen, the Green's function is obtained by applying the Fourier transform.

$$G_\ell(q_b, q_a; E_{n,l}) = i \left[h'(q_a) h'(q_b) \right]^{1/2} \sum_{n=0}^{Nm} \frac{\chi_{\ell,n}^{(k_1,k_2)}(q_b) \chi_{\ell,n}^{*(k_1,k_2)}}{i \left[\frac{(E_{n,\ell} - A' - C')}{\alpha^2} - E_n^{MPT} \right]}, \tag{3.46}$$

the denominators containing the energy eigenvalues of the GIQY potential.

Obtaining the poles of the Green's function allows for the extraction of the energy spectrum [101].

$$\widetilde{E}^2 = \alpha^2 E_n^{MPT} + A + C, \tag{3.47}$$

thus

$$\widetilde{E}^2 = -\frac{\alpha^2 \hbar^2}{2M} \left[2(k_1 - k_2 - n) - 1 \right]^2 + A + C. \tag{3.48}$$

Via the insertion of k_1 and k_2 into (3.48), we get at

$$\widetilde{E}^2 = -\frac{\alpha^2}{2} \left[\frac{1}{4}(s + 2n + 1)^2 + \frac{4A^2}{\alpha^4 (s + 2n + 1)^2} \right]^2 + C, \tag{3.49}$$

this leads to

$$\begin{aligned} E_{n,\ell}^2 - M^2 &= -\alpha^2 \left[\frac{1}{4} \left(\sqrt[2]{1 - 8\lambda(E_{n,\ell} + M) + 4\ell(\ell+1)} + 2n + 1 \right)^2 \right. \\ &\quad \left. + \frac{4((E_{n,\ell} + M)(2\lambda\alpha - \delta))^2}{\alpha^2 \left(\sqrt[2]{1 - 8\lambda(E_{n,\ell} + M) + 4\ell(\ell+1)} + 2n + 1 \right)^2} \right]^2 \\ &\quad -2(E_{n,\ell} + M)(2\lambda\alpha^2 - \delta\alpha + a), \end{aligned} \tag{3.50}$$

thus

$$\begin{aligned}E_{n,\ell}^2 - M^2 &= -\alpha^2\left(n+\sqrt[2]{\frac{1}{4}+\ell(\ell+1)-2\lambda(E_{n,\ell}+M)}+\frac{1}{2}\right)^2\\ &\quad -\frac{\left((E_{n,l}+M)(2\lambda\alpha-\delta)\right)^2}{\left(n+\sqrt[2]{\frac{1}{4}+\ell(\ell+1)-2\lambda(E_{n,\ell}+M)}+\frac{1}{2}\right)^2}\\ &\quad -2(E_{n,\ell}+M)(2\lambda\alpha^2-\delta\alpha+a), \end{aligned} \tag{3.51}$$

the associated wavefunctions

$$\begin{aligned}\psi &= \left[\left(\alpha+\frac{4A}{\alpha(s+2n+1)^2}\right)\frac{(2k_1-2n-s-2)n!\Gamma(2k_1-n-1)}{\Gamma(n+s+1)\Gamma(2k_1-s-n-12k_1-s-n-1)}\right]^{1/2}\\ &\quad \times(1-\exp(-2\alpha r))^{\frac{s+1}{2}}\exp(k_1-s/2-n-1)\\ &\quad \times P_n^{(2k_1-2n-s-2,s)}(1-2\exp(-2\alpha r)), \end{aligned} \tag{3.52}$$

3.4 Discussion

The energy numerical values (in fm^{-1}) of a relativistic spin-0 particle in GIQY potential, expressed in units $\hbar = c = 1$, are displayed in Table (3.1). In order to compare our results with the parametric Nikiforov-Uvarov method [80], we set $\alpha = 0.015, M = 5.0, a = 1.0$, $\lambda = 1.0$ and $\delta = 2.0$.

It is observed that the outcomes of the two methods are in good agreement.

Now, we adjust the alpha parameter to find solutions of some special implicit cases in GIQY potential.

3.4.1 Modified Screened Coulomb Plus Inversely Quadratic Yukawa Potential

With $a = 0$, the GIQY potential has the following form:

$$V(r) = -\delta\frac{e^{-\alpha r}}{r} - \lambda\frac{e^{-2\alpha r}}{r^2}, \tag{3.53}$$

this is known as Modified Screened Coulomb Plus Inversely Quadratic Yukawa potential (MSC-IQY) and its energy eigenvalues achieve

n	ℓ	$E_{n,\ell}$ (current results)	$E_{n,\ell}$ [80]	n	ℓ	$E_{n,\ell}$ (current results)	$E_{n,\ell}$ [80]
0	0	-4.999972084	-4.999975083	2	2	-4.999302039	-4.999377032
0	1	-4.999888330	-4.999900329	2	3	-4.998994882	-4.999102892
0	2	-4.999748737	-4.999775737	3	0	-4.999553469	-4.999601369
0	3	-4.999553298	-4.999601302	3	1	-4.999302091	-4.999377052
1	0	-4.999888347	-4.999900335	3	2	-4.998994921	-4.999102907
1	1	-4.999748748	-4.999775741	3	3	-4.998631883	-4.998778901
1	2	-4.999553309	-4.999601306	4	0	-4.999302352	-4.999377155
1	3	-4.999302017	-4.999377023	4	1	-4.998995011	-4.999102943
2	0	-4.999748804	-4.999775763	4	2	-4.998631945	-4.998778925
2	1	-4.999553336	-4.999601317	4	3	-4.998213008	-4.998405041

Table 3.1: Relativistic energy eigenvalues (in $1/fm$) of a spinless particle in the GIQY potential in units $\hbar = c = 1$, with $M = 5.0$, $\alpha = 0.015$, $a = 1.0$, $\delta = 2.0$ and $\lambda = 1.0$ for comparison with the parametric Nikiforov–Uvarov method.

$$\begin{aligned} E_{n,\ell}^2 - M^2 \;\; &= \;\; -\alpha^2 \left(n + \sqrt[2]{\frac{1}{4} + \ell(\ell+1) - 2\lambda(E_{n,\ell}+M)} + \frac{1}{2} \right)^2 \\ &\quad - \frac{((E_{n,\ell}+M)(2\lambda\alpha - \delta))^2}{\left(n + \sqrt[2]{\frac{1}{4} + \ell(\ell+1) - 2\lambda(E_{n,\ell}+M)} + \frac{1}{2} \right)^2} \\ &\quad -2(E_{n,\ell}+M)(2\lambda\alpha^2 - \delta\alpha), \end{aligned} \tag{3.54}$$

The energy eigenvalues (in fm^{-1}) of a spin 0 particle in the MSC-IQY potential are shown in Table (3.2) in units $\hbar = c = 1$. For the sake of comparison with the formula method [102], we set $\alpha = 0.0015, M = 5.0,\ \lambda = 1.0, a = 0,$ and $\delta = 1.0$.

It is clear from this comparison that the current results are very close to the results of the formula method.

3.4.2 Kratzer Potential

Setting $a = 0$, $\alpha = 0$, $\delta = 2D_e r_e$ and $\lambda = D_e r_e^2$, the GIQY potential reduces to the Kratzer Potential of the form

$$V_k(r) = -2D_e \left(\frac{r_e}{r} - \frac{1}{2}\frac{r_e^2}{r^2} \right), \tag{3.55}$$

where D_e represents the dissociation energy and r_e is the length of the equilibrium bond.

Consequently, the Kratzer energy eigenvalues are obtained as

n	ℓ	$E_{n,\ell}$ [101] (our results)	$E_{n,\ell}$ [102]
0	0	-4.9999997750674696705	-4.9999999437584356030
0	1	-4.9999991002695481483	-4.9999999437626403576
0	2	-4.9999979756061342984	-4.9999999437640417676
0	3	-4.9999964010769130787	-4.9999999437647424398
1	0	-4.9999991002706275025	-4.9999997750337892266
1	1	-4.9999979756068628624	-4.9999996938061064226
1	2	-4.9999964010776532075	-4.9999996485099273334
1	3	-4.9999943766822614265	-4.9999996198343021830
2	0	-4.9999979756105056902	-4.9999994938261254003
2	1	-4.9999964010793801748	-4.9999993110537383272
2	2	-4.9999943766837069914	-4.9999991879009274725
2	3	-4.9999919024214943076	-4.9999991001797651496
3	0	-4.9999964010880150563	-4.9999991001355010632
3	1	-4.9999943766870799773	-4.9999988099427962315
3	2	-4.9999919024239922457	-4.9999985939958475737
3	3	-4.9999889782941175377	-4.9999984287369271941
4	0	-4.9999943767039450639	-4.9999985939619655650
4	1	-4.9999919024298207725	-4.9999981940359903837
4	2	-4.9999889782980841748	-4.9999978777804448350
4	3	-4.9999856042995155398	-4.9999976238601311777

Table 3.2: Relativistic energy eigenvalues (in $1/fm$) of a spinless particle in the MSC-IQY potential in units $\hbar = c = 1$, with $M = 5.0$, $\alpha = 0.0015$, $a = 0$ and $\delta = 1$, $\lambda = 1.0$ for comparison with the results of the formula method.

$$E_{n,\ell}^2 - M^2 = -\frac{\left(\delta(E_{n,\ell}+M)\right)^2}{\left(n + \sqrt[2]{\frac{1}{4} + \ell(\ell+1) - 2c(E_{n,\ell}+M)} + \frac{1}{2}\right)^2}, \tag{3.56}$$

therefore

$$E_{n,\ell}^2 - M^2 = -\frac{\left(2D_e r_e(E_{n,\ell}+M)\right)^2}{\left(n + \sqrt[2]{\frac{1}{4} + \ell(\ell+1) - 2D_e r_e^2(E_{n,\ell}+M)} + \frac{1}{2}\right)^2}. \tag{3.57}$$

If we restrict equation (39) of reference [103] to three dimensions $d = 3$, then this relationship agrees perfectly with it.

3.4. Discussion

3.4.3 Yukawa Potential

For $\lambda = 0$ and $a = 0$, eq. (2.57) takes the Yukawa potential form

$$V(r) = -\delta \frac{e^{-\alpha r}}{r}, \tag{3.58}$$

as a result, its corresponding energies satisfy

$$\begin{aligned} E_{n,\ell}^2 - M^2 &= -\alpha^2 \left(n + \sqrt[2]{\frac{1}{4} + \ell(\ell+1)} + \frac{1}{2} \right)^2 \\ &- \frac{\left((E_{n,\ell} + M)\delta\right)^2}{\left(n + \sqrt[2]{\frac{1}{4} + \ell(\ell+1)} + \frac{1}{2} \right)^2} + 2\delta\alpha(E_{n,\ell} + M), \end{aligned} \tag{3.59}$$

In Table (3.3), the energy eigenvalues (in fm^{-1}) of a spinless particle in Yukawa potential in units $\hbar = c = 1$ are displayed. We set , $\alpha = 0.0015$, $M = 5.0$, $a = 0, \lambda = 0$ and $\delta = 1.0$ for comparison with the proper quantization rule [104].

This comparison, like the previous ones, gives a positive impression of the validity of this study.

3.4.4 Inversely Quadratic Yukawa Potential

when $a = 0$ and $\delta = 0$, eq. (2.57) takes the Inversely Quadratic Yukawa potential (IQY) formula

$$V(r) = -\lambda \frac{e^{-2\alpha r}}{r^2}, \tag{3.60}$$

So we can deduce the energy eigenvalue expression

$$\begin{aligned} E_{n,\ell}^2 - M^2 &= -\alpha^2 \left(n + \sqrt[2]{\frac{1}{4} + \ell(\ell+1) - 2\lambda(E_{n,\ell} + M)} + \frac{1}{2} \right)^2 \\ &- \frac{\left((E_{n,\ell} + M)2\lambda\alpha\right)^2}{\left(n + \sqrt[2]{\frac{1}{4} + \ell(\ell+1) - 2\lambda(E_{n,\ell} + M)} + \frac{1}{2} \right)^2} - 4\lambda\alpha^2(E_{n,\ell} + M), \end{aligned} \tag{3.61}$$

Table (3.4): Displays energy eigenvalues (in fm^{-1}) of the Inversely Quadratic Yukawa potential s states in units $\hbar = c = 1$. We take $\alpha = 0.0015$, $M = 5.0$, $a = 0$, $\delta = 0$, $\lambda = 1.0$ and $\ell = 0$ for comparison with the results of the Nikiforov-Uvarov Method [105].

Where we notice the great convergence between the results of the two methods.

n	ℓ	$E_{n,\ell}$ [101] (current results)	$E_{n,\ell}$ [104]
0	0	-4.9999997750674696402	-4.9999999437584356020
0	1	-4.9999991002698178653	-4.9999999437626530077
0	2	-4.9999979756068625893	-4.9999999437640586340
0	3	-4.9999964010783003347	-4.9999999437647614141
1	0	-4.9999991002698178653	-4.9999997750337386130
1	1	-4.9999979756068625893	-4.9999996938061251265
1	2	-4.9999964010783003347	-4.9999996485099816896
1	3	-4.9999943766837062328	-4.9999996198343817366
2	0	-4.9999979756068625893	-4.9999994938258976473
2	1	-4.9999964010783003347	-4.9999993110537092553
2	2	-4.9999943766837062328	-4.9999991879009818289
2	3	-4.9999919024225340227	-4.9999991001798808071
3	0	-4.9999964010783003347	-4.9999991001348937292
3	1	-4.9999943766837062328	-4.9999988099426420034
3	2	-4.9999919024225340227	-4.9999985939958475507
3	3	-4.9999889782941160508	-4.9999984287370349346
4	0	-4.9999943766837062328	-4.9999985939607002925
4	1	-4.9999919024225340227	-4.9999981940356091514
4	2	-4.9999889782941160508	-4.9999978777803223114
4	3	-4.9999856042976632698	-4.9999976238601764801

Table 3.3: Relativistic energy eigenvalues (in $1/fm$) of a spinless particle in Yukawa potential in units $\hbar = c = 1$. We set $M = 5.0$, $\alpha = 0.0015$, $a = 0$, $\delta = 1.0$ and $\lambda = 0$ for comparison with the proper quantization rule.

3.4.5 Coulomb potential

As $\alpha = 0$, $a = 0$ and $\lambda = 0$, eq. (2.57) reduces to the Coulomb potential of the form

$$V(r) = -\frac{\delta}{r}, \tag{3.62}$$

The Coulomb Potential's energy eigenvalues can be found as

$$E_{n,\ell}^2 - M^2 = -\frac{\left((E_{n,\ell}+M)\delta\right)^2}{\left(n + \sqrt[2]{\frac{1}{4}+\ell(\ell+1)} + \frac{1}{2}\right)^2}, \tag{3.63}$$

this relationship fully accords with the findings in Ref. [103]'s Eq. (19).

n	E_n (present)	E_n [105]
0	-4.9999997750	-4.9999994938
1	-4.9999991000	-4.9999989926
2	-4.9999979750	-4.9999980920
3	-4.9999964000	-4.9999967741
4	-4.9999943750	-4.9999950297
5	-4.9999919000	-4.9999928527

Table 3.4: s states relativistic energy eigenvalues (in $1/fm$) of a spinless particle in the IQY potential in units $\hbar = c = 1$. We take $\alpha = 0.0015$, $M = 5.0$, $\lambda = 1.0$, $a = 0$, $\delta = 0$ and $\ell = 0$ for comparison with the resullts of the Nikiforov-Uvarov Method.

3.5 Conclusion

The path integral solution of a relativistic spin-0- particle moving in equal scalar and vector Generalized Inverse Quadratic Yukawa potential has been covered in this chapter.

As we have seen, we first showed the Green's function that corresponds to the Klein Gordon equation. Next, using a few mathematical techniques, we were able to express the propagator of this equation in a manner that is comparable to the non-relativistic case. By utilizing an appropriate space-time transformation and applying approximations for the centrifugal terms, we were able to reduce the problem at hand to a known one, that ultimately produced eigenfunctions and energy eigenvalues expressions.

Specific cases and numerical outcomes were taken into consideration. They serve as a check to ensure the accuracy of our findings.

Chapter 4

A Dirac Particle in GIQY Potential

4.1 Introduction

In relativistic quantum mechanics, the wave equation used to describe the behavior of a spin-1/2 particle is called Dirac equation. It was formulated by Paul Dirac in 1928 [106] while he was looking for a covariant first order equation that is linear differential in both space and time to be an alternate for the Klein-Gordon equation. The goal of this work is to study k-states solutions of the Dirac equation for a Generalized Inverse Quadratic Yukawa (GIQY) potential in the presence of pseudospin and spin symmetries.

In fact, it has been found within the physics of the Dirac equation [107, 108, 109] that when vector and scalar potentials diverge by a constant amount (i.e., $V(r) - S(r) = constant$), spin symmetry arises; Whereas when their sum equals a constant ($i.e., V(r) + S(r) = constant$), pseudo-spin symmetry occurs.

This chapter is organized as follows: in Section 2, we wrote the Dirac equation for vector and scalar potential in spherical coordinates, which resulted in two second-order differential equations. In section 3, two Schrödinger-like equations were established for spin and pseudospin symmetries, as well as their path integrals representations. The solutions were available after using approximations to the centrifugal terms and performing a space-time transformation by the Duru-Kleinert method. special cases as Coulomb potential, inversely quadratic Yukawa potential, Yukawa potential, Kratzer potential and modified screened coulomb plus inversely quadratic Yukawa potential were discussed in section 4, here, full agreement appeared between our results and the results based on other methods in the literatures. Closing remarks were included in section 5.

4.2 Dirac equation

A spin-1/2 particle of mass M and momentum $p = i\ \nabla$ moving in in scalar and vector potential satisfies the relativistic Dirac equation, in natural units with $\hbar = c = 1$,

$$[\alpha p + \beta(M + S(r))]\,\psi(r) = [E - V(r)]\,\psi(r), \tag{4.1}$$

where α and β are the 4×4 Dirac matrices defined by

$$\alpha = \begin{pmatrix} 0 & \sigma_i \\ \sigma_i & 0 \end{pmatrix}, \qquad \beta = \begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix}, \tag{4.2}$$

with I is the 2×2 unit matrix and σ_i are Pauli matrices

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \qquad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \qquad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \tag{4.3}$$

since the GIQY potential is a spherically symmetric potential, it is preferable to write eq.(4.1) in spherical coordinates

$$\left[\alpha_r P_r + \frac{i\alpha_r \beta K}{r} + \beta(M + S(r))\right]\psi(r) = [E - V(r)]\,\psi(r), \tag{4.4}$$

where $\alpha_r = \begin{pmatrix} 0 & \sigma_r \\ \sigma_r & 0 \end{pmatrix}$ is the velocity operator, $P_r = -i\left(\frac{\partial}{\partial r} + \frac{1}{r}\right)$ is the radial momentum operator and $K = \beta(\sigma.L + 1)$ is the spin-orbit coupling operator,with L is the orbital angular momentum.

It is worthy noting that the dirac Hamiltonian is compatible with J^2, J_z and K, where $J = L + S$ is the total angular momentum operator and J_z is it's projection on the z-axis, accordingly, the set $(H, K,\ J^2, J_z\ )$ forms a complete set of of common eigenfunctions,

all these things make it convincing to write Dirac wave functions in the following form

$$\psi_{n,k}(r) = \frac{1}{r}\begin{pmatrix} F_{nk}(r) Y^{\ell}_{jm}(\theta,\varphi) \\ iG_{nk}(r) Y^{\bar{\ell}}_{jm}(\theta,\varphi) \end{pmatrix}, \tag{4.5}$$

where $Y^{\ell}_{jm}(\theta,\varphi)$ and $Y^{\bar{\ell}}_{jm}(\theta,\varphi)$ are the spherical spinors constructed by combining the spatial spherical harmonics $y_{\ell m_\ell}$ with the two-component spin wavefunctions, which are eigenstates of S^2 and S_z, here m denote the projection of the total angular momentum on the third axis and $\bar{\ell}$ is pseudo-orbital angular momentum, which is defined as $\bar{\ell} = \ell + 1$ for the aligned spin $j = \ell - \frac{1}{2}$ and $\bar{\ell} = \ell - 1$ for the unaligned spin $j = \ell + \frac{1}{2}$.

$F_{nk}(r)$, $G_{nk}(r)$ represent the upper and lower radial components of the Dirac spinors.

Substituting (4.5) on (4.4) and using the properties

$$\begin{cases} \sigma_r Y^{\ell}_{jm}(\theta,\varphi) = -Y^{\bar{\ell}}_{jm}(\theta,\varphi); \\ \sigma_r Y^{\bar{\ell}}_{jm}(\theta,\varphi) = -Y^{\ell}_{jm}(\theta,\varphi), \end{cases} \tag{4.6}$$

$$\begin{cases} KY^{\ell}_{jm}(\theta,\varphi) = kY^{\ell}_{jm}(\theta,\varphi); \\ KY^{\bar{\ell}}_{jm}(\theta,\varphi) = -kY^{\bar{\ell}}_{jm}(\theta,\varphi), \end{cases} \tag{4.7}$$

where the eigenvalues of K operator are $k = \pm(j + 1/2)$ for $j = \ell \pm \frac{1}{2}$, one can easily reduce the four coupled partial differential equations included in eq.(4.4) to the following two coupled first-order ordinary differential equations,

$$\left(\frac{d}{dr} + \frac{k}{r}\right) F_{nk}(r) = \left[M + E_{nk} - (V(r) - S(r))\right] G_{nk}(r), \tag{4.8}$$

$$\left(\frac{d}{dr} - \frac{k}{r}\right) G_{nk}(r) = \left[M - E_{nk} + (V(r) + S(r))\right] F_{nk}(r), \tag{4.9}$$

by introducing the abbreviations

$$\begin{cases} \Delta(r) = V(r) - S(r); \\ \Sigma(r) = V(r) + S(r), \end{cases} \tag{4.10}$$

we can write

$$\left(\frac{d}{dr} + \frac{k}{r}\right) F_{nk}(r) = \left[M + E_{nk} - \Delta(r)\right] G_{nk}(r), \tag{4.11}$$

$$\left(\frac{d}{dr} - \frac{k}{r}\right) G_{nk}(r) = \left[M - E_{nk} + \Sigma(r)\right] F_{nk}(r), \tag{4.12}$$

from eq.(4.11) we have

$$G_{nk}(r) = \frac{\left(\frac{d}{dr} + \frac{k}{r}\right) F_{nk}(r)}{\left[M + E_{nk} - \Delta(r)\right]}, \tag{4.13}$$

inserting this into eq.(4.12), we find the second-order differential equation satisfied by the upper component $F_{nk}(r)$

$$\left(\frac{d^2}{dr^2} - \frac{k(k+1)}{r^2} - \left[M + E_{nk} - \Delta(r)\right]\left[M - E_{nk} + \Sigma(r)\right] - \frac{\frac{d\Delta(r)}{dr}\left(\frac{d}{dr} + \frac{k}{r}\right)}{\left[M + E_{nk} - \Delta(r)\right]}\right) F_{nk}(r) = 0, \tag{4.14}$$

In the same way, it is possible to prove that the lower component $G_{nk}(r)$ satisfies

$$\left(\frac{d^2}{dr^2} - \frac{k(k-1)}{r^2} - \left[M - E_{nk} + \Sigma(r)\right]\left[M + E_{nk} - \Delta(r)\right] - \frac{\frac{d\Sigma(r)}{dr}\left(\frac{d}{dr} - \frac{k}{r}\right)}{\left[M - E_{nk} + \Sigma(r)\right]}\right) G_{nk}(r) = 0, \tag{4.15}$$

If we apply these last two formulas to the spin and pseudospin symmetries, respectively, we obtain a Schrödinger-like differential equations, which can be represented by path integral as we shall describe below.

4.3 Solutions to the Dirac equation

4.3.1 Spin symmetry

in the case of exact spin symmetry we have $\Delta(r) = cst \equiv \xi$, thus $\frac{d\Delta(r)}{dr} = 0$ and $\Sigma(r) = V(r)$

thus, eq. (4.14) becomes

$$\left(\frac{d^2}{dr^2} - \frac{k(k+1)}{r^2} - [M + E_{nk} - \xi]\,[M - E_{nk} + V(r)]\right) F_{nk}(r) = 0, \tag{4.16}$$

therefore

$$\left(-\frac{1}{2}\frac{d^2}{dr^2} + \frac{k(k+1)}{2r^2} + \frac{[M + E_{nk} - \xi]\,[M - E_{nk}]}{2} + \frac{(M + E_{nk} - \xi)}{2}V(r)\right) F_{nk}(r) = 0, \tag{4.17}$$

Obviously, this equation looks like a radial Schrödinger equation, thus we can easily establish it's path integral representation in the form [110]

$$P_k(r_b, t_b; r_a, t_a) = \left(\frac{1}{r_a r_b}\right) \lim_{N\to\infty} \left(\frac{1}{2\pi i\hbar\varepsilon}\right)^{\frac{1}{2}(N+1)} \times \left[\prod_{j=1}^{N} \int_0^{\infty} dr_j\right] \exp(i\ A_n), \tag{4.18}$$

where
$$\begin{cases} t_b = t_{N+1}; t_a = t_0; \\ r_b = r_{N+1}; r_a = r_0, \end{cases}$$
and

$$A_n = \sum_{j=1}^{N+1} \left[\frac{1}{2\varepsilon}(\Delta r_j)^2 - \varepsilon(V_{eff}(r_j) - \widetilde{E})\right], \tag{4.19}$$

with the abbreviations

$$\begin{aligned} V_{eff}(r_j) &= \frac{k(k+1)}{2r^2} + \frac{(M + E_{nk} - \xi)}{2}V(r); \\ \widetilde{E} &= -\frac{[M + E_{nk} - \xi]\,[M - E_{nk}]}{2}, \end{aligned} \tag{4.20}$$

the GIQY potential has the form

$$V(r) = -a - \delta\,\frac{e^{-\alpha r}}{r} - \lambda\,\frac{e^{-2\alpha r}}{r^2}, \tag{4.21}$$

accordingly, the effective potential can be written as

$$V_{eff}(r_j) = \frac{\frac{k(k+1)}{2} - (M + E_{nk} - \xi)\frac{\lambda}{2}\,e^{-2\alpha r}}{r^2} - \frac{(M + E_{nk} - \xi)\frac{\delta}{2}\,e^{-\alpha r}}{r} - (M + E_{nk} - \xi)\frac{a}{2}, \tag{4.22}$$

since the difficulties of performing the integral (4.18) imposed by the terms r^{-2} and r^{-1}, we consider the following approximation

$$\frac{1}{r}=\frac{-2\alpha e^{-\alpha r}}{e^{-2\alpha r}-1}, \tag{4.23}$$

and consequently

$$\frac{1}{r^2}=\frac{4\alpha^2 e^{-2\alpha r}}{(e^{-2\alpha r}-1)^2}, \tag{4.24}$$

it is worth pointing out that these approximations become more accurate with decreasing the value of α.

So, by substituting (4.23) and (4.24) into (4.22), and introducing the new variables

$$\begin{cases} A=(M+E_{nk}-\xi)\left(\alpha^2\lambda\ -\frac{\alpha\delta}{2}\right); \\ B=\frac{\alpha^2 k(k+1)}{2}-(M+E_{nk}-\xi)\frac{\alpha^2\lambda}{2}; \\ C=-(M+E_{nk}-\xi)\left(\alpha^2\lambda\ -\alpha\frac{\delta}{2}+\frac{a}{2}\right), \end{cases} \tag{4.25}$$

we obtain an equation of the form

$$V_{eff}(r)=A\ \coth(\alpha r)+\frac{B}{\sinh^2(\alpha r)}+C\ , \tag{4.26}$$

In fact, dealing with Green's function is better than the propagator (4.18), especially when extracting the energy spectrum and wave functions.

The Green's function can be obtained by simply transforming the propagator by Fourier transformation

$$G_k(r_b,r_a;\widetilde{E})=\int P_k(r_b,t_b;r_a,t_a)dt, \tag{4.27}$$

therefore

$$G_k(r_b,r_a;\widetilde{E})=\int dT\int Dr(t)\exp\left[i\int_0^T\left\{\frac{1}{2}\dot{r}^2-V_{eff}(r)-\widetilde{E}\right\}dt\right]. \tag{4.28}$$

In the same way Duru and Kleinert solved the Coulomb problem in 1979 [12, 83], we use here a space-time transformation for the Green's function

$$\begin{aligned} r &\ \to\ q\Leftrightarrow r=h(q)=\frac{1}{\alpha}\arg\coth(2\coth^2(q)-1), \\ t &\ \to\ s\Leftrightarrow dt=\left[h'(q(s))\right]^2 ds. \end{aligned} \tag{4.29}$$

The transformed Green's function can be written as

$$\begin{aligned} G_k(q_b, q_a; \widetilde{E}^2) &= i\ [h'(q_a)h'(q_b)]^{1/2} \int_0^s ds \int Dq(s) \\ &\exp\left[i \int_0^s \left\{ \frac{1}{2}\dot{q}^2 - h'^2(V_{eff}(q) - \widetilde{E}) - \Delta V(q) \right\} ds \right], \end{aligned} \tag{4.30}$$

where we extended the action by the quantum potential $\Delta V(q)$ in order to be related to the original Green's function (4.28) [83]

$$\Delta V(q) = \frac{1}{2}\left(3\frac{h''^2}{h'^2} - 2\frac{h'''}{h'}\right) = \frac{1}{2}\left(\frac{1}{\cosh^2(q)} + \frac{1}{\sinh^2(q)}\right), \tag{4.31}$$

the effective potential with the new variables reads

$$V_{eff}(q) = A(2\coth^2(q) - 1) + 2B(2\coth^2(q) - 2)\coth^2(q) + C\ , \tag{4.32}$$

therefore

$$\begin{aligned} h'^2(V_{eff}(q) - \widetilde{E}) + \Delta V(q) &= \frac{1}{2}\left(\frac{\frac{8B}{\alpha^2} + \frac{3}{4}}{\sinh^2(q)} + \frac{\frac{2}{\alpha^2}(\widetilde{E} + A - C) + \frac{1}{4}}{\cosh^2(q)} \right) \\ &\quad - \frac{1}{\alpha^2}(\widetilde{E} - A - C). \end{aligned} \tag{4.33}$$

Thus, we can re-express the transformed Green's function as

$$\begin{aligned} G_k(q_b, q_a; \widetilde{E}^2) &= i\ [h'(q_a)h'(q_b)]^{1/2} \int_0^s ds \int Dq(s) \\ &\exp\left[\frac{i}{\hbar} \int_0^s \left\{ \frac{1}{2}\dot{q}^2 - \frac{1}{2}\left(\frac{\eta(\eta-1)}{\sinh^2(q)} + \frac{\upsilon(\upsilon-1)}{\cosh^2(q)} \right) \right\} ds \right] \\ &\times \exp\left[i\frac{1}{\alpha^2}(\widetilde{E} - A - C)s \right], \end{aligned} \tag{4.34}$$

with the notations

$$\begin{cases} \eta = \frac{1}{2} \pm \sqrt{1 + \frac{8B}{\alpha^2}}; \\ \upsilon = \frac{1}{2} \pm \sqrt{-\frac{2}{\alpha^2}(\widetilde{E}^2 + A - C)}. \end{cases} \tag{4.35}$$

Eq. (4.34) can be rephrased in another, more inspiring way

$$G_k(q_b, q_a; \widetilde{E}^2) = i\,[h'(q_a)h'(q_b)]^{1/2} \int_0^s ds \exp\left[i\frac{1}{\alpha^2}(\widetilde{E} - A - C)s \right] K_\ell^{MPT}, \tag{4.36}$$

where K_{ℓ}^{MPT} represent a propagator of the form [99]

$$K_{k}^{MPT}=\int Dq(s)\exp\left[i\int_{0}^{s}\left\{\frac{1}{2}\dot{q}^{2}-\frac{1}{2}\left(\frac{\eta(\eta-1)}{\sinh^{2}(q)}-\frac{\upsilon(\upsilon-1)}{\cosh^{2}(q)}\right)\right\}ds\right], \tag{4.37}$$

In fact, this integration is one of the problems that have already been exactly solved in previous studies, it is the modified Pöschl-Teller problem, and it can be written as

$$K_{k}^{MPT}=\sum_{n=0}^{Nm}\exp(-isE_{n}^{MPT})\chi_{k,n}^{(k_1,k_2)}(q_b)\chi_{k,n}^{*(k_1,k_2)}(q_a), \tag{4.38}$$

where $\chi_{k,n}^{(k_1,k_2)}$ and $\chi_{k,n}^{*(k_1,k_2)}$ are the associated wave functions [111]

$$\begin{aligned}\chi_{k,n}^{(k_1,k_2)}(q) &= N_{n}^{(k_1,k_2)}(\sinh(q))^{2k_2-1/2}(\cosh(q))^{-2k_2+3/2}\\ &\quad\times{}_2F_1(-n,-2k_1+2k_2+n;2k_2;-\sinh^{2}(q))\\ &= \left[\frac{2n!(2k_1-1)\Gamma(2k_1-n-1)}{\Gamma(2k_2+n)\Gamma(2k_1-2k_2-n)}\right]^{1/2}\\ &\quad\times(\sinh(q))^{2k_2-1/2}(\cosh(q))^{2n-2k_1+3/2}\\ &\quad\times P_{n}^{(2k_2-1,2(k_1-k_2-n)-1)}\left(\frac{1-\sinh^{2}(q)}{\cosh^{2}(q)}\right),\end{aligned} \tag{4.39}$$

and the energy eigenvalues

$$E_{n}^{MPT}=-\frac{1}{2}\left[2(k_1-k_2-n)-1\right]^{2}, \tag{4.40}$$

consequently, the corresponding Green's function will be

$$\begin{aligned}G_k(q_b,q_a;\widetilde{E}^{2}) &= i\left[h'(q_a)h'(q_b)\right]^{1/2}\int_{0}^{s}ds\sum_{n=0}^{Nm}\exp\left(is\left[\frac{(\widetilde{E}-A-C)}{\alpha^{2}}-E_{n}^{MPT}\right]\right)\\ &\quad\times\chi_{k,n}^{(k_1,k_2)}(q_b)\chi_{k,n}^{*(k_1,k_2)}(q_a),\end{aligned} \tag{4.41}$$

leading to the spectral representation; it arises by simply integrating (4.41) over ds

$$G_k(q_b,q_a;E_{n,\ell})=i\left[h'(q_a)h'(q_b)\right]^{1/2}\sum_{n=0}^{Nm}\frac{\chi_{k,n}^{(k_1,k_2)}(q_b)\chi_{k,n}^{*(k_1,k_2)}}{i\left[\frac{(E_{n,l}-A'-C')}{\alpha^{2}}-E_{n}^{MPT}\right]}, \tag{4.42}$$

the quantities k_1 and k_2 are given by [111]

$$\begin{cases}k_1=\frac{1}{2}\left(1+\frac{1}{2}(s+2n+1)-\frac{2A}{\alpha^{2}(s+2n+1)}\right);\\ k_2=\frac{1}{2}\left(1+\sqrt{1+\frac{8B}{\alpha^{2}}}\right)\equiv\frac{1}{2}\left(1+s\right),\end{cases} \tag{4.43}$$

with

$$s=\sqrt{1+\frac{8B}{\alpha^2}}. \tag{4.44}$$

The energy eigenvalues lie at the poles of the integrated Green's function (4.42) where

$$\widetilde{E}=\alpha^2E_n^{MPT}+A+C, \tag{4.45}$$

thus

$$\widetilde{E}=-\frac{\alpha^2}{2}\left[2(k_1-k_2-n)-1\right]^2+A+C. \tag{4.46}$$

Inserting the expressions of k_1, k_2 and $\widetilde{E}$ in (4.46) one obtain

$$\left[M+E_{nk}-\xi\right]\left[M-E_{nk}\right]=\alpha^2\left[\frac{1}{4}(s+2n+1)^2+\frac{4A^2}{\alpha^4(s+2n+1)^2}\right]-2C, \tag{4.47}$$

which leads to [110]

$$\begin{aligned}\left[M+E_{nk}-\xi\right]\left[M-E_{nk}\right] &= \alpha^2\left(\sqrt{\frac{1}{4}+k(k+1)-(M+E_{nk}-\xi)\lambda}+n+\frac{1}{2}\right)^2\\ &+\frac{(M+E_{nk}-\xi)^2\left(\alpha\lambda\ -\frac{\delta}{2}\right)^2}{\left(\sqrt{\frac{1}{4}+k(k+1)-(M+E_{nk}-\xi)\lambda}+n+\frac{1}{2}\right)^2}\\ &+(M+E_{nk}-\xi)\left(2\alpha^2\lambda\ -\alpha\delta+a\right).\end{aligned} \tag{4.48}$$

The corresponding calculated values (in fm^{-1}) are listed in Tables (4.1) and (4.2) in units $\hbar=c=1$, for comparison with the parametric Nikiforov-Uvarov method [112]. The following parameters were used: $\alpha=0.015$, $M=5.0$, $\xi=6$, $\lambda=1.0$, $\delta=2.0$ and $a=1.0$.

These results presented in Tables (4.1) and (4.2) show the degenerate states for the spin symmetry of the GIQY potential. Specifically, it is observed that the following pairs of orbitals exhibit the same energy: $(0p_{1/2}=0p_{3/2})$, $(0d_{3/2}=0d_{5/2})$, $(0f_{5/2}=0f_{7/2})$, $(0g_{7/2}=0g_{9/2})$, $(1p_{1/2}=1p_{3/2})$, $(1d_{3/2}=1d_{5/2})$, $(1f_{5/2}=1f_{7/2})$ and $(1g_{7/2}=1g_{9/2})$. Consequently, they can be considered spin doublets.

from the residues of (4.42) we extract the upper components of the wavefunctions

$$\begin{aligned}F_{nk}(r) &= \left[\left(\alpha+\frac{4A}{\alpha(s+2n+1)^2}\right)\frac{(2k_1-2n-s-2)n!\Gamma(2k_1-n-1)}{\Gamma(n+s+1)\Gamma(2k_1-s-n-12k_1-s-n-1)}\right]^{1/2}\\ &\times(1-\exp(-2\alpha r))^{\frac{s+1}{2}}\exp(k_1-s/2-n-1)\\ &\times P_n^{(2k_1-2n-s-2,s)}(1-2\exp(-2\alpha r)),\end{aligned} \tag{4.49}$$

ℓ	n	k	$(\ell, j=\ell+1/2)$	$E_{n,k}$ (our result)	$E_{n,k}$ [112]
1	0	-2	$0p_{3/2}$	2.786421054, 1.000297081	3.548970670, 1.000681826
2	0	-3	$0d_{5/2}$	3.595958210, 1.000668520	3.760489854, 1.001212357
3	0	-4	$0f_{7/2}$	3.814480865, 1.001188689	3.842392207, 1.001894749
4	0	-5	$0g_{9/2}$	3.898657006, 1.001857741	3.882740822, 1.002729209
1	1	-2	$1p_{3/2}$	3.229212185, 1.000668480	3.736363776, 1.001212315
2	1	-3	$1d_{5/2}$	3.789006080, 1.001188649	3.836893867, 1.001894703
3	1	-4	$1f_{7/2}$	3.892889088, 1.001857698	3.880924589, 1.002729159
4	1	-5	$1g_{9/2}$	3.938135847, 1.002675827	3.904706802, 1.003715941

Table 4.1: Relativistic energy eigenvalues (in $1/fm$) of a spin 1/2 particle in the GIQY potential in units $\hbar = c = 1$ (spin symmetry), with parameters $M = 5.0$, $\alpha = 0.015$ and $a = 1.0$, $\delta = 2.0$, $\lambda = 1.0$ and $\xi = 6$ for comparison with the parametric Nikiforov–Uvarov method.

ℓ	n	k	$(\ell, j=\ell-1/2)$	$E_{n,k}$ (our result)	$E_{n,k}$ [112]
1	0	1	$0p_{1/2}$	2.786421054, 1.000297081	................., 1.000075738
2	0	2	$0d_{3/2}$	3.595958210, 1.000668520	2.767863869, 1.000302992
3	0	3	$0f_{5/2}$	3.814480865, 1.001188689	3.548970670, 1.000681826
4	0	4	$0g_{7/2}$	3.898657006, 1.001857741	3.760489854, 1.001212357
1	1	1	$1p_{1/2}$	3.229212185, 1.000668480	.................., 1.000302931
2	1	2	$1d_{3/2}$	3.789006080, 1.001188649	3.215030796, 1.000681785
3	1	3	$1f_{5/2}$	3.892889088, 1.001857698	3.736363776, 1.001212315
4	1	4	$1g_{7/2}$	3.938135847, 1.002675827	3.836893867, 1.001894703

Table 4.2: Relativistic energy eigenvalues (in $1/fm$) of a spin 1/2 particle in the GIQY potential in units $\hbar = c = 1$ (spin symmetry), with parameters $M = 5.0$, $\alpha = 0.015$ and $a = 1.0$, $\delta = 2.0$, $\lambda = 1.0$ and $\xi = 6$ for comparison with the parametric Nikiforov–Uvarov method.

for the lower component of the wavefunction we have

$$G_{nk}(r) = \frac{1}{[M + E_{nk} - \xi]} \left(\frac{d}{dr} + \frac{k}{r} \right) F_{nk}(r), \tag{4.50}$$

thus

$$\begin{aligned} G_{nk}(r) &= \frac{\exp(k_1 - s/2 - n - 1)}{[M + E_{nk} - \xi]} \\ & \left[\left(\alpha + \frac{4A}{\alpha(s+2n+1)^2} \right) \frac{(2k_1 - 2n - s - 2)n!\Gamma(2k_1 - n - 1)}{\Gamma(n+s+1)\Gamma(2k_1 - s - n - 12k_1 - s - n - 1)} \right]^{1/2} \\ & \left[\begin{array}{c} \left((s+1)\alpha \exp(-2\alpha r)(1 - \exp(-2\alpha r))^{\frac{s-1}{2}} + \frac{k(1-\exp(-2\alpha r))^{\frac{s+1}{2}}}{r} \right) \\ \times P_n^{(2k_1 - 2n - s - 2, s)}(1 - 2\exp(-2\alpha r)) \\ + \left((1 - \exp(-2\alpha r))^{\frac{s+1}{2}} 2\alpha \exp(-2\alpha r)(2k_1 - n - 1) \right) \\ \times P_{n-1}^{(2k_1 - 2n - s - 2 + 1, s+1)}(1 - 2\exp(-2\alpha r)) \end{array} \right]. \end{aligned} \tag{4.51}$$

4.3.2 Pseudospin symmetry

In the case of exact pseudospin symmetry we have $\Sigma(r) = \beta = cst$, thus $\frac{d\Sigma(r)}{dr} = 0$ and $\Delta(r) = V(r)$,

after substituting these conditions in eq(4.15) , the lower component satisfies

$$\left(\frac{d^2}{dr^2} - \frac{k(k-1)}{r^2} - [M - E_{nk} + \Sigma(r)] [M + E_{nk} - \Delta(r)] \right) G_{nk}(r) = 0 \tag{4.52}$$

therefore

$$\left(-\frac{1}{2} \frac{d^2}{dr^2} + \frac{k(k-1)}{2r^2} + \frac{[M - E_{nk} + \beta] [M + E_{nk}]}{2} + V(r) \frac{(M - E_{nk} + \beta)}{2} \right) G_{nk}(r) = 0 \tag{4.53}$$

introducing the new variables V_{eff} and $\widetilde{E}$

$$\begin{aligned} V_{eff} &= \frac{k(k-1)}{2r^2} + \frac{(M + \beta - E_{nk})}{2} V(r), && (4.54) \\ \widetilde{E} &= -\frac{[M + \beta - E_{nk}] [M + E_{nk}]}{2}, && (4.55) \end{aligned}$$

then becomes

$$\left(-\frac{1}{2} \frac{d^2}{dr^2} + V_{eff}(r) - \widetilde{E} \right) G_{nk}(r) = 0 \tag{4.56}$$

this equation is quite similar to the radial Schrödinger equation, it's path integral representation can be shown in the form

$$G_k(r_b, r_a; E) = \int dT \int Dr(t) \exp\left[i \int_0^T \left\{ \frac{1}{2}\dot{r}^2 - V_{eff}(r) - \widetilde{E} \right\} dt \right], \tag{4.57}$$

using the same previous approximations(4.23,4.24), the effective potential can be written in a new simple form

$$V_{eff}(r_j) = A' \ \coth(\alpha r) + \frac{B'}{\sinh^2(\alpha r)} + C' \ , \tag{4.58}$$

with the notations

$$\begin{cases} A' = \alpha \left(M - E_{nk} + \beta \right) \left(\alpha\lambda \ - \frac{\delta}{2} \right); \\ B' = \frac{\alpha^2 k(k-1)}{2} - \left(M - E_{nk} + \beta \right) \frac{\alpha^2 d}{2}; \\ C' = -\left(M - E_{nk} + \beta \right) \frac{\left(2\alpha^2\lambda \ -\alpha\delta + a \right)}{2}, \end{cases} \tag{4.59}$$

using the same previous space-time transformation, one can find

$$\begin{aligned} G_k(q_b, q_a; \widetilde{E}^2) \ &= \ i \left[h'(q_a) h'(q_b) \right]^{1/2} \int_0^s ds \int Dq(s) \\ &\times \exp\left[\frac{i}{\hbar} \int_0^s \left\{ \frac{1}{2}\dot{q}^2 - \frac{1}{2} \left(\frac{\eta(\eta-1)}{\sinh^2(q)} + \frac{\upsilon(\upsilon-1)}{\cosh^2(q)} \right) \right\} ds \right] \\ &\times \exp\left[i \frac{1}{\alpha^2} (\widetilde{E} - A' - C') s \right], \end{aligned} \tag{4.60}$$

with

$$\begin{cases} \eta = \frac{1}{2} \pm \sqrt{1 + \frac{8B'}{\alpha^2}}; \\ \upsilon = \frac{1}{2} \pm \sqrt{-\frac{2}{\alpha^2} (\widetilde{E}^2 + A' - C')}, \end{cases} \tag{4.61}$$

which permit us to re-express eq(4.60) in terms of the non-relativistic modified Pöschl-Teller propagator K_ℓ^{MPT} as follow

$$G_k(q_b, q_a; \widetilde{E}^2) = i \left[h'(q_a) h'(q_b) \right]^{1/2} \int_0^s ds \ K_k^{MPT} \times \exp\left[i \frac{1}{\alpha^2} (\widetilde{E} - A' - C') s \right], \tag{4.62}$$

where K_k^{MPT} is defined by

$$K_k^{MPT} = \int Dq(s) \exp\left[i \int_0^s \left\{ \frac{1}{2}\dot{q}^2 - \frac{1}{2} \left(\frac{\eta(\eta-1)}{\sinh^2(q)} - \frac{\upsilon(\upsilon-1)}{\cosh^2(q)} \right) \right\} ds \right], \tag{4.63}$$

which is very similar to that of the modified Pöschl-Teller problem, and it's solutions are available in previous studies and can be expressed by means of wavefunctions and energy eigenvalues.

$$K_k^{MPT} = \sum_{n=0}^{N_m} \exp(-isE_n^{MPT})\chi_{k,n}^{(k_1,k_2)}(q_b)\chi_{k,n}^{*(k_1,k_2)}(q_a), \tag{4.64}$$

with

$$\begin{aligned}\chi_{k,n}^{(k_1,k_2)}(q) &= N_n^{(k_1,k_2)}(\sinh(q))^{2k_2-1/2}(\cosh(q))^{-2k_2+3/2}\\ &\quad\times 2F_1(-n,-2k_1+2k_2+n;2k_2;-\sinh^2(q))\\ &= \left[\frac{2n!(2k_1-1)\Gamma(2k_1-n-1)}{\Gamma(2k_2+n)\Gamma(2k_1-2k_2-n)}\right]^{1/2}\\ &\quad\times(\sinh(q))^{2k_2-1/2}(\cosh(q))^{2n-2k_1+3/2}\\ &\quad\times P_n^{(2k_2-1,2(k_1-k_2-n)-1)}\left(\frac{1-\sinh^2(q)}{\cosh^2(q)}\right),\end{aligned} \tag{4.65}$$

the actual Green's function therefore takes the form

$$G_k(q_b,q_a;E_{n,k}) = i\left[h'(q_a)h'(q_b)\right]^{1/2}\sum_{n=0}^{Nm}\frac{\chi_{k,n}^{(k_1,k_2)}(q_b)\chi_{k<,n}^{*(k_1,k_2)}}{i\left[\frac{(\widetilde{E}-A'-C')}{\alpha^2}-E_n^{MPT}\right]}. \tag{4.66}$$

the poles of eq. (4.66) give the energy spectrum

$$\widetilde{E} = -\frac{\alpha^2}{2}\left[\frac{1}{4}\left(\sqrt{1+\frac{8B'}{\alpha^2}}+2n+1\right)^2+\frac{4A'^2}{\alpha^4\left(\sqrt{1+\frac{8B'}{\alpha^2}}+2n+1\right)^2}\right]+C', \tag{4.67}$$

leading to [110]

$$\begin{aligned}\left[M-E_{nk}+\beta\right]\left[M+E_{nk}\right] &= \alpha^2\left(\sqrt{\frac{1}{4}+k(k-1)-\left(M-E_{nk}+\beta\right)\lambda}+n+\frac{1}{2}\right)^2\\ &\quad+\frac{\left(M-E_{nk}+\beta\right)^2\left(\alpha\lambda\ -\frac{\delta}{2}\right)^2}{\left(\sqrt{\frac{1}{4}+k(k-1)-\left(M-E_{nk}+\beta\right)\lambda}+n+\frac{1}{2}\right)^2}\\ &\quad+\left(M-E_{nk}+\beta\right)\left(2\alpha^2\lambda\ -\alpha\delta+a\right),\end{aligned} \tag{4.68}$$

The corresponding calculated values of GIQY energies (in fm^{-1}) are listed in Tables (4.3) and (4.4) in units $\hbar = c = 1$, with parameters: $M = 5.0$, $\alpha = 0.015, \beta = 0$, $a = 1.0$, $\delta = 2.0$ and $\lambda = 1.0$ for comparison with the parametric Nikiforov–Uvarov method [112].

4.3. Solutions to the Dirac equation

$\widetilde{\ell}$	n	k	(ℓ, j)	$E_{n,k}$ (our result)	$E_{n,k}$ [112]
1	1	-1	$1s_{1/2}$	-3.229212185, -1.000668480	..................., -1.000407408
2	1	-2	$1p_{3/2}$	-3.789006080, -1.001188649	-5.438375582, -1.000724340
3	1	-3	$1d_{5/2}$	-3.892889088, -1.001857698	-5.715675962, -1.001131883
4	1	-4	$1f_{7/2}$	-3.938135847, -1.002675827	-5.810728576, -1.001630082
1	2	-1	$2s_{1/2}$	..................., -1.001188554	..................., -1.000724305
2	2	-2	$2p_{3/2}$	-3.879477822, -1.001857619	-5.651303287, -1.001131854
3	2	-3	$2d_{5/2}$	-3.934814412, -1.002675751	-5.798924985, -1.001630054
4	2	-4	$2f_{7/2}$	-3.961366006, -1.003643201	-5.854398360, -1.002218963

Table 4.3: Relativistic energies (in $1/fm$) of a spin 1/2 particle in the GIQY potential in units $\hbar = c = 1$ (pseudospin symmetry). We set $M = 5.0$, $\alpha = 0.015$, $a = 1.0$, $\delta = 2.0$, $\lambda = 1.0$ and $\beta = 0$ for comparison with the parametric Nikiforov–Uvarov method

$\widetilde{\ell}$	n	k	(ℓ, j)	$E_{n,k}$ (our result)	$E_{n,k}$ [112]
1	1	2	$0d_{3/2}$	-3.229212185, -1.000668480	..................., -1.000407408
2	1	3	$0f_{5/2}$	-3.789006080, -1.001188649	-5.438375582, -1.000724340
3	1	4	$0g_{7/2}$	-3.892889088, -1.001857698	-5.715675962, -1.001131883
4	1	5	$0h_{9/2}$	-3.938135847, -1.002675827	-5.810728576, -1.001630082
1	2	2	$1d_{3/2}$	..................., -1.001188554	..................., -1.000724305
2	2	3	$1f_{5/2}$	-3.879477822, -1.001857619	-5.651303287,-1.001131854
3	2	4	$1g_{7/2}$	-3.934814412, -1.002675751	-5.798924985, -1.001630054
4	2	5	$1h_{9/2}$	-3.961366006, -1.003643201	-5.854398360, -1.002218963

Table 4.4: Relativistic energies (in $1/fm$) of a spin 1/2 particle in the GIQY potential in units $\hbar = c = 1$ (pseudospin symmetry). We set $M = 5.0$, $\alpha = 0.015$, $a = 1.0$, $\delta = 2.0$, $\lambda = 1.0$ and $\beta = 0$ for comparison with the parametric Nikiforov–Uvarov method.

From Tables (4.3) and (4.4) degeneracy for the pseudospin symmetry of the GIQY potential can be seen in the following states: $(1s_{1/2},\ 0d_{3/2})$, $(1p_{3/2}, 0f_{5/2})$, $(1d_{5/2}, 0g_{7/2})$, $(1f_{7/2}, 0g_{9/2})$, $(2s_{1/2}, 1d_{3/2})$, $(2p_{3/2}, 1f_{5/2})$, $(2d_{5/2}, 1g_{7/2})$ and $(2f_{7/2}, 1h_{9/2})$.

the residues of eq. (4.66) give the expression of the lower component of the wavefunction

$$\begin{aligned} G_{nk}(r) &= \left[\left(\alpha + \frac{4A'}{\alpha(s+2n+1)^2}\right)\frac{(2k_1-2n-s-2)n!\Gamma(2k_1-n-1)}{\Gamma(n+s+1)\Gamma(2k_1-s-n-12k_1-s-n-1)}\right]^{1/2} \\ &\quad \times(1-\exp(-2\alpha r))^{\frac{s+1}{2}}\exp(k_1-s/2-n-1) \\ &\quad \times P_n^{(2k_1-2n-s-2,s)}(1-2\exp(-2\alpha r)), \end{aligned} \tag{4.69}$$

for the upper component of the wavefunction we have

$$F_{nk}(r) = \frac{1}{[M-E_{nk}+\beta]}\left(\frac{d}{dr}-\frac{k}{r}\right)G_{nk}(r), \tag{4.70}$$

therefore

$$\begin{aligned} F_{nk}(r) &= \frac{\exp(k_1-s/2-n-1)}{[M-E_{nk}+\beta]} \\ &\quad \left[\left(\alpha + \frac{4A'}{\alpha(s+2n+1)^2}\right)\frac{(2k_1-2n-s-2)n!\Gamma(2k_1-n-1)}{\Gamma(n+s+1)\Gamma(2k_1-s-n-12k_1-s-n-1)}\right]^{1/2} \\ &\quad \left(\begin{array}{c} \left[(s+1)\alpha\exp(-2\alpha r)(1-\exp(-2\alpha r))^{\frac{s-1}{2}} - k\frac{(1-\exp(-2\alpha r))^{\frac{s+1}{2}}}{r}\right] \\ \times P_n^{(2k_1-2n-s-2,s)}(1-2\exp(-2\alpha r)) \\ +\left[(1-\exp(-2\alpha r))^{\frac{s+1}{2}}2\alpha\exp(-2\alpha r)(2k_1-n-1)\right] \\ \times P_{n-1}^{(2k_1-2n-s-1,s+1)}(1-2\exp(-2\alpha r)) \end{array}\right). \end{aligned} \tag{4.71}$$

4.4 Discussion

In this section, we discuss some special cases whose solutions can be derived directly by modifying parameters a, δ, λ and α in the general solution.

4.4.1 Modified Screened Coulomb Plus Inversely Quadratic Yukawa Potential

Setting $a = 0$ eq. (2.57) reduces to the form

$$V(r) = -\delta\frac{e^{-\alpha r}}{r} - \lambda\,\frac{e^{-2\alpha r}}{r^2}, \tag{4.72}$$

which is a combination between a Modified Screened Coulomb and Inversely Quadratic Yukawa potential (MSC-IQY). The energy eigenvalues for the spin symmetry case satisfy

$$\begin{aligned}
&[M+E_{nk}-\xi]\,[M-E_{nk}]=\alpha^2\left(\sqrt{\frac{1}{4}+k(k+1)-(M+E_{nk}-\xi)\lambda}+n+\frac{1}{2}\right)^2\\
&+\frac{(M+E_{nk}-\xi)^2\left(\alpha\lambda\ -\frac{\delta}{2}\right)^2}{\left(\sqrt{\frac{1}{4}+k(k+1)-(M+E_{nk}-\xi)\lambda}+n+\frac{1}{2}\right)^2}\\
&+(M+E_{nk}-\xi)\left(2\alpha^2\lambda\ -\alpha\delta\right),
\end{aligned} \tag{4.73}$$

while for the pseudospin symmetry we have

$$\begin{aligned}
[M-E_{nk}+\beta]\,[M+E_{nk}] \;=\;& \alpha^2\left(\sqrt{\frac{1}{4}+k(k-1)-(M-E_{nk}+\beta)\,\lambda}+n+\frac{1}{2}\right)^2\\
&+\frac{(M-E_{nk}+\beta)^2\left(\alpha\lambda\ -\frac{\delta}{2}\right)^2}{\left(\sqrt{\frac{1}{4}+k(k-1)-(M-E_{nk}+\beta)\,\lambda}+n+\frac{1}{2}\right)^2}\\
&+(M-E_{nk}+\beta)\left(2\alpha^2\lambda\ -\alpha\delta\right).
\end{aligned} \tag{4.74}$$

4.4.2 Kratzer Potential

For $\alpha=0,\ a=0, \delta=2D_e r_e$ and $\lambda=D_e r_e^2$, eq. (2.57) reduces to the Kratzer Potential given by

$$V_k(r)=-2D_e\left(\frac{a}{r}-\frac{1}{2}\frac{a^2}{r^2}\right), \tag{4.75}$$

where D_e is the dissociation energy and a is the equilibrium bond length.
The spin symmetry energy eigenvalues of the Kratzer Potential are then

$$[M-\xi+E_{nk}]\,[M-E_{nk}]=+\frac{(M-\xi+E_{nk})^2(D_e a)^2}{\left(\sqrt{\frac{1}{4}-(M-\xi+E_{nk})D_e a^2+k(k+1)}+n+\frac{1}{2}\right)^2}, \tag{4.76}$$

and for the pseudospin symmetry we have

$$[M+\beta-E_{nk}]\,[M+E_{nk}]=+\frac{(M+\beta-E_{nk})^2\,(D_e a)^2}{\left(\sqrt{\frac{1}{4}-(M+\beta-E_{nk})\,D_e a^2+k(k-1)}+n+\frac{1}{2}\right)^2}, \tag{4.77}$$

for $k=0$, these last relationships become in complete agreement with eq. (3.9) and eq. (3.13) of Ref. [113].

4.4.3 Yukawa Potential

As $\lambda = 0$ and $a = 0$, the GIQY potential takes the form of Yukawa potential [114]

$$V(r) = -\delta \frac{e^{-\alpha r}}{r}, \tag{4.78}$$

consequently, the spin symmetry energy eigenvalues achieve

$$\begin{aligned}[M - \xi + E_{nk}]\,[M - E_{nk}] &= \frac{(M + E_{nk} - \xi)^2 \delta^2}{4\,(k+n+1)^2} \\ &\quad + \alpha^2\,(k+n+1)^2 - \alpha\delta(M + E_{nk} - \xi),\end{aligned} \tag{4.79}$$

while, the pseudospin symmetry energy eigenvalues satisfy

$$[M + \beta - E_{nk}]\,[M + E_{nk}] = \alpha^2\,(k+n)^2 + \frac{(M - E_{nk} + \beta)^2\,\delta^2}{4\,(k+n)^2} - \alpha\delta\,(M - E_{nk} + \beta)\,. \tag{4.80}$$

Eq. (4.79) is very similar to eq. (35) of Ref. [115]

4.4.4 Inversely Quadratic Yukawa Potential

When $a = 0$ and $\delta = 0$, the GIQY potential takes the form of the Inversely Quadratic Yukawa potential (IQY) of the form

$$V(r) = -\lambda \frac{e^{-2\alpha r}}{r^2}, \tag{4.81}$$

the energy eigenvalue expression for the spin symmetry becomes

$$\begin{aligned}&[M - \xi + E_{nk}]\,[M - E_{nk}] = \alpha^2 \left(\sqrt{\frac{1}{4} - (M - \xi + E_{nk})\lambda + k(k+1)} + n + \frac{1}{2} \right)^2 \\ &+ \frac{(M - \xi + E_{nk})^2\,(\alpha\lambda\,)^2}{\left(\sqrt{\frac{1}{4} - (M + E_{nk} - \xi)\lambda + k(k+1)} + n + \frac{1}{2} \right)^2} \\ &+ 2\alpha^2\lambda\,(M - \xi + E_{nk}),\end{aligned} \tag{4.82}$$

and for the pseudospin symmetry

$$\begin{aligned}[M + \beta - E_{nk}]\,[M + E_{nk}] &= \alpha^2 \left(\sqrt{\frac{1}{4} - (M - E_{nk} + \beta)\,\lambda + k(k-1)} + n + \frac{1}{2} \right)^2 \\ &\quad + \frac{(M + \beta - E_{nk})^2\,(\alpha\lambda\,)^2}{\left(\sqrt{\frac{1}{4} - (M + \beta - E_{nk})\,\lambda + k(k-1)} + n + \frac{1}{2} \right)^2} \\ &\quad + 2\alpha^2\lambda\,(M + \beta - E_{nk})\ ,\end{aligned} \tag{4.83}$$

the eqs. (4.82) and (4.83) are largely consistent with equations (38) and (30) of Ref. [79].

4.4.5 Coulomb potential

For $\alpha = 0$, $a = 0$ and $\lambda = 0$, eq. (2.57) reduces to the Coulomb potential of the form

$$V(r) = -\frac{b}{r}, \tag{4.84}$$

which is called the Coulomb potential.

The energy eigenvalues of the Coulomb potential are obtained as

$$[M + E_{nk} - \xi]\,[M - E_{nk}] = \frac{(M + E_{nk} - \xi)^2\delta^2}{4\,(k+n+1)^2},$$

for the spin symmetry, and

$$[M - E_{nk} + \beta]\,[M + E_{nk}] = \frac{(M - E_{nk} + \beta)^2\,\delta^2}{4\,(k+n)^2}, \tag{4.85}$$

for the pseudospin symmetry.

These two equations are in full agreement with the results in eq. (12) and eq. (17) of Ref. [116].

4.5 Conclusion

In this chapter, the Dirac equation for the Generalized Inverse Quadratic Yukawa potential has been solved under spin and pseudo-spin symmetries. Dirac equation has been reduced to a two couple Schrödinger-like differential equations, which allows to establish the path integral representation. Using a suitable space-time transformation the actual kernel is transformed to another one similar to that of the non-relativistic modified Pöschl-Teller problem, the energy eigenvalues expressions are extracted from the integrated Green's function, also the upper and the lower components are obtained in terms of Jacobi polynomial. In the end, we have also discussed the energy spectrum for a number of particular cases, which constitute tangible confirmation of the validity of our results.

Conclusion

In this dissertation, after having briefly presented the formalism of Feynman's path integrals covering in particular the time-sliced propagator, its spectral representation and the Green's function and gave some insights on the techniques commonly used within the framework of the path integral method, namely the formulation of the path integral in spherical coordinates to deal with the problem of a potential spherical symmetry, space-time transformation method, we have taken up in an original way the complete study of a set of quantum systems composed of particles in motion in models of central potentials widely used in theoretical physics and quantum chemistry.

In the context of non-relativistic quantum mechanics, we first in Chapter Two consider the two problems of a moving particle in the trigonometric Pöschl-Teller potential and a moving particle in the modified Pöschl-Teller potential. Both problems have been the subject of many works using different analysis techniques, the results of which have been valid. Our addition to this presentation takes into account ℓ solutions to both problems by adopting the Greene-Aldrich approximation to the centrifugal term. The results obtained by the path integration method were satisfactory, especially after comparing them with other analysis techniques.

In the same non-relativistic context, also in Chapter Two we touched on the issue of the Generalized Inverse Quadratic Yukawa potential in an approximate manner. By using approximations to $1/r$ and $1/r^2$ terms, and using the appropriate spatiotemporal transformation we were able to reduce the ℓ-states problem of the studied potential to the modified Pöschl-Teller s-states problem. This allowed us to find an expression for the energy and wave functions

In the context of relativistic quantum mechanics, we have re-examined in Chapter Three the problem of a spinless particle of mass M in the presence of an equal vector potential $V(r)$ and a scalar potential $S(r)$ of the Generalized Inverse Quadratic Yukawa type. Our results are original and compared with those obtained through the resolution of the Klein Gordon equation.

The Fourth Chapter is devoted to presenting a relativistic study of a spin-1/2 particle in the Generalized Inverse Quadratic Yukawa potential. Path integration theory allowed us to represent this problem. We were able to develop an expression for the energy and wave functions by using approximations for centrifugal terms and a suitable spatiotemporal transformation. Spin and pseudospin symmetry were both examined in this work.

It can be noted that our results seem to be correct, as the energy spectrum corresponding to several cases well-known in the literature, which can be used as tests, has been found.

Finally, in light of the results obtained, it should be emphasized that the Feynman path integral formalism constitutes a serious alternative to other quantum mechanical formalisms. It can be considered a very powerful and effective working tool for finding the propagator associated with many quantum physics problems, including relativistic and non-relativistic problems, which can cross the most difficult areas of physics. The results of this method (energy spectrum and wave functions) are fairly satisfactory.

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