

الجمهورية الجزائرية الديمقراطية الشعبية
People's Democratic Republic of Algeria
وزارة التعليم العالي والبحث العلمي

Ministry of Higher Education and Scientific Research

University Center
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المركز الجامعي
عبد الحفيظ بوصوف ميله

Institute: Mathematics and Computer Science
Order N°:
Registration number:

Department: Mathematics
Field: Mathematics
Specialty: Mathematics and applications

www.centre-univ-mila.dz

Thesis

Submitted for the degree of
Doctorate LMD

Spectral study of some problems in quantum mechanics

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University year: 2024/2025

Dedication

To my parents

To my sisters

To my uncle Kamel Zemmouri

To the memory of my grandfather Messaoud Ladjeroud

I dedicate this work

Acknowledgements

I extend my deepest gratitude to my supervisor, Pr. Badredine Boudjedaa, for his unwavering support and insightful critiques throughout my research journey. His deep commitment to academic excellence and meticulous attention to detail have significantly shaped this dissertation, his guidance and advice carried me through all stages of my Ph.D journey. I am equally thankful to the members of my thesis committee : Pr. Mohammed Salah Abdelouahab, Dr. Rabeh Bououden, Pr. Tahar Boudjedaa, Pr. Saleh Haouat and Dr. Issam Bousafsaf.

This thesis is a reflection of the unwavering support and boundless love I received from my family during this challenging academic pursuit. I owe an immense debt of gratitude to my parents, my sisters : Meriem, Wissame and Alae, and my uncle Kamel Zemmouri for their support.

Amal

Abstract

In this thesis, we resolved Schrödinger equation spectral problem, for few central potentials, a single potential is the sum of the generalized Cornell potential plus an exponential potential, in the framework of quasi-exactly solvable problems. The exponential potentials that were treated are : Morse potential, the generalized Pöschl-Teller potential, Yukawa class potential, Schiöberg potential and Manning-Rosen potential. After inserting the central potential in the radial equation, the effective potential became a combination of terms that made the resolution of the radial equation not trivial to find, for this purpose, an approximation scheme was used to transform the radial equation into the normal form of biconfluent Heun's equation, where the solutions are known, hence the approximate bound states of Schrödinger equation and their energy eigenvalues are obtained in explicit form. At the end, for given values of the parameters, some of the approximate bound states and their energy levels were given.

Keywords:

Schrödinger equation, the generalized Cornell potential, quasi-exactly solvable problems, : Morse potential, the generalized Pöschl-Teller potential, Yukawa class potential, Schiöberg potential, Manning-Rosen potential, biconfluent Heun's equation, approximate bound states.

Résumé :

Dans cette thèse, nous avons résolu le problème spectral de l'équation de Schrödinger, pour quelques potentiels centraux, un seul potentiel est la somme du potentiel de Cornell généralisé plus un potentiel exponentiel, dans le cadre de problèmes quasi-exactement solubles. Les potentiels exponentiels qui ont été traités sont : le potentiel de Morse, le potentiel de Pöschl-Teller généralisé, le potentiel de Yukawa, le potentiel de Schiöberg et le potentiel de Manning-Rosen. Pour ce potentiel et par un schéma d'approximation bien précis on a pu transformer l'équation radiale en l'équation de Heun biconfluente, où on a déterminé les états liés approximatifs de l'équation de Schrödinger et leurs niveaux d'énergie correspondante sous une forme explicite. À la fin, pour des valeurs données des paramètres, certains des états liés approximatifs et leurs niveaux d'énergie associée ont été donnés.

Mots clés :

Équation de Schrödinger, potentiel de Cornell généralisé, problèmes quasi-exactement solubles, potentiel de Morse, potentiel de Pöschl-Teller généralisé, potentiel de classe de Yukawa, potentiel de Schiöberg, potentiel de Manning-Rosen, équation de Heun biconfluente, états liés approximatifs.

ملخص

في هذه الأطروحة، قمنا بحل المشكلة الطيفية لمعادلة شرودنجر (Schrödinger)، لبعض الكمونات المركزية، الكمون الواحد هو مجموع الكمون المعمم لكورنل (Cornell) بالإضافة إلى كمون أسي، في إطار المشاكل الشبه قابلة الحل. الكمونات الأسية التي تمت معالجتها هي: كمون مورس (Morse) ، الكمون المعمم لبوشل-تالر (Pöschl-Teller)، كمون فئة يوكاوا (Yukawa)، كمون شيوبرغ (Schiöberg) و كمون مانينغ-روزن (Manning-Rosen). بعد إدخال الكمون المركزي في المعادلة القطرية، الكمون الفعلي يصبح دمج لحدود التي تجعل حل المعادلة القطرية ليس بديهيا، لهذا الغرض مخطط تقريب سوف يستعمل لتحويل المعادلة القطرية إلى الصيغة العادية لمعادلة هون بيكونفلوننت (Heun Biconfluyente) ، أين الحلول تكون معروفة، ومنه الحالات المقيدة لمعادلة شرودنجر (Schrödinger) و القيم الذاتية للطاقة الخاصة بها يتحصل عليها بصورة صريحة. في النهاية، لبعض قيم المتغيرات المعطاة، بعض الحالات المقيدة التقريبية و مستويات الطاقة الخاصة بها تعطى.

الكلمات المفتاحية

معادلة شرودنجر (Schrödinger) ، كمون كورنل (Cornell) المعمم، مشاكل شبه قابلة الحل، كمون مورس (Morse) ، الكمون المعمم لبوشل-تالر (Pöschl-Teller)، كمون فئة يوكاوا (Yukawa)، كمون شيوبرغ (Schiöberg)، كمون مانينغ-روزن (Manning-Rosen)، معادلة هون بيكونفلوننت (Heun Biconfluyente) ، حالات مقيدة تقريبية.

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CHAPTER 1

INTRODUCTION

The foundation of classical mechanics was created at the beginning of the seventeenth century, by Newton who published in 1687 his work "Philosophiae Naturalis Principia Mathematica", since three centuries ago, he gave rise to the foundation of Newtonian mechanics, which is the branch of physics that predicts and describes perfectly the motion of macroscopic object. Beside to the theory of electromagnetism founded by Maxwell, enabled physicists to develop a comprehensive understanding of a wide range of observed phenomena in nature, they are a deterministic theories, but, how about the microscopic world? When the physicists tried to extend the principles of these theories to puzzle out the world at the atomic and subatomic scale, they found that the classical laws aren't applicable and they break down at this levels, they were unable to answer questions that classical theories could not explain like the black body radiation problem, stability of atoms or Young's double-slit experiment, then they released that infinitely objects are governed by other types of laws. Consequently, quantum mechanics came to us as

a result of the failure of newtonian mechanics and Maxwell theory to describe the microscopic world behaviour, hence, the eventful transition from classical to non-classical laws of physics and then, the creation of the new branch of physics, under the name of quantum mechanics. In the universe one distinguishes two kinds of object: radiation and matter, matter is made of localized particles where the state of particle is defined perfectly at any instant by its position and velocity, that are derived from Newton's laws, in the other side radiation that has been treated as a wave in which it can not be localized, since it is impossible to split radiation into small particles obeys Maxwell's laws of electromagnetism. Quantum mechanics foundation made a truly revolutionary theory of physics, by its rejection of the absolute ideas of classical understanding of physical events and concepts. The first who gave the act of birth of Quantum Mechanics was Planck in 1900 work [1], by its assumption of quantization of energy, he argued that the exchange of energy between electromagnetic waves and matter occurs only in discrete form, in this way he was able to find an answer to the black body radiation problem. Where in fact, classically the energy is treated as a continuous entity and this make the classical picture of energy is not able to account for predict the black body spectral properties. Planck discovered a new universal constant which bears his name, thus, he created the first building block of a new theory. Followed by Planck, by the time when it was universally accepted that light was treated as a wave among physicists, which is experimentally proved by the existence of diffraction and interference pattern in double slit experiment, Einstein by his hypothesis of quantum nature of light in 1905, he was inspired by the black-body problem solution of Planck, that led him to resolve the paradox of the photoelectric

effect, leading to particle-wave duality of light, he proposed that light of fixed energy is composed of small units, a single unit called photon and its energy is given by the following expression $E = hf$ where f represents the frequency of light and h is Planck's constant. In parallel with this discoveries, the structure of atoms were studied, where in the year 1913, the physicist Niels Bohr was able to explicate the hydrogen atom stability besides to the discreteness in the energy levels spectrum, just by partially rejecting the classical concepts, he proposed a model of atoms where there is the electrons evolving around the nucleus, on orbits with well-defined discrete energy levels and they can only absorb well-defined energies. Since light exhibit both wave and particle behaviour, in 1924, de Broglie in his doctoral dissertation took the critical step, he extended the wave-particle duality behaviour to all microscopic objects, since there was no manifestation of wave nature of matter until it was experimentally proven by the two scientists Davisson and Germer in the year 1927, where they by chance proved the interference and diffraction of electron. Another proof of the wavelike properties of the electron was in the same year by Thomson, after the subatomic particle the so-called neutron were discovered by Chadwick in 1932, the experiment of Young's double slit were carried out using this subatomic particle. The real birth of quantum mechanics was by Heisenberg publishing his work in 1925, who put for the first time a mathematical background for the new theory based on non-commutative multiplication rule as matrices, this work on matrix mechanics, that appeared in the early days of twentieth century, was indeed advanced in significant way by physicists such as Born and Jordan. Later, both Born and Wiener explored the concept of physical variables as linear operators, leading to the modern mathemat-

ical framework where physical quantities are represented as matrices. This revolutionary development allowed for a more rigorous and abstract understanding of quantum mechanics, paving the way for future advancements in the field, including the formulation of Heisenberg's matrix mechanics and the eventual unification with wave mechanics. In 1927, Heisenberg derived his uncertainty principle that imposes limits on the concurrent measurability of both momentum and position of particles, this principle arises from the inherent wave-particle duality of quantum entities, indicating that the more precisely one property is measured, the less precisely the other can be determined, if one try to know exactly the position which is a corpuscular aspect of the particle, all information about its momentum is lost where the momentum is a wave characteristic. In 1926, Schrödinger proposed wave mechanics, instead of matrices, he dealt with partial differential equations, he proposed his famous equation. Matrix mechanics was difficult to understand by the physicists so wave mechanics was more accessible and intuitive, Schrödinger in 1926 showed that they are equivalent. The standard tool in wave mechanics is the wave equation the so-called Schrödinger equation, it is valid for any non-relativistic system, where the solution is called a wave function that is still without a physical meaning and in 1927 Bohr suggested the probabilistic interpretation of the wave function known as Copenhagen interpretation of quantum mechanics, he stated that its square modulus is a probability density of the system under consideration, hence the notion of determinism in the atomic world is abandoned by quantum mechanics. It is postulated in the context of non-relativistic quantum mechanics, that every information about the physical system for a given instant is derived starting from the knowledge of the solu-

tion of Schrödinger equation, namely the wave function. Then Dirac suggested a simple formulation of quantum mechanics named Dirac Algebra, he dealt with the general concepts by introducing the operators, ket and bras vectors. In parallel with the construction of the new theory, a very important discovery were made that contribute to more overall formulation later, where Ulhenbeck and Goudsmit proposed in 1925 the existence of an intrinsic magnet moment of the electron that they called spin, that was discovered by Stern and Gerlach in 1922 where they proved experimentally the quantification of the magnetic moment of atoms. The proposed quantum mechanics theory by Schrödinger and Heisenberg is valid only when dealing with non-relativistic phenomena. For particles with mass and by combining between special relativity and quantum mechanics, the origins of the first relativistic wave equation known as Klein-Gordon equation was obtained, the early versions of the equation were due to several physicists, it was proposed simultaneously by many physicists among them Klein, Schrödinger, Kudar and Fock in 1926, it is the relativistic extension of Schrödinger equation in which it describes a free electrically-charged spin-0 particle. In 1928 Dirac published his equation that was named after him, he extended quantum mechanics to relativistic phenomena for particles with spin where his equation deals with spin $1/2$ particles, in 1930 Dirac predicted the existence of antiparticles while he tried to overcome the difficulties of Klein-Gordon equation negative probability densities [2, 3, 4, 5, 6, 7]. Quantum mechanics theory is the basic theory that is still leading to modern development in technologies that are based on principles of quantum phenomenon, it has a lot of important applications in which it offers significant advantages and create new capabilities in comput-

ing, communication , cryptography, measurement, etc. One of quantum mechanics applications the characterization of matter in laboratory and chemical analysis is based on the principle of absorption of photons from the photoelectric effect, the phenomenon of diffraction allows to access to the crystallographic structure of matter besides to visualize matter at the smallest details using electron microscopes that use electrons instead of light and the scanning tunneling microscopes are other type of microscopes that was invented by Gerd Binnig and Heinrich Rohrer in 1981 that uses the tunneling effect to image surfaces of materials, the magnet resonance imaging (MRI) that is used to diagnose diseases works thanks to the property of spin to generate images of human bodies, laser which is a beam of focused monochromatic light widely used in medicine for eye surgery or the treatment of local lesions, lasers are used also for optical disk storage (DVDs), for industry there is laser cutting which has been used since 1980, it is a manufacturing process that uses laser to make cuts in materials like metals with high precision. One of the most transformative features of quantum principles is its application in quantum computing which employs superposition and entanglement to process information in ways unlike classical computers, such that instead of using bits that represents either 0 or 1, quantum computing uses qubit that use them simultaneously as a superposition, this feature allows the quantum computer to make many operations at once, this will improve data analysis and accelerate the performance. Quantum sensing is an advanced sensor technology that highly improves the accuracy of measurement, it measure changes at the atomic level with higher degree of precision, and the Global Positioning System (GPS) is one of Quantum sensing realizations, it uses very accurate atomic clocks for geolocation.

In this thesis, we resolved some problems that are in relation with non-relativistic quantum mechanics in the framework of quasi-exactly solvable problems, particularly we resolved Schrödinger equation for few central potentials and a single potential is in the form of the generalized Cornell plus some exponential potentials, where the quasi-exactly solvability of Schrödinger equation came from approximating the radial equation to the biconfluent Heun's equation using an appropriate approximation scheme such that the normalized solutions of this equation are possible after imposing some specific conditions on the equation, the thing that gives only a finite portion of the discrete spectrum with the associated eigenfunctions in analytic form. The thesis is composed of three chapters, the first chapters is for introducing some mathematical tools that are basic to understand quantum mechanics such as the notion of linear operators and the different kinds of spectrum of these operators, where they have a fundamental role in quantum mechanics since they provide a mathematical framework for describing the observables of physical and the evolution of quantum systems, for example many physical quantities like energy, position, momentum and spin have been represented by linear operators. at the other side, the notion of discrete spectrum is also important in the quantum theory because it plays a crucial role in explaining and understanding the behavior of quantum systems, especially in terms of measurement outcomes of the observables, then we give a brief introduction about Heun's biconfluent equation with the associated canonical form and its polynomial solutions that leads to the approximate normalized eigensolutions of Schrödinger equation. The second chapter is dedicated to the basic notions that

formulated the theory of quantum mechanics such as the fundamental principles that form the foundation of the entire framework of quantum mechanics, known as the postulates of quantum mechanics, these postulates are essential because they define the mathematical background and the conceptual structure that governs the behavior of physical systems at microscopic scales, where classical physics does not apply. Besides to the fundamental equation of quantum mechanics "Schrödinger equation", it is crucial to understand the world at the microscopic scale, because it governs how the solution the so-called wavefunction evolves over time allowing us to predict the system future states from its initial conditions. In the third chapter, we give approximate bound states of Schrödinger equation for few central potentials, where one potential is formed as the generalized Cornell potential plus an exponential potential, starting by transforming the radial equation to the biconfluent Heun's equation, then using the results from chapter one about the solutions of biconfluent Heun's equation to construct the analytic approximate eigensolutions of Schrödinger equation and for given values of the parameters, we compute some approximate bound states of Schrödinger equation.

CHAPTER 2

PRELIMINARY NOTIONS

For this chapter, we are going to expose the preliminary notions that are useful in this thesis, we present the mathematical background of quantum mechanics

For the next sections, the considered vector spaces are defined on a field $\mathbb{K}$ such that $\mathbb{K} = \mathbb{R}$ or $\mathbb{K} = \mathbb{C}$.

2.1 Hilbert space

2.1.1 Sesquilinear forms

Definition 1. [8] Let consider X to be a vector space over a field $\mathbb{K}$. the following mapping $q : X \times X \rightarrow \mathbb{K}$ is called a sesquilinear form on the vector space X if for $\forall x, y, z \in X$ and $\forall \alpha, \beta \in \mathbb{K}$

$$i) q(\alpha x + \beta y, z) = \alpha q(x, z) + \beta q(y, z),$$

$$ii) q(x, \alpha y + \beta z) = \bar{\alpha} q(x, y) + \bar{\beta} q(x, z).$$

A sesquilinear form is said to be Hermitian if for every element x and y from X

we have

$$q(x, y) = \overline{q(y, x)}.$$

A sesquilinear form is a non-negative on X if for every element $x \in X$ where x we have

$$q(x, x) \geq 0.$$

Definition 2. [8] The following mapping

$$(\cdot, \cdot) : X \times X \rightarrow \mathbb{K}$$

is a scalar product if and only if for every element $x, y, z \in X$ and for every scalar $\alpha \in \mathbb{K}$ we have the following

$$i) (x + y, z) = (x, z) + (y, z),$$

$$ii) (\alpha x, y) = \alpha(x, y),$$

$$iii) (x, y) = \overline{(y, x)},$$

$$iv) (x, x) \geq 0,$$

$$v) (x, x) > 0 \text{ if } x \neq 0.$$

Definition 3. A pre-Hilbert space by definition is a vector space with scalar product where a norm which is defined as follows

$$\|x\| = \sqrt{(x, x)}.$$

Theorem 1. (Cauchy-Schwartz) [9] For every elements x and y that are belonging to the pre-Hilbert space X we have

$$|(x, y)| \leq \|x\| \|y\|.$$

Definition 4. A Hilbert space by definition is a pre-Hilbert space which is complete according to the norm induced by that scalar product.

Example 1. Every pre-Hilbert space of finite dimensions is a Hilbert space in particular $\mathbb{C}^n$ with the following scalar product

$$(x, y) = \sum_{k=1}^n x_k \overline{y_k},$$

is a finite dimensional Hilbert space for the norm

$$\|x\| = \sqrt{\sum_{k=1}^n x_k^2}.$$

Example 2. $L^2([a, b])$ the space of square integrable functions defined on the interval $[a, b]$ with the scalar product

$$(f, g) = \int_a^b f(x) \overline{g(x)} dx,$$

is a Hilbert space for the norm

$$\|f\| = \sqrt{\int_a^b |f(x)|^2 dx}.$$

Proposition 1. Let be X a pre-Hilbert space, $\forall x, y \in X$ we have the following identities

i) **The parallelogram law**

$$\|x + y\|^2 + \|x - y\|^2 = 2\|x\|^2 + 2\|y\|^2,$$

ii) **Polarisation identity**

Complex case:

$$4(x, y) = \|x + y\|^2 - \|x - y\|^2 + i\|x + iy\|^2 - i\|x - iy\|^2,$$

Real case:

$$4(x, y) = \|x + y\|^2 - \|x - y\|^2,$$

iii) **The triangular inequality**

$$\|x + y\| \leq \|x\| + \|y\|.$$

2.2 Orthogonality

Definition 5. Two vectors x and y from a pre-Hilbert space X are said to be orthogonal if the scalar product of these vectors vanishes, which means that

$$(x, y) = 0.$$

Definition 6. Let consider Q to be a subspace of pre-Hilbert space X , then its orthogonal is defined as

$$Q^\perp = \{y \in X; x \perp y, \forall x \in Q\},$$

it is the set of vectors where each vector is orthogonal all vectors of Q .

$Q^\perp$ is called the orthogonal complement of Q .

Proposition 2. $Q^\perp$ is a closed subspace of X .

Corollary 1. [9] Let be Q a closed linear subspace of a Hilbert space H , then

$$Q = (Q^\perp)^\perp,$$

and we have

$$X = Q \oplus Q^\perp.$$

Theorem 2. [9] Let be H a Hilbert space and Q is a closed linear subspace. Let consider a vector $x \in H$, then we have

i) there exists a unique $q \in Q$ such that

$$\|x - q\| = \min_{z \in Q} \|x - z\|,$$

ii) the vector q is the only vector from Q such that

$$x - q \in Q^\perp.$$

Theorem 3. (Orthogonal decomposition)[9] Let Q be a closed linear space of a Hilbert space H , then each vector $x \in H$ is uniquely representable as

$$x = q + p,$$

where $q \in Q$ is called the orthogonal projection of x upon Q and $p \in Q^\perp$.

Proposition 3.

Let X be a pre-Hilbert space, then we have

$$i) \{0\}^\perp = X \text{ and } X^\perp = \{0\}.$$

$$ii) A \subset B \Rightarrow B^\perp \subset A^\perp$$

Definition 7. (Orthogonal projection) Let Q be a closed subspace of a Hilbert space H , the mapping

$$P_Q : X \rightarrow Q$$

$$x \mapsto P_Q x = q$$

is called orthogonal projection of x on Q .

The mapping P_Q has the following properties

$$i) P_Q \text{ is linear,}$$

$$ii) P_Q^2 = P_Q,$$

$$iii) \|P_Q x\| \leq \|x\| \text{ for every vector } x \text{ of } H,$$

$$iv) \|P_Q\| = 1.$$

Definition 8. Let E be a linear space and $\mathbb{K}$ is a field. The mapping

$$f : E \rightarrow \mathbb{K}$$

$$x \mapsto f(x),$$

that verifies

$$f(\alpha x + \beta y) = \alpha f(x) + \beta f(y),$$

for every elements x and y from E while α and β from $\mathbb{K}$ is called a linear functional.

Definition 9. A linear functional f defined on a normed space E is bounded if it exists a constant c strictly positive that

$$|f(x)| \leq c\|x\|,$$

for every $x \in E$.

Theorem 4. (Riesz representation theorem)[9] Let be f a bounded linear functional defined on a Hilbert space H , then it exist some vector $a \in H$ such that

$$f(x) = (x, a)$$

for every element $x \in H$ in addition

$$\|f\| = \|a\|.$$

2.3 Hilbertian base

Definition 10. Let H be a Hilbert space. A set $(e_i)_0^n$ is said to be an orthonormal system if

$$(e_i, e_j) = \delta_{i,j}.$$

Theorem 5. [9] Let H be a Hilbert space. By considering the orthonormal system $(e_k)_{k \in \mathbb{N}}$, the following expressions are obtained

1) for any vector $x \in H$

$$\sum_{k=1}^{\infty} |(x, e_k)|^2 \neq \|x\|^2,$$

2) for any vector $x \in H$, the following serie converges

$$\sum_{k=1}^{\infty} (x, e_k) e_k,$$

3) for any vector $x \in H$ we have the following equality

$$\sum_{k=1}^{\infty} |(x, e_k)|^2 = \|x\|^2,$$

for

$$x = \sum_{k=1}^{\infty} (x, e_k) e_k.$$

Definition 11. Let H is considered as a Hilbert space, then an orthonormal system $(e_k)_{k \in \mathbb{N}}$ is called a hilbertian basis if for every element of H we have

$$x = \sum_{k=1}^{\infty} (x, e_k) e_k.$$

Example 3. By considering the Hilbert space l_2 of sequences that are square summable for the scalar product

$$(x, y) = \sum_{k \geq 1} x_k \overline{y_k},$$

then the following family that is given by

$$e_i = (0, 0, \dots, 0, 1, 0, \dots), \quad i \geq 1,$$

where the vector number i presents a sequences of zeros except for the position i is an orthonormal basis for this space.

Theorem 6. (Gram-Schmidt Orthonormalization process)

Gram-Schmidt Orthonormalization process is an algorithm that transfer a set of vectors of a Hilbert space which they are linear independent into an orthonormal vectors.

Let consider $\{z_k, \quad 1 \neq k \neq n\}$ a set of linear independent vectors, then an

orthogonal set $(w_k)_{k=1}^n$ starting from the set of vectors where they are linearly independent is constructed as follows

$$w_1 = z_1,$$

$$w_2 = z_2 - \frac{(z_2, w_1)}{(w_1, w_1)} w_1,$$

$$w_3 = z_3 - \frac{(z_3, w_1)}{(w_1, w_1)} w_1 - \frac{(z_3, w_2)}{(w_2, w_2)} w_2,$$

$\vdots$

$\vdots$

$$w_n = z_n - \sum_{k=1}^{n-1} \frac{(z_n, w_k)}{(w_k, w_k)} w_k,$$

by normalizing this vectors the orthonormal set is obtained.

2.4 Linear operator

Definition 12. Let consider the set $\mathcal{X}$ and the set $\mathcal{Y}$ to be linear spaces .

The mapping $\mathcal{A} : \mathcal{D}(\mathcal{A}) \rightarrow \mathcal{Y}$ where the domain $\mathcal{D}(\mathcal{A})$ is a subspace of $\mathcal{X}$ is called a linear operator if

$$\mathcal{A}(x_1 + x_2) = \mathcal{A}(x_1) + \mathcal{A}(x_2),$$

$$\mathcal{A}(\alpha x_1) = \alpha \mathcal{A}(x_1),$$

whenever $x_1, x_2 \in \mathcal{D}(\mathcal{A})$ and α is a scalar.

Definition 13. Let $\mathcal{X}$ and $\mathcal{Y}$ be linear spaces, α is a complex number and $\mathcal{A} : \mathcal{D}(\mathcal{A}) \rightarrow \mathcal{Y}$ is a linear operator. We define the operator $\alpha \mathcal{A}$ as follows

$$\alpha \mathcal{A} : \mathcal{D}(\mathcal{A}) \rightarrow \mathcal{Y},$$

such that for every element $x \in \mathcal{D}(\mathcal{A})$ we have

$$(\alpha \mathcal{A})x = \alpha(\mathcal{A}x).$$

Definition 14. Let $\mathcal{X}_1, \mathcal{X}_2$ and $\mathcal{Y}$ be linear spaces .

Two linear operators $\mathcal{A}_1$ and $\mathcal{A}_2$ are defined as

$$\mathcal{A}_1 : \mathcal{D}(\mathcal{A}_1) \rightarrow \mathcal{Y},$$

and

$$\mathcal{A}_2 : \mathcal{D}(\mathcal{A}_2) \rightarrow \mathcal{Y}.$$

For the two operators $\mathcal{A}_1$ and $\mathcal{A}_2$, the sum $\mathcal{A}_1 + \mathcal{A}_2$ is defined by

$$\mathcal{A}_1 + \mathcal{A}_2 : \mathcal{D}(\mathcal{A}_1 + \mathcal{A}_2) \rightarrow \mathcal{Y},$$

where

$$\mathcal{D}(\mathcal{A}_1 + \mathcal{A}_2) = \mathcal{D}(\mathcal{A}_1) \cap \mathcal{D}(\mathcal{A}_2),$$

and

$$(\mathcal{A}_1 + \mathcal{A}_2)x = \mathcal{A}_1x + \mathcal{A}_2x,$$

while the product of the two operators $\mathcal{A}_1$ and $\mathcal{A}_2$ is defined by

$$\mathcal{A}_1\mathcal{A}_2 : \mathcal{D}(\mathcal{A}_1\mathcal{A}_2) \rightarrow \mathcal{Y},$$

where

$$\mathcal{D}(\mathcal{A}_1\mathcal{A}_2) = \{x \in \mathcal{D}(\mathcal{A}_2) \text{ and } \mathcal{A}_2x \in \mathcal{D}(\mathcal{A}_1)\},$$

and

$$(\mathcal{A}_1\mathcal{A}_2)x = \mathcal{A}_1(\mathcal{A}_2x).$$

Definition 15. A linear operator $\mathcal{A}_2$ where

$$\mathcal{A}_2 : \mathcal{D}(\mathcal{A}_2) \rightarrow \mathcal{Y},$$

is called an extension of a linear operator $\mathcal{A}_1$ which is defined by

$$\mathcal{A}_1 : \mathcal{D}(\mathcal{A}_1) \rightarrow \mathcal{Y},$$

if

$$\mathcal{D}(\mathcal{A}_1) \subset \mathcal{D}(\mathcal{A}_2),$$

and

$$\mathcal{A}_1x = \mathcal{A}_2x, \quad \forall x \in \mathcal{D}(\mathcal{A}_1).$$

Definition 16. The set $\mathcal{R}(\mathcal{A})$ is called the range of the operator $\mathcal{A}$, it is given by

$$\mathcal{R}(\mathcal{A}) = \{\mathcal{A}x, x \in \mathcal{D}(\mathcal{A})\}.$$

Definition 17. $\text{Ker}(\mathcal{A})$ is the nul space of the operator $\mathcal{A}$, it is given by

$$\text{Ker}(\mathcal{A}) = \{x \in \mathcal{D}(\mathcal{A}) , \mathcal{A}x = 0\}.$$

Lemma 1. $\text{Ker}(\mathcal{A})$ is a subspace of $\mathcal{X}$ and $\mathcal{R}(\mathcal{A})$ is a subspace of $\mathcal{Y}$.

Definition 18. Let $\mathcal{X}$ and $\mathcal{Y}$ be linear spaces .

The linear operator $\mathcal{A} : \mathcal{X} \rightarrow \mathcal{Y}$ is surjective if

$$\mathcal{R}(\mathcal{A}) = \mathcal{Y},$$

and it is injective if

$$\mathcal{A}x = \mathcal{A}y \quad \Rightarrow \quad x = y.$$

Definition 19. Let consider $\mathcal{A} : \mathcal{X} \rightarrow \mathcal{Y}$ to be a linear operator where the set $\mathcal{X}$ and the set $\mathcal{Y}$ are normed spaces. Then the operator $\mathcal{A}$ is said to be bounded if and only if it exists a positive constant c such that

$$\|\mathcal{A}x\| \leq c\|x\|, \quad \forall x \in \mathcal{X}.$$

Proposition 4. Let be $\mathcal{A} : \mathcal{X} \rightarrow \mathcal{Y}$ a linear operator where $\mathcal{X}$ and $\mathcal{Y}$ are normed spaces. Then the following statements are equivalent:

- $\mathcal{A}$ is continuous at 0.

- $\mathcal{A}$ is continuous on $\mathcal{X}$.
- It exists a positive number $c > 0$ such that $\|\mathcal{A}x\| \leq c\|x\|$, $\forall x \in \mathcal{X}$.
- It exists a positive number $c > 0$ such that $\|\mathcal{A}x\| \leq c\|x\|$, $\forall x \in \mathcal{X}$ where $\|x\| \leq 1$.

We denote by $\mathcal{L}(\mathcal{X})$ the space of bounded linear operators from $\mathcal{X}$ in $\mathcal{X}$.

Definition 20. Let $\mathcal{X}$ and $\mathcal{Y}$ be a Banach spaces. The linear operator

$$\mathcal{A} : \mathcal{X} \rightarrow \mathcal{Y},$$

is said to be invertible if it exist a linear operator $\mathcal{B} : \mathcal{Y} \rightarrow \mathcal{X}$ such that

$$\mathcal{A}\mathcal{B} = I_{\mathcal{X}},$$

$$\mathcal{B}\mathcal{A} = I_{\mathcal{Y}},$$

then, in this case we put

$$\mathcal{B} = \mathcal{A}^{-1}.$$

Definition 21. (Continuously invertible operator) We say that a linear operator $\mathcal{A}$ is continuously invertible if

i) $\mathcal{A}^{-1}$ exists.

ii) $\mathcal{A}^{-1}$ is bounded.

2.5 Adjoint operator

Definition 22. [10] Let consider a linear operator $\mathcal{A} : \mathcal{D}(\mathcal{A}) \subset \mathcal{X} \rightarrow \mathcal{Y}$ with dense domain $\mathcal{D}(\mathcal{A})$, (The density of the domain $\mathcal{D}(\mathcal{A})$ is a necessary condition for the uniqueness of the adjoint).

The adjoint of the operator $\mathcal{A}$ is the linear operator

$$\mathcal{A}^* : \mathcal{D}(\mathcal{A}^*) \subset \mathcal{Y}' \rightarrow \mathcal{X}',$$

defined as

$$\langle f, \mathcal{A}x \rangle = \langle \mathcal{A}^* f, x \rangle \quad , \quad \forall x \in \mathcal{D}(\mathcal{A}) \quad , \quad \forall f \in \mathcal{D}(\mathcal{A}^*),$$

where

$$\mathcal{D}(\mathcal{A}^*) = \{f \in \mathcal{Y}' \mid \exists c > 0 \quad |\langle f, \mathcal{A}x \rangle| \leq c\|x\|, \quad \forall x \in \mathcal{D}(\mathcal{A})\},$$

while $\mathcal{X}'$ and $\mathcal{Y}'$ present respectively the dual space of $\mathcal{X}$ and $\mathcal{Y}$ while $\langle , \rangle$ is the product of duality.

2.5.1 The adjoint operator on Hilbert space

Definition 23. Let be H_1 and H_2 two Hilbert spaces and a linear operator $\mathcal{A}$ densely defined from H_1 into H_2 .

The operator $\mathcal{B}$ is called the adjoint of $\mathcal{A}$ if we have

$$(\mathcal{A}x, y) = (x, \mathcal{B}y),$$

and we put $\mathcal{B} = \mathcal{A}^*$, if $\mathcal{A}^* = \mathcal{A}$ then $\mathcal{A}$ is called self-adjoint operator.

Properties: Let be $\mathcal{A}, \mathcal{B} \in \mathcal{L}(\mathcal{H})$ and λ is a scalar, then we have

$$i) (\lambda \mathcal{A})^* = \bar{\lambda} \mathcal{A},$$

$$ii) (\mathcal{A} + \mathcal{B})^* = \mathcal{A}^* + \mathcal{B}^*,$$

$$iii) (\mathcal{A}\mathcal{B})^* = \mathcal{B}^* \mathcal{A}^*.$$

Definition 24. A linear operator defined from a Hilbert space into itself is hermitian if

$$\mathcal{A} = \mathcal{A}^*.$$

Definition 25. Let be $\mathcal{A}$ and $\mathcal{B}$ two linear operator from $\mathcal{L}(\mathcal{H})$ such that $\mathcal{H}$ is a Hilbert space. The commutator of two operators is defined by

$$[\mathcal{A}, \mathcal{B}] = \mathcal{A}\mathcal{B} - \mathcal{B}\mathcal{A}.$$

If we have $[\mathcal{A}, \mathcal{B}] = 0$ we say that the two operators commute.

Properties

Let be $\mathcal{A}, \mathcal{B}$ and $\mathcal{C}$ linear operator from $\mathcal{L}(\mathcal{H})$ where $\mathcal{H}$ is a Hilbert space, then we have the following properties

i) $[\mathcal{A}, \mathcal{B}] = -[\mathcal{B}, \mathcal{A}].$

ii) $[\mathcal{A}, \mathcal{B} + \mathcal{C}] = [\mathcal{A}, \mathcal{B}] + [\mathcal{A}, \mathcal{C}].$

iii) $[\mathcal{A}, \mathcal{B}\mathcal{C}] = [\mathcal{A}, \mathcal{B}]\mathcal{C} + \mathcal{B}[\mathcal{A}, \mathcal{C}].$

iv) If the operators $\mathcal{A}$ and $\mathcal{B}$ are hermitians, then we have

$$[\mathcal{A}, \mathcal{B}]^* = -[\mathcal{B}, \mathcal{A}].$$

v) $[\mathcal{A}, [\mathcal{B}, \mathcal{C}]] = [\mathcal{B}, [\mathcal{C}, \mathcal{A}]] + [\mathcal{C}, [\mathcal{A}, \mathcal{B}]].$

2.6 Spectrum of an operator

Let $\mathcal{A}$ be a linear operator defined from a Banach space to itself with domain $\mathcal{D}(\mathcal{A})$ and λ is a complex number.

Definition 26. The scalar λ is called a regular point of a linear operator $\mathcal{A}$ if the operator defined by $\mathcal{A} - \lambda I$ is continuously invertible. which means that $(\mathcal{A} - \lambda I)^{-1}$ exists and it is bounded.

The set of every regular point of the operator $\mathcal{A}$ is called the resolvent set and it is given by

$$\rho(\mathcal{A}) = \{\lambda \in \mathbb{C}, \quad \mathcal{A} - \lambda I \text{ is continuously invertible}\},$$

and the following operator $(\mathcal{A} - \lambda I)^{-1}$ is called the resolvent of $\mathcal{A}$.

The complement of the resolvent set $\rho(\mathcal{A})$ in $\mathbb{C}$ is called the spectrum of the

operator $\mathcal{A}$, it is the set of point where $\mathcal{A} - \lambda I$ fails to be continuously invertible and it is denoted by $\sigma(\mathcal{A})$.

The resolvent set is an open set, then $\sigma(\mathcal{A})$ is a closed set.

Definition 27. The spectrum of an operator is represented in the union of 3 sets:

i) **The point spectrum** it is the set

$$\sigma_p(\mathcal{A}) = \{\lambda \in \mathbb{C} \text{ such that } \text{Ker}(\mathcal{A} - \lambda I) \neq \{0\}\},$$

if λ belongs to the point spectrum it exist an element $x \neq 0$ such that

$$\mathcal{A}x = \lambda x,$$

then the element x is called an eigenvector associated to the eigenvalue λ , which means that the operator $\mathcal{A} - \lambda I$ is not injective.

ii) **continuous spectrum** it is the set:

$$\sigma_c(\mathcal{A}) = \{\lambda \in \mathbb{C} \text{ such that } \mathcal{A} - \lambda I \text{ is injective and } \mathcal{R}(\mathcal{A} - \lambda I) \text{ is dense but } (\mathcal{A} - \lambda I)^{-1} \text{ is not bounded}\}.$$

iii) **residual spectrum** it is the set:

$$\sigma_r(\mathcal{A}) = \{\lambda \in \mathbb{C} \text{ such that } \mathcal{A} - \lambda I \text{ is injective and } \mathcal{R}(\mathcal{A} - \lambda I) \text{ is not dense}\}$$

then the spectrum of an operator is the following union

$$\sigma(\mathcal{A}) = \sigma_p(\mathcal{A}) \cup \sigma_c(\mathcal{A}) \cup \sigma_r(\mathcal{A}),$$

and we have

$$\mathbb{C} = \rho(\mathcal{A}) \cup \sigma_p(\mathcal{A}) \cup \sigma_c(\mathcal{A}) \cup \sigma_r(\mathcal{A}).$$

Theorem 7. [11] Let be $\mathcal{A}$ a bounded linear hermitian operator, then its spectrum $\sigma(\mathcal{A})$ is on the real axis, in particular we have

i) All of its eigenvalues are real.

ii) Two eigenvectors that are associated to two different eigenvalues are orthogonal.

2.6.1 Spectral decomposition of an auto-adjoint operator

Definition 28. [10] Let A be a self-adjoint operator on a Hilbert space H , then, there exists a projection-valued measure $E(\lambda)$ on the spectrum $\sigma(A) \subset \mathbb{R}$,

such that

$$A = \int_{\sigma(A)} \lambda dE(\lambda). \quad (2.1)$$

2.7 Heun's differential equations

After Heun's equation appeared in 1889 which is a second order linear ordinary differential equation that possesses 4 singular points, it has been involved in many fields of applied sciences and it has a lot of applications in many domains like quantum physics, special relativity, chemistry and optics.

Heun's differential equation in his general form is given by [12]

$$\frac{d^2 y}{dx^2} + \left(\frac{\gamma}{x} + \frac{\delta}{x-1} + \frac{\epsilon}{x-a} \right) \frac{dy}{dx} + \frac{\alpha\beta x - q}{x(x-1)(x-a)} y = 0, \quad (2.2)$$

such that y is the function and x is the variable while $\alpha, \beta, \gamma, \delta, \epsilon, q$ and a are arbitrary parameters related by this relation

$$\gamma + \epsilon + \delta = \alpha + \beta + 1, \quad (2.3)$$

with the parameter a is different from 1 and 0.

The equation has 3 regular singular point at the finite complex plane at $x = 0, 1, a$ and one regular singular point at infinity. The exponents of these singularities are respectively $\{0, 1 - \gamma\}$, $\{0, 1 - \delta\}$, $\{0, 1 - \epsilon\}$, $\{\alpha, \beta\}$ and the sum of these exponents has to take the value 2.

2.7.1 Normal form of Heun's differential equation and its confluent cases

Heun's differential equation has 4 confluent cases confluent: there is the confluent, biconfluent, double confluent and triconfluent Heun's equation and their normal form are given by

i) Heun's equation

$$\frac{d^2 y}{dx^2} + \left(\frac{A}{x} + \frac{B}{x-1} + \frac{C}{x-a} + \frac{D}{x^2} + \frac{E}{(x-1)^2} + \frac{F}{(x-a)^2} \right) y = 0. \quad (2.4)$$

ii) Confluent Heun's equation

$$\frac{d^2 y}{dx^2} + \left(A + \frac{B}{x} + \frac{C}{x-1} + \frac{D}{x^2} + \frac{E}{(x-1)^2} \right) y = 0. \quad (2.5)$$

iii) Biconfluent Heun's equation

$$\frac{d^2 y}{dx^2} + \left(Ax^2 + Bx + C + \frac{D}{x} + \frac{E}{x^2} \right) y = 0. \quad (2.6)$$

iv) Double confluent Heun's equation

$$\frac{d^2 y}{dx^2} + \left(A + \frac{B}{x} + \frac{C}{x^2} + \frac{D}{x^3} + \frac{E}{x^4} \right) y = 0. \quad (2.7)$$

v) Triconfluent Heun's equation

$$\frac{d^2 y}{dx^2} + \left(Ax^4 + Bx^3 + Cx^2 + Dx + E \right) y = 0. \quad (2.8)$$

in each case of the above cases, the parameters that appear in the equations are not all independent, where some relations emerge between them in addition for the equation 2.4 we have the condition

$$A + B + C = 0. \quad (2.9)$$

2.8 Biconfluent Heun's equation

The canonical form of the biconfluent Heun's equation is given by

$$xy'' + \left(1 + \alpha - \beta x - 2x^2\right)y' + \left((\gamma - \alpha - 2)x - \frac{1}{2}(\delta + (1 + \alpha)\beta)\right)y = 0, \quad (2.10)$$

it is an ordinary linear differential equation with two irregular singular points, the first irregular singular point is 0 and the second one is ∞ with rank 2 such that α, β, γ and δ are arbitrary parameters.

Using the following transformation [13]

$$y(x) = x^{-\frac{1+\alpha}{2}} e^{\frac{\beta x + x^2}{2}} z(x), \quad (2.11)$$

the canonical form becomes in the normal form as

$$\frac{d^2 z}{dx^2} + \left(Ax^2 + Bx + C + \frac{D}{x} + \frac{E}{x^2}\right)z = 0. \quad (2.12)$$

where the parameters that appear in the equation (2.12) are given by

$$A = -1, \quad B = -\beta, \quad C = \gamma - \frac{\beta^2}{4}, \quad D = -\frac{\delta}{2}, \quad E = \frac{1 - \alpha^2}{4}. \quad (2.13)$$

2.9 Serie solution to the canonical form of bi-confluent Heun's equation

To construct a power serie solutions to the canonical form of biconfluent Heun's equation let consider the following expansion

$$z(x) = \sum_{n \geq 0} c_n x^{n+\rho}. \quad (2.14)$$

After deriving and substituting in equation (2.10) we get the following conditions

$$\begin{aligned} \rho(\rho + \alpha) &= 0, \\ (\rho + 1)(\rho + 1 + \alpha)c_1 - \left(\beta\rho + \frac{1}{2}(\delta + \beta(1 + \alpha)) \right) c_0 &= 0, \\ (\rho + 2 + n)(\rho + 2 + \alpha + n)c_{n+2} - \left(\beta(\rho + 1 + n) + \frac{1}{2}(\delta + \beta(1 + \alpha)) \right) c_{n+1} \\ &+ \left(\gamma - 2 - \alpha - 2(\rho + n) \right) c_n = 0. \end{aligned} \quad (2.15)$$

When α is not a negative integer, we denote the solution by $N(\alpha, \beta, \gamma, \delta, x)$ obtained for the value $\rho = 0$ and $c_0 = 1$, we write

$$N(\alpha, \beta, \gamma, \delta, x) = \sum_{n \geq 0} \frac{A_n}{(1 + \alpha)_n} \frac{x^n}{n!}, \quad (2.16)$$

such that the coefficients of the entire function $(A_n)_{n \geq 0}$ can be calculated using the following recurrence relation

$$\begin{aligned} A_0, \quad A_1 &= \frac{1}{2}(\delta + \beta(1 + \alpha))A_0, \\ A_{n+2} &= \left((n + 1)\beta + \frac{1}{2}(\delta + \beta(1 + \alpha)) \right) A_{n+1} \\ &- (n + 1)(n + 1 + \alpha)(\gamma - 2 - \alpha - 2n)A_n, \quad n \geq 0 \end{aligned} \quad (2.17)$$

where

$$(1 + \alpha)_n = \frac{\Gamma(1 + \alpha + n)}{\Gamma(1 + \alpha)}.$$

If α is a negative integer $\alpha = -m$ for $m \geq 1$ it is possible to put the function N as

$$N(-m, \beta, \gamma, \delta, x) = x^m N(m, \beta, \gamma, \delta, x), \quad (2.18)$$

and it is still a solution to the canonical form of biconfluent Heun's equation.

Proposition 5. *The following identities are obtained [12]*

i) *when α is not a negative integer*

$$N(\alpha, \beta, \gamma, \delta, x) = e^{\beta x + x^2} N(\alpha, -i\beta, -\gamma, i\delta, -ix), \quad (2.19)$$

$$N(\alpha, \beta, \gamma, \delta, x) = N(\alpha, -\beta, \gamma, -\delta, -x). \quad (2.20)$$

ii) *when α is a negative integer ($\alpha = -m, m \geq 1$)*

$$N(-m, \beta, \gamma, \delta, x) = i^m e^{\beta x + x^2} N(-m, -i\beta, -\gamma, i\delta, -ix), \quad (2.21)$$

$$N(-m, \beta, \gamma, \delta, x) = (-1)^m N(-m, -\beta, \gamma, -\delta, -x). \quad (2.22)$$

2.9.1 Polynomial solutions of the biconfluent Heun's equation

By returning to the recurrence relation (2.17), the function N becomes a polynomial of degree n if and only if the following conditions are verified at the same time

$$\gamma - \alpha - 2 = 2n, \quad (2.23)$$

$$A_{n+1} = 0,$$

the condition $A_{n+1} = 0$ means that A_{n+1} is a polynomial of degree $n + 1$ in $\omega = -\frac{1}{2}(\delta + \beta(1 + \alpha))$, and it exists at most $n + 1$ value of δ that are denoted by

$$\delta_k, \quad 0 \leq k \leq n,$$

in addition, if $1 + \alpha > 0$ and $\beta \in R$ then A_{n+1} have at most $n + 1$ real root.

For more details see the following references [\[8, 9, 10, 11, 12, 13\]](#).

CHAPTER 3

SCHRÖDINGER EQUATION

3.1 Introduction

Newtonian mechanics is founded upon some principles and postulates that determine perfectly the position and the velocity of any physical system, it is based on principle of perfect determinism where every property of a physical system can be perfectly determined and measured at any instant using Newton's laws of motion that give rise to the concept of trajectory. the duality nature of light namely wavelike and corpuscular aspect is one of the most important characteristic that is connected directly to the birth of quantum theory, that led to the principle of superposition, the idea that a quantum system can exist in more than one state simultaneously until it is measured, where de Broglie generalized the principle of duality to all microscopic object. the main properties of the wavelike behaviour are obtained by analogy with optics, by tracking the analogy between matter waves and classical wave, one can ask if it is considerable to establish a unified theory and found a wave equation that describe corpuscular wave nature of matter once and for all microscopic particles, and to replace the classical theory by a wave theory where the wave would play the role played by the electromagnetic field in the theory of radiation, to answer that and inspired by the works of de Broglie, Schrödinger established his equation from a very simple correspondence rule that allowed to obtain that fundamental equation starting from the Hamiltonian of the corresponding classical system. Quantum mechanics similarly to the classical theories stands upon some postulates that provide the framework for understanding and predicting the behavior of quantum world, these postulates are typically organized into a serie of statements that describe the physical and mathematical structure of

quantum mechanics.

3.2 Postulates of quantum mechanics

In classical mechanics, the state of objects is known for an instant t by the knowledge of some functions of some dynamical variables which they are fundamental, these variables are the position and the momentum and any other measured quantity is defined by calculations in function of these dynamical variables, in addition the prediction of the values of the variables is possible using Hamilton's equations at any later time t' . However, concerning the quantum mechanical counterpart one must answer these questions

- how the state of the system at the microscopic scale can be fundamental mathematically for a given instant?
- how can one calculate a physical quantity of quantum system?
- by knowing the state of this system, how can the state be determined at a later time?
- how to determine the time evolution of the physical system?

To describe the state of quantum state of particles, quantum mechanics has been developed from some postulates that permit to determine the state of the physical system. These postulates cannot be derived, they are a result of experimental justification. They represent the minimum collection of assumptions that is needed to found the theory of quantum mechanics, they have been verified through a wide number

of experiments and have led to remarkable technological advancements. The postulates of quantum mechanics have been incredibly accurate and have passed numerous experimental tests. The predictions derived from quantum mechanics have been confirmed in many areas, from atomic and molecular interactions to subatomic particles, and more recently, quantum computing and quantum information

First postulate: Description of the of the system state[14]

The information about a physical system at the microscopic level is contained in state vector where the first postulate is formulated as [14]:

at a time instant t_0 , the state of a physical system is defined by a function $\psi(t_0)$ that belongs to a hilbert space the so-called: the state space.

Because Schrödinger equation is linear and homogeneous the state of a system have the property of superposition which means if two or more quantum states are solutions of the Schrödinger equation, then any linear combination of these states is also a valid solution. This feature permits the building of wave functions that can stand for several possible states simultaneously, which is one of the cornerstones in the field of quantum mechanics, such that if we consider a state vector ψ_1 and another state vector ψ_2 for two scalars λ_1, λ_2 then the function

$$\psi = \lambda_1\psi_1 + \lambda_2\psi_2 \quad (3.1)$$

presents a state vector.

The first postulate asserts that the particle and the associated wavefunction are inseparable aspects of a microscopic object, it adds to it the wave nature behavior of particles, comparable to the superposition principle for light waves. One wave function is not required to express a system's

state; two or more wave functions can be superposed to represent it. A vibrating string serves as an example from the macroscopic world; its state can be shown by either a single wave or the superposition of (linear combination) of several waves. This clearly contradicts the classical treatment of a material object. It is impossible to describe the nature of the relationships that the Superposition principle demands exist between any system's states using familiar physical concepts, where it is given no wave properties to them, and brings into profound conflict with our intuitions from a lifetime of experience with macroscopic objects. The objects of the everyday world in simple way do not behave as some inseparable combination of particle and wave nature. However, for quantum mechanics to be able to anticipate anything about the processes that take place at the atomic level of matter, particle and wave must merge. The first postulate is important because it asserts that a quantum system's whole description is contained in this wavefunction and that the system exists in a superposition of all conceivable states defined by this wavefunction prior to any measurements being taken.

Second postulate: Description of physical quantities

Properties that observed or measured of the physical system are called observables, they are modeled by Hermitian operators, the dynamical variables that appears in classical mechanics, they are represented mathematically by Hermitian operators, then the second postulate is formulated as [14]:

For one measurable physical quantity it corresponds an operator A acting on the state vector that describe this physical quantity

Because the laws governing classical systems are deterministic, it is pos-

sible to ascertain a particle's trajectory and all other properties in classical mechanics by knowing its position and momentum. On the other hand, quantum mechanics presents a radically different paradigm in which state vectors in a complex Hilbert space represent a system's state. Quantum mechanics provides probabilities and uncertainties in place of exact trajectories, and operators acting on these state vectors represent physical quantities. In stark contrast to classical determinism, this change emphasizes the significance of superposition and the probabilistic interpretation inherent in quantum systems. The operators are linear and they act on the state vectors the so-called wavefunction. Each observable is guaranteed to have orthonormal eigenfunctions and real eigenvalues by the premise of hermiticity.

Third postulate: The measurement of physical quantities

Possible results of measurement

From the eigenvalue problem of the stationary equation one can conclude that the only possible energies are eigenvalues of the Hamiltonian, this result can be generalized to all physical quantity where the third postulate states that [14]:

In quantum mechanics, when a measurement is performed on a physical quantity represented by an observable (an operator), the only possible outcomes are the eigenvalues of that operator.

The quantum system "collapses" to one of the operator's eigenstates following a measurement if the system is in a superposition of eigenstates of some observable, and the measurement's result is the associated eigenvalue.

Suppose that A is an operator that models an observable and we have

$$A\psi_j = a_j\psi_j \quad (3.2)$$

then ψ_j and a_j represents the j^{th} eigenstate and eigenvalue for the operator A and if the system is in the state ψ_j then the measurement gives the value a_j .

If the spectrum is discrete then the results of measurement are quantized.

In quantum mechanics, this postulate radically changes how we think about measurement. Position, momentum, and other quantities are directly measured in classical mechanics, and the results are always certain. A wavefunction, on the other hand, describes the system in quantum mechanics, and it is only through measurement that the system "chooses" a specific value for the observable based on the eigenvalues of the corresponding operator.

Fourth postulate: Principle of spectral decomposition

Let consider a state of a system ψ which is normalized which means that the norm of the state vector is 1, if we want to predict the result of measurement of a quantity that is characterized by an observable A then this prediction is probabilistic and we are going to give the rules how to calculate the amount probability of obtaining any eigenvalue a_n of an operator A :

The case of discrete spectrum

If the operator A has an entirely discrete spectrum and the eigenvalues a_n of A are with multiplicity one which means for a given eigenvalue it exists only an eigenvector, we write

$$Au_n = a_nu_n. \quad (3.3)$$

Because A represents an observable, then if the vectors u_n constitutes a basis in the state space then the vector ψ is expressed as

$$\psi = \sum_n c_n u_n, \quad (3.4)$$

then the probability of finding the result $a_n : \mathcal{P}(a_n)$, of finding the result a_n after the measurement is

$$\mathcal{P}(a_n) = |c_n|^2 = |(u_n, \psi)|^2. \quad (3.5)$$

The fourth postulate for a spectrum which is discrete and not degenerate states that [14]:

When an observable is measured on physical system such that this system is in a state which is normalized ψ , then to compute the probability $\mathcal{P}(a_n)$ of obtaining the eigenvalue a_n the following expression is applied

$$\mathcal{P}(a_n) = |(u_n, \psi)|^2, \quad (3.6)$$

where the eigenvector u_n is normalized and it is associated to the operator A which corresponds to the eigenvalue a_n .

Now when an degenerate eigenvalue is obtained which mean that it exist several eigenvectors u_n^i associated to the same eigenvalue a_n for the operator A

$$A u_n^i = a_n u_n^i, \quad i = 1, 2, \dots, g_n \quad (3.7)$$

then ψ is still can be written as an expansion in terms of the basis $\{u_n^i\}$ as

$$\psi = \sum_n \sum_{i=1}^{g_n} c_n^i u_n^i \quad (3.8)$$

and the probability $\mathcal{P}(a_n)$ is given by

$$\mathcal{P}(a_n) = \sum_{i=1}^{g_n} |c_n^i|^2 = \sum_{i=1}^{g_n} |(u_n^i, \psi)|^2. \quad (3.9)$$

Another statement of the fourth postulates in the case of degenerate eigenvalue is the following [14]:

When a physical system is in a normalized state, and the observable is measured, then the probability of getting the eigenvalue a_n given by $\mathcal{P}(a_n)$ is given by the expression

$$\mathcal{P}(a_n) = \sum_{i=1}^{g_n} |(u_n^i, \psi)|^2, \quad (3.10)$$

such that the integer g_n represents the degree of degeneracy that is associated to eigenvalue a_n and the set of vectors $\{u_n^i\}(i = 1, 2, \dots, g_n)$ is orthonormal that constitutes a basis for the eigenspace associated to the eigenvalue a_n .

The probability $\mathcal{P}(a_n)$ do not dependent on the basis of the eigenspace associated to the eigenvalue.

The case of continuous spectrum

In this part, let us assume that the operator A spectrum is continuous and not degenerate for sake of simplicity, we have the orthonormal system v_α in the generalized sense of A

$$Av_\alpha = \alpha v_\alpha, \quad (3.11)$$

constitutes a continuous basis in the space of states, the state ψ is written as

$$\psi = \int c(\alpha) v_\alpha d\alpha, \quad (3.12)$$

and the probability of getting a value between α and $\alpha + d\alpha$ is given by

$$\mathcal{P}(\alpha) = \rho(\alpha) d\alpha, \quad (3.13)$$

with

$$\rho(\alpha) = |c(\alpha)|^2 = |(v_\alpha, \psi)|^2, \quad (3.14)$$

and the fourth postulate for a spectrum which is not degenerate is the following [14]:

When measuring an observable on a system in the normalized state ψ , the probability of obtaining a measurement result within the interval $[\alpha, \alpha + d\alpha]$ is determined by

$$\mathcal{P}(\alpha) = |\langle v_\alpha, \psi \rangle|^2 d\alpha, \quad (3.15)$$

such that $|v_\alpha\rangle$ is a generalized eigenvector for the value α of the observable A .

These postulates give rise to the principle of indeterminism in quantum mechanics by introducing the probabilistic characteristics of measurement of different quantities, this probabilistic nature emerges because the quantum state of a system does not provide definite values for physical quantities after measurement that leads to probabilities of various possible outcomes, then the act of measurement forces the system to take one of those outcomes.

Fifth postulate: Reduction of the wave packet

By assuming that we want to measure a physical quantity at any given time, If we know the system's condition right before the measurement and it is represented by a ket ψ , according to the fourth postulate we can predict the probability of various possible outcomes, but obviously after the measurement only a result is obtained, therefore, the state just after the measurement of the system is different from ψ .

Let consider a case where the measurement result yields a non-degenerate eigenvalue a_n , then the system state just after the measurement is in the state u_n which represents the eigenvector for the eigenvalue

a_n

$$\psi \Rightarrow u_n,$$

and if another measurement is performed after the first one, the result that will be found is a_n and the system state is u_n and not ψ anymore.

When the eigenvalue a_n is degenerate, then there is a generalization as follows:

we write the expansion of the state of the system as

$$\psi = \sum_n \sum_{i=1}^{g_n} c_n^i u_n^i, \quad (3.16)$$

then the modified state after the measurement is expressed as follows

$$\psi \Rightarrow \frac{1}{\sqrt{\sum_{i=1}^{g_n} |c_n^i|^2}} \sum_{i=1}^{g_n} c_n^i u_n^i, \quad (3.17)$$

where the vector $\sum_{i=1}^{g_n} c_n^i u_n^i$ is a projection of ψ onto the eigensubspace of the eigenvalue a_n , the vector is normalized because it is more convenient to deal with states with norm 1, then we can write the new state in the form

$$\psi \Rightarrow \frac{P_n \psi}{\sqrt{(\psi, P_n \psi)}}, \quad (3.18)$$

and the fifth postulate is formulated as [14]:

If the measurement of an observable is in the state ψ yields the result a_n , then one can have that the state just after the measurement is the following projection that is normalized as

$$\psi \Rightarrow \frac{P_n \psi}{\sqrt{(\psi, P_n \psi)}} \quad (3.19)$$

of ψ onto the eigensubspace associated with a_n .

Before a measurement is made, the state of a quantum system is often

described by a superposition of different possible states. The reduction of the wave packet is of probabilistic nature. The wave function provides a probability distribution for the possible outcomes of a measurement, but it does not predict the special outcome. Instead, it gives the probability of obtaining a particular result.

Sixth postulate: The system Time evolution

In quantum mechanics the sixth postulates states that the time evolution of a given quantum physical system is obtained by Schrödinger equation that is given by

$$i\hbar \frac{d}{dt} \psi(\mathbf{r}, t) = \mathcal{H} \psi(\mathbf{r}, t), \quad (3.20)$$

such that $\mathcal{H}$ is the Hamiltonian operator, it is associated to the system total energy. The Hamiltonian operator is given by

$$\mathcal{H} = -\frac{\hbar^2}{2m} \Delta + V(\mathbf{r}, t), \quad (3.21)$$

in which its solution, the wave function encoded all information about the physical system. Stated differently, the wave function's time evolution is deterministic and does not require the specification of extra initial or final data.

3.3 Schrödinger equation

The Schrödinger equation constitutes the most important element of Wave Mechanics, it is the basic equation for a non-relativistic framework, that describes how the quantum system state changes over time. Essentially, Schrödinger equation enables us to predict and compute the dynamics of particles in a way that classical mechanics cannot, where one can predict the observable quantities like energy levels. The high level

of validity of this equation is up to the agreement of these predictions compared to experimental results, it has been one of the most successful and predictive equations in physics history, providing accurate descriptions and predictions for a wide range of physical phenomena. Since the foundations of quantum mechanics, because the Schrödinger equation solution, the wave function, encoded every information about the system, resolving a such equation had attracted the attention of researchers, where they resolved the equation using many techniques and tools such as the NU method and its extended version that were used widely [15, 16, 17, 18, 19, 20], Feynman path integral [21, 22, 23, 24, 25], asymptotic iteration method [26, 27], or by using Laplace transform [28, 29] and recently Schrödinger equation solutions has been obtained by resolving Heun type equations [30, 31, 32, 33], where the solutions has been found for many type of potentials, either for central potentials where they depend only on the radius not the orientation or non-central ones where an angular dependency is added to it, like Alberg and Wilets who resolved Schrödinger equation for the Coulomb [34] that models the electrostatic interaction between particles, Fernández who treated the equation for the harmonic oscillator with singular terms [35], Dong et al who dealt with a new anharmonic oscillator [36], Gareev et al found solutions for Woods-Saxon potential [37], Ikhdair and Sever constructed polynomial solutions to Mie potential [38], Dong et al obtained approximate solutions to Eckart potential [39], Drigi Filho and Riccota used the method of supersymmetric quantum mechanics to resolve the equation for Hulthen potential [40], Dong and Garcia-Ravelo resolved Schrödinger equation for Manning-Rosen potential [41], Morales got solutions for Morse potential [42], Aktaş and Sever has the exact solutions for the ring-shaped har-

monic oscillator [43], Dong et al and Garcia-Martinez obtained solutions for exponential type potentials [44, 45], Hamzavi and Ikhdair obtained solutions for the trigonometric Pöschl-Teller while Qiang and Dong got solutions for Scarf potentials [46, 47]. Schrödinger equation is given for a non-relativistic particle with mass m by

$$i\hbar \frac{d}{dt} \psi(\mathbf{r}, t) = \mathcal{H} \psi(\mathbf{r}, t), \quad (3.22)$$

where $\hbar$ is the reduced Planck's constant and $\mathbf{r}$ is the position vector, $\mathcal{H}$ is the Hamiltonian operator, the operator that is associated to the total energy of the system, it is Hermitian and given by

$$\mathcal{H} = -\frac{\hbar^2}{2m} \Delta + V(\mathbf{r}, t). \quad (3.23)$$

For Cartesian coordinates $\mathbf{r} = (x, y, z)$ one deduces the equation

$$i\hbar \frac{d}{dt} \psi(\mathbf{r}, t) = -\frac{\hbar^2}{2m} \left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \right) \psi(\mathbf{r}, t) + V(\mathbf{r}, t) \psi(\mathbf{r}, t), \quad (3.24)$$

the function V is known as the potential function.

for a potential function independent of time, Schrödinger equation becomes

$$i\hbar \frac{d}{dt} \psi(\mathbf{r}, t) = \left(-\frac{\hbar^2}{2m} \Delta + V(\mathbf{r}) \right) \psi(\mathbf{r}, t), \quad (3.25)$$

when the system is not subjected to any potential function, then Schrödinger equation takes the form

$$i\hbar \frac{d}{dt} \psi(\mathbf{r}, t) = \frac{\hbar^2}{2m} \Delta \psi(\mathbf{r}, t). \quad (3.26)$$

Schrödinger equation is a linear PDE of first order according to time variable and of second order for space variable, its solution is the so-called wave function ψ , it has a probabilistic interpretation that makes

the concept of trajectory at the microscopic level is lost such that in quantum mechanics, the probabilistic interpretation, as formulated by Max Born, implies that the wave function $|\psi\rangle$ does not provide a deterministic trajectory for a particle. Instead, the square of the absolute value of the wave function, gives the probability density of finding the particle at a position x at time t . This fundamentally shifts the understanding of motion at the microscopic level, as it challenges the classical notion of a well-defined trajectory, leading to the realization that particles exhibit behavior that can only be described in terms of probabilities rather than precise paths, we write [14]

$$d\mathcal{P}(\mathbf{r}, t) = C|\psi(\mathbf{r}, t)|^2 d\mathbf{r}, \quad (3.27)$$

where C is a normalization constant.

From the formula (3.27) one concludes that Schrödinger equation solution must be square integrable function which means that

$$\int |\psi(\mathbf{r}, t)|^2 d\mathbf{r} < \infty, \quad (3.28)$$

Hence the normalization constant that manifests in (3.27) is obtained by the following relation

$$\frac{1}{C} = \int |\psi(\mathbf{r}, t)|^2 d\mathbf{r}. \quad (3.29)$$

The hermiticity of the Hamiltonian operator allows to get only real values of the energy, This guarantees that the energies are physically meaningful, measurable quantities. This feature is important because it ensures that probabilities (which are the squares of the wavefunction amplitudes) remain conserved over time.

3.4 Time independent Schrödinger equation stationary solution

Let give Schrödinger equation in the case of a potential that do not depend on time

$$i\hbar \frac{d}{dt}\psi(\mathbf{r}, t) = \left(-\frac{\hbar^2}{2m}\Delta + V(\mathbf{r}) \right)\psi(\mathbf{r}, t), \quad (3.30)$$

For a potential which is independent of time, the Hamiltonian becomes explicitly independent of time and this led to a conservative system where the energy is a constant of motion [14, 48]. We look for wave function ψ that has a well-defined energy.

By using separation of variables method, we seek solutions for the Schrödinger equation to be in the form

$$\psi(\mathbf{r}, t) = X(\mathbf{r})T(t), \quad (3.31)$$

substituting the function (3.31) in the equation (3.30) leads to the following equation

$$i\hbar X(\mathbf{r})T'(t) = T(t) \left(-\frac{\hbar^2}{2m}\Delta X(\mathbf{r}) \right) + T(t)V(\mathbf{r})X(\mathbf{r}), \quad (3.32)$$

if both sides are divided (3.32) by $X(\mathbf{r})T(t)$ we get

$$\frac{i\hbar}{T(t)}T'(t) = \frac{1}{X(\mathbf{r})} \left(-\frac{\hbar^2}{2m}\Delta X(\mathbf{r}) \right) + V(\mathbf{r}). \quad (3.33)$$

The right side is dependent only on x equates the left side that is dependent only on t , therefore, both sides have to be equal to a constant that we note by E and we write

$$\frac{i\hbar}{T(t)}T'(t) = \frac{1}{X(\mathbf{r})} \left(-\frac{\hbar^2}{2m}\Delta X(\mathbf{r}) \right) + V(\mathbf{r}) = E, \quad (3.34)$$

then, we have

$$i\hbar T'(t) = ET(t), \quad (3.35)$$

$$-\frac{\hbar^2}{2m}\Delta X(\mathbf{r}) + V(\mathbf{r})X(\mathbf{r}) = EX(\mathbf{r}). \quad (3.36)$$

The equation (3.36) is written as

$$\mathcal{H}X(\mathbf{r}) = EX(\mathbf{r}). \quad (3.37)$$

Equation (3.35) solution is written explicitly by

$$T(t) = Ae^{-i\frac{Et}{\hbar}}, \quad (3.38)$$

where A is a constant.

The equation (3.37) is the so-called the time-independent Schrödinger equation or the stationary equation. In the language of differential equations, it represents an eigenvalue problem where the function X is an eigenfunction that is associated to the eigenvalue E .

The function

$$X(\mathbf{r})e^{-i\frac{Et}{\hbar}}, \quad (3.39)$$

is a stationary solution to Schrodinger equation, it gives a probability density that does not depend on time

$$d\mathcal{P}(\mathbf{r}, t) = C|X(\mathbf{r})|^2 d\mathbf{r}. \quad (3.40)$$

By introducing an index $n \in \mathbb{N}$ we can have the function $X_n(x)$ as a solution to the stationary equation for the eigenvalue E_n

$$\mathcal{H}X_n(\mathbf{r}) = E_n X_n(\mathbf{r}). \quad (3.41)$$

Using the superposition principle, the general solution to Schrödinger equation is written as

$$\psi(\mathbf{r}, t) = \sum_{n \geq 0} C_n e^{-i\frac{E_n t}{\hbar}} X_n(\mathbf{r}), \quad (3.42)$$

where the coefficients C_n depend on the initial condition

$$\psi(\mathbf{r}, 0) = \sum_{n \geq 0} C_n X_n(\mathbf{r}). \quad (3.43)$$

Local conservation of probability: Probability densities and probability current

In this part, we confine ourselves to the case where the system under consideration is one non-relativistic particle.

If the state vector $|\psi\rangle$ is normalized, then

$$\rho(\mathbf{r}, t) = |\psi(\mathbf{r}, t)|^2, \quad (3.44)$$

is a probability density, and the probability of finding a particle in a region dx of space at a time t is given by

$$d\mathcal{P}(\mathbf{r}, t) = \rho(\mathbf{r}, t) d\mathbf{r}. \quad (3.45)$$

Using classical vector analysis, the local conservation of electrical charge can be written in the following expression

$$\frac{\partial}{\partial t} \rho(\mathbf{r}, t) + \text{div} \mathbf{J}(\mathbf{r}, t) = 0, \quad (3.46)$$

we are going to prove that is possible to find a vector $\mathbf{J}(\mathbf{r}, t)$ that represents a probability current in which it verifies the equation (3.46), in this case we said that there is a local conservation of probability.

At the beginning, let assume that the particle is influenced by a scalar potential $V(\mathbf{r}, t)$, then, under the principle of correspondance given by

$$P = -i\hbar \nabla, \quad (3.47)$$

the Hamiltonian is written as

$$H = \frac{P^2}{2m} + V(\mathbf{r}, t), \quad (3.48)$$

then, Schrödinger equation is given by

$$i\hbar \frac{\partial}{\partial t} \psi(\mathbf{r}, t) = -\frac{\hbar^2}{2m} \Delta \psi(\mathbf{r}, t) + V(\mathbf{r}, t) \psi(\mathbf{r}, t), \quad (3.49)$$

in our case, the potential $V(\mathbf{r}, t)$ has to be real so that the Hamiltonian H is Hermitian. Writing the complex conjugate of equation (3.49) gives

$$-i\hbar \frac{\partial}{\partial t} \psi^*(\mathbf{r}, t) = -\frac{\hbar^2}{2m} \Delta \psi^*(\mathbf{r}, t) + V(\mathbf{r}, t) \psi^*(\mathbf{r}, t). \quad (3.50)$$

By multiplying both sides of the equation (3.49) by $\psi^*(\mathbf{r}, t)$ and both sides of the equation (3.50) by $-\psi(\mathbf{r}, t)$ and by adding them the following equation is obtained

$$i\hbar \frac{\partial}{\partial t} [\psi(\mathbf{r}, t) \psi^*(\mathbf{r}, t)] = -\frac{\hbar^2}{2m} [\psi^*(\mathbf{r}, t) \Delta \psi(\mathbf{r}, t) - \psi(\mathbf{r}, t) \Delta \psi^*(\mathbf{r}, t)], \quad (3.51)$$

that is written as

$$\frac{\partial}{\partial t} \rho(\mathbf{r}, t) + \frac{\hbar}{2mi} [\psi^*(\mathbf{r}, t) \Delta \psi(\mathbf{r}, t) - \psi(\mathbf{r}, t) \Delta \psi^*(\mathbf{r}, t)] = 0, \quad (3.52)$$

if we set

$$\mathbf{J}(\mathbf{r}, t) = -\frac{\hbar^2}{2m} [\psi^*(\mathbf{r}, t) \Delta \psi(\mathbf{r}, t) - \psi(\mathbf{r}, t) \Delta \psi^*(\mathbf{r}, t)], \quad (3.53)$$

then

$$\mathbf{J}(x, t) = \frac{1}{m} \text{Re} \left(\psi^*(\mathbf{r}, t) \left(\Delta \psi(\mathbf{r}, t) \right) \right). \quad (3.54)$$

Hence, the equation (3.52) can be put in the form of equation (3.46) [14].

3.5 Schrödinger equation for some solvable potentials

The study of the Schrödinger equation has been a central focus in quantum mechanics since its inception, particularly for exactly solvable potentials. These potentials allow for the analytical determination of their

associated eigenvalues and eigenfunctions, facilitating a deeper understanding of quantum systems. The exact solvability of Schrödinger equation is allowed only for few quantum problems such as the hydrogen atom, harmonic oscillator, Morse and other potentials.

Here we give the exact eigensolutions for Schrödinger equation in 1-dimension for some exactly solvable potentials [49]:

3.5.1 Morse potential

The one dimensional Morse potential is given by the following expression

$$V(x) = V_0(e^{-2\alpha x} - 2e^{-\alpha x}), \quad V_0 > 0, x \geq 0 \quad (3.55)$$

where V_0 is the depth of the potential and α is related to its range.

The one dimensional Schrödinger equation is given by:

$$-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} \psi(x) + V(x)\psi(x) = E\psi(x). \quad (3.56)$$

By substituting Morse potential expression (3.55) in the one dimensional Schrödinger equation (3.56) we obtain

$$-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} \psi(x) + V_0(e^{-2\alpha x} - 2e^{-\alpha x})\psi(x) = E\psi(x). \quad (3.57)$$

By considering the following constants and variable

$$\begin{aligned} v &= \sqrt{\frac{8mV_0}{\alpha^2 \hbar^2}}, \\ s &= \sqrt{\frac{-2mE}{\alpha^2 \hbar^2}}, \\ y &= ve^{-\alpha x}, \end{aligned}$$

the equation (3.57) becomes

$$\frac{d^2}{dy^2} \psi(y) + \frac{1}{y} \psi(y) + \left(\frac{v}{2y} - \frac{s^2}{y^2} - \frac{1}{4} \right) \psi(y) = 0. \quad (3.58)$$

By taking the following ansatz

$$\psi(y) = e^{\frac{y}{2}} y^s F(y), \quad (3.59)$$

the equation (3.58) is written as

$$y \frac{d^2}{dy^2} F(y) + (2s + 1 - y) \frac{d}{dy} F(y) - \left(s + \frac{1 - \nu}{2} \right) F(y) = 0, \quad (3.60)$$

where the solutions are the confluent hypergeometric functions that are given as

$$F(y) = F\left(s + \frac{1 - \nu}{2}, 2s + 1, y\right). \quad (3.61)$$

By putting the following condition

$$s + \frac{1 - \nu}{2} = -n,$$

the solutions ψ of the differential equation (3.57) are given in terms of the associated Laguerre polynomials L_n^{2s} as

$$\psi_n^\nu = N_n^\nu e^{\frac{y}{2}} y^s L_n^{2s}(y),$$

and the factor N_n^ν is the normalization constant which is given by

$$N_n^\nu = \sqrt{\frac{\alpha(\nu - 2n - 1)\Gamma(n + 1)}{\Gamma(\nu - n)}}, \quad (3.62)$$

while the energy is given by the expression

$$E_n = -\frac{\alpha^2 \hbar^2}{2m} \left(\sqrt{\frac{2mV_0}{\alpha^2 \hbar^2}} - n - \frac{1}{2} \right)^2. \quad (3.63)$$

3.5.2 The Harmonic oscillator

The harmonic oscillator potential is given by the expression [49]

$$V(x) = \frac{1}{2} m \omega^2 x^2, \quad x \in \mathbb{R}, \quad (3.64)$$

where m is the mass of the particle and ω is the frequency of the oscillator.

The one dimensional Schrödinger equation for the harmonic oscillator is given by

$$-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} \psi(x) + \frac{1}{2} m \omega^2 x^2 \psi(x) = E \psi(x). \quad (3.65)$$

Let consider the following parameters

$$\tau = \frac{2E}{\hbar\omega},$$

$$\alpha = \sqrt{\frac{m\omega}{\hbar}},$$

and the following variable

$$y = \alpha x,$$

then, the differential equation (3.65) becomes

$$\frac{d^2}{dy^2} \psi(y) + (\tau - y^2) \psi(y) = 0. \quad (3.66)$$

We take the following ansatz of the wave function

$$\psi(y) = e^{-\frac{y^2}{2}} H(y). \quad (3.67)$$

By substituting the ansatz (3.67) into the differential equation (3.66), we get the following equation

$$\frac{d^2}{dy^2} H(y) - 2y \frac{d}{dy} H(y) + (\tau - 1) H(y) = 0. \quad (3.68)$$

The solutions of the differential equation (3.68) are nothing but Hermite polynomials $H_n(y)$ with the relation

$$\tau - 1 = 2n$$

that permits to obtain the eigenvalues as follows

$$E_n = \hbar\omega \left(n + \frac{1}{2} \right), \quad (3.69)$$

while the corresponding eigenfunctions can be written as

$$\psi_n(x) = N_n e^{-\frac{\alpha^2 x^2}{2}} H_n(\alpha x), \quad (3.70)$$

the normalization constant can be derived starting from the normalization condition of the wave functions

$$\int_{-\infty}^{+\infty} \psi_n(x) dx = 1 \quad (3.71)$$

as

$$N_n = \left(\frac{\alpha}{\sqrt{\pi} 2^n n!} \right)^{\frac{1}{2}} \quad (3.72)$$

3.5.3 The pseudoharmonic oscillator

Let us begin by presenting the pseudoharmonic oscillator expression as [49]

$$V(x) = \frac{1}{2} m \omega^2 x^2 + \frac{\hbar^2}{2m} \frac{\alpha}{x^2}, \quad x \in R \quad (3.73)$$

where m represents the mass of the particle while α represents the strength of the external field.

The one dimensional Schrödinger equation for the pseudoharmonic oscillator is written as

$$-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} \psi(x) + \left(\frac{1}{2} m \omega^2 x^2 + \frac{\hbar^2}{2m} \frac{\alpha}{x^2} \right) \psi(x) = E \psi(x). \quad (3.74)$$

By taking $\hbar = m = \omega = 1$ and by defining the new variable

$$y = x^2, \quad (3.75)$$

the differential equation (3.74) can be written as

$$\frac{d^2}{dy^2} \psi(y) + \frac{1}{2y} \frac{d}{dy} \psi(y) - \left(\frac{1}{4} + \frac{\alpha}{4y^2} - \frac{E}{2y} \right) \psi(y) = 0. \quad (3.76)$$

Let be the following parameter

$$s = \frac{1 + \sqrt{1 + 4\alpha}}{4}, \quad (3.77)$$

and the following ansatz of the wave function

$$\psi(y) = y^s e^{-\frac{y}{2}} \omega(y). \quad (3.78)$$

Substituting the function (3.78) into the differential equation (3.76) leads to this differential equation

$$y \frac{d^2}{dy^2} \omega(y) + \left(2s + \frac{1}{2} - y\right) \frac{d}{dy} \omega(y) + \left(\frac{E}{2} - s - \frac{1}{4}\right) \omega(y) = 0. \quad (3.79)$$

The solutions of the differential equation (3.79) are the confluent hypergeometric functions

$$F\left(s - \frac{E}{2} + \frac{1}{4}, 2s + \frac{1}{2}, y\right).$$

Starting from the quantum condition

$$s - \frac{E}{2} + \frac{1}{4} = -n,$$

we obtain the energy expression as

$$E_n = 1 + 2n + \sqrt{\alpha + \frac{1}{4}}. \quad (3.80)$$

when $s - \frac{E}{2} + \frac{1}{4} = -n$, then, we use the following relation

$$L_n^\beta(x) = \frac{\Gamma(\beta + n + 1)}{n! \Gamma(\beta + 1)} F(-n, \beta + 1, x), \quad (3.81)$$

and the integral

$$\int_0^\infty x^\beta e^{-x} L_n^\beta(x) L_m^\beta(x) dx = \frac{\Gamma(n + \beta + 1)}{n!} \delta_{n,m}, \quad (3.82)$$

in order to obtain the normalized wave functions as

$$\psi(y) = N_n y^s e^{-\frac{y}{2}} L_n^{2s-\frac{1}{2}}(y), \quad (3.83)$$

where $y = x^2$ and N_n is the normalization constant that is given by

$$N_n = \sqrt{\frac{n!}{\Gamma\left(n + 2s + \frac{1}{2}\right)}}. \quad (3.84)$$

3.5.4 Pöschl-Teller like potential

The studied Pöschl-Teller like potential is given by [49]

$$V(x) = V_0 \tan^2\left(\frac{\pi x}{L}\right), \quad x \in \left[-\frac{L}{2}, \frac{L}{2}\right], \quad (3.85)$$

where V_0 and L are two constants where $L > 0$.

Schrödinger equation for Pöschl-Teller like potential is given by

$$-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} \psi(x) + V_0 \tan^2\left(\frac{\pi x}{L}\right) \psi(x) = E \psi(x), \quad (3.86)$$

such that the solutions must satisfy the boundary conditions

$$\psi\left(\frac{L}{2}\right) = \psi\left(-\frac{L}{2}\right) = 0. \quad (3.87)$$

By introducing the parameters

$$\epsilon = \frac{2mL^2}{\pi^2 \hbar^2} (E + V_0), \quad (3.88)$$

$$W = \frac{2mL^2}{\pi^2 \hbar^2} V_0, \quad (3.89)$$

and the new variable

$$y = \frac{\pi x}{L}, \quad (3.90)$$

then, substituting them into the differential equation (3.86) we obtain the following equation

$$\frac{d^2}{dy^2} \psi(y) + \left(\epsilon - \frac{W}{\cos^2 y} \right) \psi(y) = 0. \quad (3.91)$$

Let us consider the following ansatz of the wave function

$$\psi(y) = P_n(t) \cos^\lambda y, \quad \lambda > 0, \quad (3.92)$$

where

$$t = \sin y.$$

Substitution of the ansatz function into the differential equation (3.91) allows us to have the following equation

$$(1 - t^2) \frac{d^2}{dt^2} P_n(t) - (1 + 2\lambda) t \frac{d}{dt} P_n(t) + (\epsilon - \lambda^2) P_n(t) = 0, \quad (3.93)$$

with the notation

$$W = \lambda(\lambda - 1)$$

and the condition $\lambda \neq 0, 1$.

From the differential equation for the Gegenbauer polynomials given by

$$\frac{d^2}{dt^2} F(t) + \frac{t(1 + 2\lambda)}{t^2 - 1} \frac{d}{dt} F(t) - \frac{n(2\lambda + n)}{t^2 - 1} F(t) = 0, \quad (3.94)$$

it is concluded that the solutions of the differential equation (3.93) are nothing but the Gegenbauer polynomials $C_n^\lambda(t)$ where the expression of the wave functions is obtained as

$$\psi_n(y) = N_n C_n^\lambda(y) \sin y \cos^\lambda y, \quad (3.95)$$

where N_n is the normalization constant that will be calculated below from the normalization condition

$$\int_{-\frac{\pi}{2}}^{\frac{\pi}{2}} |\psi(x)|^2 dx = 1, \quad (3.96)$$

for this Let recall an important formula

$$\int_{-1}^1 (1 - x^2)^{\nu - \frac{1}{2}} |C_n^\nu|^2 dx = \frac{\pi 2^{(1-2\nu)} \Gamma(n + 2\nu)}{n! (n + \nu) \Gamma^2(\nu)}, \quad \operatorname{Re} \nu > -\frac{1}{2}, \quad (3.97)$$

finally the normalization constant is given by

$$N_n = \sqrt{\frac{n!(n+\lambda)\Gamma^2(\lambda)}{L2^{(1-2\lambda)}\Gamma(n+2\lambda)}}. \quad (3.98)$$

From the following condition

$$\epsilon_n = (n + \lambda)^2, \quad n = 0, 1, 2, \dots \quad (3.99)$$

the eigenvalues of the corresponding quantum system are obtained as

$$E_n = \frac{\pi^2 \hbar^2}{2mL^2} (n^2 + 2n\lambda + \lambda). \quad (3.100)$$

CHAPTER 4

APPLICATION

4.1 Introduction

Schrödinger equation is a crucial equation in non-relativistic quantum mechanics because according to the sixth postulate it governs the time evolution of the system under consideration [14, 48]. It is an important equation that allows us to conclude the spectral properties of any quantum physical system, Schrödinger equation also play very crucial role in many Science branches such as chemistry and spectroscopy where the solutions are used to describe the electronic distribution and structure of atoms and molecules, they provide the necessary information about the energy levels and the distribution of electrons, they are helpful in predicting the chemical properties such as bond and bond angles in which they are essential in explaining the chemical reactions, Schrödinger equation is used also to understand the composition, structure, identification and quantification of substances, it is essential to explain the absorption and emission spectra and predict the properties of molecules and atoms with their spectroscopic behavior besides to determine the thermodynamics properties, it is crucial tool in determining the energies levels and transitions of quantum physical systems that are fundamental in spectroscopy analyses [50, 51, 52]. Since the early days of quantum mechanics, the exact solvable problems of Schrödinger equation has attracted the interest of researchers, here we mean by the exact solvable Schrödinger equation the case when all the energy levels and corresponding wave functions expressions can be obtained explicitly in closed form and although this kind of quantum mechanical models such as the Coulomb and the harmonic oscillator play an important role in many fields of quantum physics, it generally they are with limited applications. Re-

cently a new class of spectral problems in quantum mechanics has been discovered [53, 54, 55], this class is with many applications more than the class of exactly solvable potentials, it took the name of quasi exactly solvable problem and it attracted the attention of researchers, the concept of quasi exactly problems in quantum mechanics has been introduced in the late of 1980s by the physicist Alexander Turbiner, in contrast to the class of exactly solvable problems, for the situation when the solvability of Schrödinger equation is quasi exact only a finite part of the discrete spectrum or their eigenfunctions are obtained exactly in full expression. The class of central potentials constitute a very important class because it models the different interactions between atoms and molecules, this potentials are used extensively in chemistry since they provide accurate predictions about vibrational properties like determining the vibrational energies and understanding molecular spectroscopy such as Morse potential and the harmonic oscillator, besides to studying the rotational properties of molecules and obtaining the rotational energy levels, add to it understanding the molecular structure [50, 51, 52]. In resolving Schrödinger equation for the situation where the potential is central, we solve directly the so-called radial equation, in general solving a such equation is not trivial due to the existence of the centrifugal term that makes the resolution of the equation not an easy task, this term add complexity to potential expression, hence in a such situation when the radial equation cannot be resolved analytically, approximate solutions are required, by approximating the effective potential using an appropriate scheme, this method allows to transform the original radial equation to another equation that can be resolved and its solutions are known [57, 58].

In this work, we search the approximate bound states for the Schrödinger equation in the case of quasi exactly Schrödinger equation problems, for some potentials that would be taken as central potentials, a single potential potential is written as

$$V(r) = V_C(r) + V_e(r), \quad (4.1)$$

where the potential V_C is called the generalized Cornell potential, it is given by

$$V_C(r) = \sum_{i=-2}^2 a_i r^i, \quad (4.2)$$

in which the parameters that appear in the expansion a_i , $i = -2, \dots, 2$ are real constants, at the other side V_e is an exponential potential, precisely the potential that will be treated in this work are:

- Schiöberg potential..
- The generalized Pöschl-Teller.
- Manning-Rosen potential.
- Morse.
- Yukawa class potential.

The generalized Cornell potential is a sum of the inverse square potential, Coulomb, the linear potential and the harmonic oscillator, this potential is important, it is one of the most applicable potential in quantum mechanics, it combine between the inverse square potential models the electrostatics force between electron and nucleus, the Coulomb potential arises in describing systems involving charged particles such as the force between the electron and proton in the hydrogen atom, the linear potential is used to approximate forces that are nearly constant or to ap-

proximate the harmonic oscillator in its equilibrium point, this potential can describe some kind of physical behavior such as the displacements from the equilibrium, or in systems that are confined the linear potential models an external electric field applied on the system, the harmonic oscillator models force proportional to its displacement from an equilibrium and vibrations of individual atoms and molecules, it models also the force that links bosons, one of the building blocks in the macroscopic scale. By combining this potentials besides to the exponential potentials, we get a better description of the forces applied on the physical system.

in the next sections, we are going to deal with the radial equation for some central potentials that are in the form of (4.1), In order to treat the radial equation for this central potentials, for each one we use an appropriate approximation scheme that allows us to transform the radial equation to a different equation where the resolution is allowed, exactly, to the biconfluent Heun's equation, then, the approximate solutions will be obtained analytically.

4.2 Schrödinger equation in the case of central potential

Schrödinger equation taken for $\hbar = 1$ is given by

$$\left(-\frac{\Delta}{2M} + V(\mathbf{r}, t) \right) \Psi(\mathbf{r}, t) = i \frac{\partial}{\partial t} \Psi(\mathbf{r}, t), \quad (4.3)$$

in which M represents the mass of the particle and Δ is the Laplacian operator, V is the potential function, $\mathbf{r}$ is the position vector and where its solution is the so-called the wave function.

Let consider the potential V to be time-independent, then, by separating

the spatial and time dependencies and by putting the wave function in the form below

$$\Psi(\mathbf{r}, t) = \psi(\mathbf{r})e^{-iEt}, \quad (4.4)$$

we obtain the time-independent Schrödinger equation or the stationary equation as

$$\left(-\frac{\Delta}{2M} + V(\mathbf{r}) \right) \psi(\mathbf{r}) = E\psi(\mathbf{r}). \quad (4.5)$$

We choose the position vector to be in spherical coordinates system $\mathbf{r} = (r, \theta, \phi)$, then the stationary equation (4.5) becomes

$$\left(-\frac{1}{2Mr^2} \left(\frac{\partial}{\partial r} \left(r^2 \frac{\partial}{\partial r} \right) - \Omega^2 \right) + V(r, \theta, \phi) \right) \psi(r, \theta, \phi) = E\psi(r, \theta, \phi), \quad (4.6)$$

where Ω^2 is given by

$$\Omega^2 = \frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial}{\partial \theta} \right) + \frac{1}{\sin^2 \theta} \frac{\partial^2}{\partial \phi^2} \quad (4.7)$$

By considering the potential function to depend only on the radius, which means that the potential is central and using, then the equation (4.6) is written as

$$\left(-\frac{1}{2Mr^2} \left(\frac{\partial}{\partial r} \left(r^2 \frac{\partial}{\partial r} \right) - \Omega^2 \right) + V(r) \right) \psi(r, \theta, \phi) = E\psi(r, \theta, \phi), \quad (4.8)$$

using the separation of variables method, we separate the radial and angular dependencies as

$$\psi(r, \theta, \phi) = \frac{R(r)Y(\theta, \phi)}{r}, \quad (4.9)$$

then we insert the function (4.9) in the equation (4.8) to have

$$\frac{d^2 R(r)}{dr^2} + 2M(E - V(r))r^2 = -\Omega^2 Y(\theta, \phi), \quad (4.10)$$

and since the equation (4.10) give a side that depends only on r equals a side that depends only on θ and ϕ which means that the both sides

equal a constant ξ

$$\frac{d^2 R(r)}{dr^2} + 2M(E - V(r))r^2 = -\Omega^2 Y(\theta, \phi) = \xi. \quad (4.11)$$

From the equation (4.10) we obtain the following system of equations

$$\frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial Y(\theta, \phi)}{\partial \theta} \right) + \frac{1}{\sin^2 \theta} \frac{\partial^2 Y(\theta, \phi)}{\partial \theta^2} = -\xi, \quad (4.12)$$

$$\frac{d^2 R(r)}{dr^2} + 2M \left(E - V(r) - \frac{\xi}{2Mr^2} \right) R(r) = 0. \quad (4.13)$$

The differential equation (4.12) admits solutions Y_l^m that are the spherical harmonics [14, 56], the eigenfunctions of the differential operator Ω^2 in which this operator eigenvalue are $l(l+1)$, here the number l represent a positive integer while the number m is a relative integer that takes its values from $-l$ to l , their expression is given by

$$Y_l^m(\theta, \phi) = NP_l^m(\cos \theta) e^{im\phi}, \quad (4.14)$$

$$N = (-1)^m \sqrt{\frac{2l+1}{4\pi} \frac{(l-m)!}{(l+m)!}}$$

where N is a normalization constant and P_l^m represents the associated Legendre function, their full expression are given by

$$P_l^m(u) = \sqrt{(1-u^2)^m} \frac{d^m}{du^m} P_l(u), \quad -1 \leq u \leq 1, \quad (4.15)$$

and P_l are Legendre polynomial written as

$$P_l(x) = \frac{1}{l!2^l} \frac{d^l}{dx^l} (x^2 - 1)^l. \quad (4.16)$$

The bound states equation (4.8) are in the following form

$$\psi_{n,l,m}(r, \theta, \phi) = \frac{R_{n,l}}{r} Y_l^m(\theta, \phi), \quad (4.17)$$

where $R_{n,l}$ are the radial eigenfunctions, the solutions to the radial equation below

$$-\frac{1}{2M} \frac{d^2 R_{n,l}(r)}{dr^2} + \left(V(r) + \frac{l(l+1)}{2Mr^2} \right) R_{n,l}(r) = E_{n,l,m} R_{n,l}(r), \quad (4.18)$$

this term

$$\frac{l(l+1)}{2Mr^2},$$

is called the centrifugal term, while the expression

$$V(r) + \frac{l(l+1)}{2Mr^2}, \quad (4.19)$$

is called the effective potential, hence solving the stationary equation in the case of central potentials is based on obtaining the radial equation solutions.

In the next parts, we are going to resolving Schrödinger equation for few potential in specific form, this potentials are are central, using an accurate approximate scheme for each case. A single central potential is composed of the generalized Cornell potential plus an exponential part. Approximating the central potentials leads to the resolution of the equation of Heun in its biconfluent form, where the analytic approximate bound states will be obtained in closed form.

4.3 Biconfluent Heun's equation polynomial solutions

The biconfluent Heun's equation in its normal form is provided by

$$\frac{d^2 U(x)}{dx^2} + \left(\frac{A}{x^2} + \frac{B}{x} + C + Dx - Fx^2 \right) U(x) = 0, \quad (4.20)$$

here the parameters that appear in the equation are real such that the parameters B and F do not vanish.

Let consider the following ansatz

$$U(x) = y^{\frac{1+\alpha}{2}} e^{-\frac{y^2+\beta y}{2}} P(y), \quad (4.21)$$

where the new variable y is given by

$$y = \sqrt[4]{F}x, \quad (4.22)$$

then the biconfluent Heun's equation normal form is transformed to the canonical form as follows

$$y \frac{d^2 P(y)}{dy^2} + \left(1 + \alpha - \beta y - 2y^2\right) \frac{dP(y)}{dy} + \left((\gamma - \alpha - 2)y - \frac{1}{2}(\delta + (1 + \alpha)\beta)\right) P(y) = 0, \quad (4.23)$$

such that the parameters α, β, γ and δ are given by

$$\begin{cases} \alpha = \sqrt{1 - 4A}, \\ \beta = -\frac{D}{\sqrt[4]{F^3}}, \\ \gamma = \frac{D^2}{4\sqrt[4]{F^3}} + \frac{C}{\sqrt{F}}, \\ \delta = -\frac{2B}{\sqrt[4]{F}}. \end{cases} \quad (4.24)$$

When α is a non-negative integer, then, the canonical equation (4.23) accepts the series solution below

$$P(y) = \sum_{k \geq 0} \frac{\Gamma(1 + \alpha) b_k}{\Gamma(1 + \alpha + k)} \frac{y^k}{k!}, \quad (4.25)$$

so that the following recurrence relation links the coefficients b_k

$$\begin{cases} b_0 = 1, \\ b_1 = -\omega b_0, \\ b_2 = -(\omega - \beta)b_1 - (1 + \alpha)(\gamma - \alpha - 2)b_0, \\ b_{k+2} = -(\omega - (k + 1)\beta)b_{k+1} - (1 + k + \alpha)(\gamma - \alpha - 2 - 2k)(k + 1)b_k, \quad k \geq 0, \end{cases} \quad (4.26)$$

where

$$\omega = -\frac{1}{2}(\delta + (1 + \alpha)\beta).$$

It is possible to infer from the recurrence relation (4.26) that the coefficient b_k represents for each $k \in \mathbb{N}$ a polynomial with a degree k in ω .

A polynomial solution is derived from the recurrence relation (4.26) provided that the two requirements listed below are met:

$$\begin{cases} \gamma - \alpha - 2 = 2n, \\ b_{n+1} = 0, \end{cases} \quad (4.27)$$

where b_{n+1} is a polynomial of degree $n+1$ in ω and when we have $1 + \alpha > 0$ and $\beta \in \mathbb{R}$, b_{n+1} has $n + 1$ real roots that we denote them by

$$\omega_{n,\mu} = -\frac{1}{2}(\delta_\mu^n + (1 + \alpha)\beta), \quad 0 \leq \mu \leq n.$$

The first five coefficients are provided by the recurrence relation (4.26)

$$b_0 = 1,$$

$$b_1 = -\omega,$$

$$b_2 = \omega^2 - \beta\omega - (\gamma - \alpha - 2)(\alpha + 1), \quad (4.28)$$

$$b_3 = -\omega^3 + 3\beta\omega^2 - \left(2\beta^2 - \sum_{i=1}^2 i(\gamma - \alpha - 2i)(\alpha + i)\right)\omega - 2\beta(\gamma - \alpha - 2)(\alpha + 1),$$

$$b_4 = \omega^4 - 6\beta\omega^3 + \left(11\beta^2 - \sum_{i=1}^3 i(\gamma - \alpha - 2i)(\alpha + i)\right)\omega^2 - \beta\left(4(\gamma - \alpha - 6)(\alpha + 3)\right.$$

$$\left. + 6\beta^2 - \sum_{i=1}^3 (i + 4)(\gamma - \alpha - 2i)(\alpha + i)\right)\omega + 3(\gamma - \alpha - 2)(\alpha + 1) \quad (4.29)$$

$$\cdot \left((\gamma - \alpha - 6)(\alpha + 3) - 2\beta^2\right). \quad (4.30)$$

4.4 Approximate eigensolutions for few central potentials

The purpose of next part is to give the analytic expressions of the eigensolutions for central potentials where the generalized Cornell potential plus an exponential component add up to a single potential. by approximating the effective potential using an appropriate approximation scheme, after that we give the closed-form of the energy levels then in the numerical application part, for given values of the parameters, For a subset of the roots $\omega_{n,\mu}$ of b_n , we compute the bound state's analytic formula.

4.4.1 Morse potential

We give Morse potential expression as follows

$$V_e(r) = V_0 e^{-2\lambda r} + V_1 e^{-\lambda r}. \quad (4.31)$$

Morse potential is an important potential in quantum mechanics and related fields such as chemistry, it was introduced for the first time in 1929 [60], named after the physicist Philip M. Morse, it is appropriate for studying vibrational and rotational properties of diatomic molecules, Morse potential is one of the available models in quantum mechanics to model the vibrations of molecules such as diatomic models and even polyatomic molecules, this potential allows to study the anharmonicity of molecular vibrations as well as the ionization besides to the stabilization of atoms and molecules electronic states [61], usually Morse potential is helpful for investigating the spectroscopic properties

of diatomic molecules and studying the anharmonic vibrational dynamics in addition to its application in analyzing the vibrational spectra of real molecules. Morse potential attracted the attention of researchers [61, 62, 63]. where Schrödinger equation has been resolved for Morse potential by many methods where Miraboutalebi and Rajaei used the Laplace transform [62] while Dayi and Duru resolved Schrödinger equation in terms of the q-canonical transformation [63], Han et al obtained solutions for Morse potential using the approach of supersymmetric quantum mechanics [64] while Arda and Sever obtained bound states using NU method [65], Berkdemir and Han applied Pekeris approximation to obtain l -state solutions using the same method [66], Yu et al used the serie solution method [67] and Barakat et al obtained exact solutions for Schrödinger equation for Morse potential by asymptotic iteration method [68].

In order to have the potential that we resolve the radial equation for, we substitute this exponential potential of Morse in (4.1) to get

$$V(r) = \frac{a_{-2}}{r^2} + \frac{a_{-1}}{r} + a_0 + a_1 r + a_2 r^2 + V_0 e^{-2\lambda r} + V_1 e^{-\lambda r}, \quad (4.32)$$

then inserting the central potential (4.32) in the radial equation (4.18) leads to the following equation

$$-\frac{1}{2M} \frac{d^2 R_{n,l}(r)}{dr^2} + \left(\frac{\frac{l(l+1)}{2M} + a_{-2}}{r^2} + \frac{a_{-1}}{r} + a_0 + a_1 r + a_2 r^2 + V_0 e^{-2\lambda r} + V_1 e^{-\lambda r} \right) R_{n,l}(r) = E R_{n,l}(r). \quad (4.33)$$

Due to the expression of the effective potential that combine between polynomial terms and exponential term, the radial equation (4.33) can't be resolved in explicit way, for this, the following approximation scheme

is adopted [59]

$$\frac{1}{1 - e^{-\lambda r}} \approx \frac{1}{\lambda r} \quad (4.34)$$

and the following figure shows that the curves of $\frac{1}{\lambda r}$ and $\frac{1}{1 - e^{-\lambda r}}$ are so close when the parameter λ is small, where it takes the value 0.1



Figure 4.1: The curves of $\frac{1}{\lambda r}$ and $\frac{1}{1 - e^{-\lambda r}}$ for $\lambda = 0.1$

in order to approximate the effective potential and have an equation that we can resolve the previous approximation scheme is used, where the left side is a good approximation of the right side and is accurate for tiny values of the parameter λ .

We take the term $\frac{1}{1 - e^{-\lambda r}}$ and we approximate it by the term $\frac{1}{\lambda r}$ in the effective potential in the radial equation (4.33), then we get the following equation

$$\frac{d^2 R_{n,l}(r)}{dr^2} + \left(\frac{A_1}{r^2} + \frac{B_1}{r} + C_1 + D_1 r + F_1 r^2 \right) R_{n,l}(r) = 0. \quad (4.35)$$

The differential equation (4.35) is the normal form of Heun's differential

equation for the following parameters

$$\begin{cases} A_1 = -2Ma_{-2} - l(l+1), \\ B_1 = -2Ma_{-1}, \\ C_1 = 2M(E - V_0 - V_1 - a_0), \\ D_1 = 2M(\lambda(2V_0 + V_1) - a_1), \\ F_1 = 2M(a_2 + V_0\lambda^2). \end{cases} \quad (4.36)$$

The normal Heun equation in his biconfluent form is transformed to the following canonical form

$$y \frac{d^2 P(y)}{dy^2} + \left(1 + \alpha_1 - \beta_1 y - 2y^2\right) \frac{dP(y)}{dy} + \left((\gamma_1 - \alpha_1 - 2)y - \frac{1}{2}(\delta_1 + (1 + \alpha_1)\beta_1)\right) P(y) = 0, \quad (4.37)$$

for this set of parameters

$$\begin{cases} \alpha_1 = \sqrt{1 + 4(l(l+1) + 2Ma_{-2})}, \\ \beta_1 = \left(a_1 - \lambda(2V_0 + V_1)\right) \sqrt[4]{\frac{2M}{(a_2 + V_0\lambda^2)^3}}, \\ \delta_1 = 2a_{-1} \sqrt[4]{\frac{8M^3}{a_2 + V_0\lambda^2}}, \\ \gamma_1 = \left(E - V_0 - V_1 - a_0\right) \sqrt{\frac{2M}{a_2 + V_0\lambda^2}} \\ + \left(\lambda(2V_0 + V_1) - a_1\right)^2 \sqrt{\frac{M}{8(a_2 + V_0\lambda^2)^3}}. \end{cases} \quad (4.38)$$

The canonical equation (4.37) has polynomial solutions in the following form

$$P(y) = \sum_{k=0}^n \frac{\Gamma(1 + \alpha_1) b_k}{\Gamma(1 + \alpha_1 + k)} \frac{y^k}{k!}, \quad (4.39)$$

And the recurrence expression (4.26) links the coefficients b_k . Hence only a portion of the eigenfunctions can be written in explicit form, which means that the case here is quasi-exactly solvability of Schrödinger equation.

Now we calculate the energy eigenvalues, by returning to the first condition in (4.27) which is given by

$$\gamma_1 - \alpha_1 - 2 = 2n, \quad (4.40)$$

to get the approximate energy values as

$$E_{n,l,m} = \frac{(\lambda(2V_0 + V_1) - a_1)^2}{4(a_2 + V_0\lambda^2)} + a_0 + V_0 + V_1 + \sqrt{\frac{a_2 + V_0\lambda^2}{2M}} \left(2 + 2n + \sqrt{1 + 4(l(l+1) + 2Ma_2)} \right) \quad (4.41)$$

for the condition $1 - 4A_1 \geq 0$ to have real values of the energy besides to the condition $F_1 > 0$.

Finally the approximate wave function of Schrödinger equation in the case of the central potential: the generalized Cornell potential plus Morse potential is given by

$$\psi_{n,l,m}(\rho, \theta, \phi) = \rho^{\frac{\alpha_1-1}{2}} e^{-\frac{\rho^2+\beta_1\rho}{2}} \left(\sum_{k=0}^n \frac{\Gamma(1+\alpha_1)b_k}{\Gamma(1+\alpha_1+k)} \frac{\rho^k}{k!} \right) (1-\cos^2 \theta)^{\frac{m}{2}} \cdot \frac{d^{l+m}}{d \cos \theta^{l+m}} (1-\cos^2 \theta)^l e^{im\phi} \quad (4.42)$$

for the following variable $\rho = \sqrt[4]{F_1}r$.

Numerical application for the approximate eigensolutions of Morse potential

We take into consideration the following numerical values of the parameters to provide some examples of the estimated bound states for the

case of Morse potential

$$\begin{cases} a_{-2} = a_0 = a_1 = a_2 = 0, \\ V_0 = 2, V_1 = 1, \\ M = 0.001, l = m = 1, \lambda = 0.01 \end{cases} \quad (4.43)$$

• For $n = 1$

The roots of the coefficient b_2 are

$$\begin{aligned} \omega_{1,0} &= -2.0039, \\ \omega_{1,1} &= 3.9921, \end{aligned} \quad (4.44)$$

choosing the root $\omega_{1,0}$ yields

$$\begin{cases} \psi_{1,1,1}(\rho, \theta, \phi) = e^{-\frac{\rho^2}{2} + 1.9882\rho} (1 - 0.501\rho) \sin \theta e^{i\phi}, \\ E_{1,1,1} = 25.1359. \end{cases} \quad (4.45)$$



Figure 4.2: The graph of the radial part of $\psi_{1,1,1}$

• For $n = 2$

The roots of the coefficient b_3 are

$$\omega_{2,0} = -4.2307, \quad (4.46)$$

$$\omega_{2,1} = 1.7889, \quad (4.47)$$

$$\omega_{2,2} = 8.4063, \quad (4.48)$$

for the case of the root $\omega_{2,1}$ we have

$$\begin{cases} \psi_{2,1,1}(\rho, \theta, \phi) = e^{-\frac{\rho^2}{2} + 1.9882\rho} (1 + 0.4472\rho - 0.4089\rho^2) \sin \theta e^{i\phi}, \\ E_{1,1,1} = 31.4605. \end{cases} \quad (4.49)$$

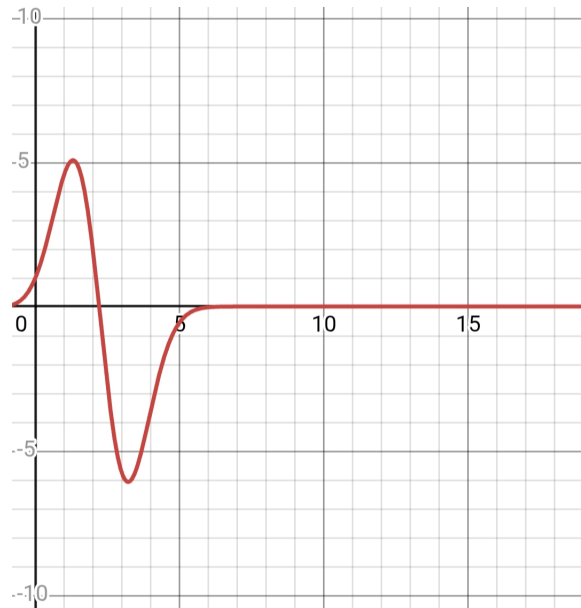


Figure 4.3: The graph of the radial part of $\psi_{2,1,1}$

- For $n = 3$

The roots of the coefficient b_4 are

$$\omega_{3,0} = -6.7 \quad (4.50)$$

$$\omega_{3,1} = -0.5571, \quad (4.51)$$

$$\omega_{3,2} = 5.9816, \quad (4.52)$$

$$\omega_{3,3} = 13.2046, \quad (4.53)$$

the root $\omega_{3,2}$ gives the following approximate energy and bound state

$$\begin{cases} \psi_{3,1,1}(\rho, \theta, \phi) = e^{-\frac{\rho^2}{2} + 1.9882\rho} \left(1 + 1.4954\rho - 0.0028\rho^2 - 0.3326\rho^3 \right) \sin \theta e^{i\phi}, \\ E_{3,1,1} = 37.7851. \end{cases} \quad (4.54)$$

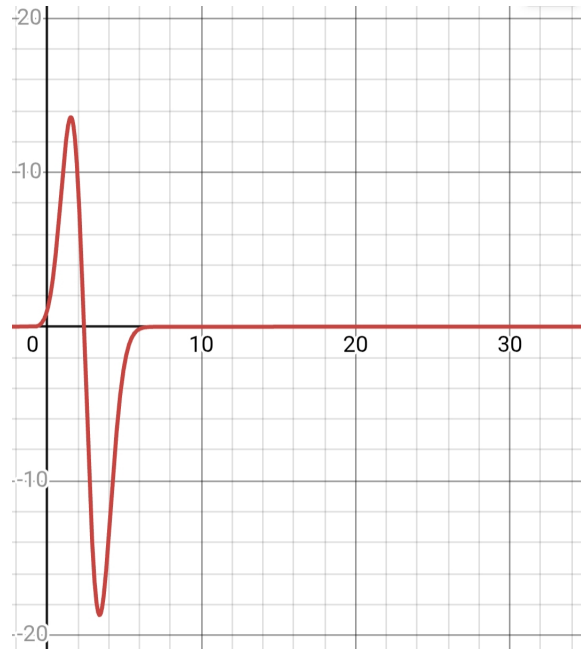


Figure 4.4: The graph of the radial part of $\psi_{3,1,1}$

• For $n = 4$

The roots of the coefficient b_5 are

$$\omega_{4,0} = -9.4248 \quad (4.55)$$

$$\omega_{4,1} = -3.0688, \quad (4.56)$$

$$\omega_{4,2} = 3.464, \quad (4.57)$$

$$\omega_{4,3} = 10.5564, \quad (4.58)$$

$$\omega_{4,4} = 18.3549, \quad (4.59)$$

selecting the root $\omega_{4,4}$ yields

$$\left\{ \begin{array}{l} \psi_{4,1,1}(\rho, \theta, \phi) = e^{-\frac{\rho^2}{2} + 1.9882\rho} \left(1 + 4.5887\rho + 6.7103\rho^2 + 3.8306\rho^3 + \right. \\ \quad \left. 0.7365\rho^4 \right) \sin \theta e^{i\phi}, \\ E_{4,1,1} = 44.1096. \end{array} \right. \quad (4.60)$$

• **For $n = 5$**

The roots of the coefficient b_6 are

$$\omega_{5,0} = -12.4108, \quad (4.61)$$

$$\omega_{5,1} = -5.7704, \quad (4.62)$$

$$\omega_{5,2} = 0.8386, \quad (4.63)$$

$$\omega_{5,3} = 7.845, \quad (4.64)$$

$$\omega_{5,4} = 23.831, \quad (4.65)$$

$$\omega_{5,5} = 15.4893, \quad (4.66)$$

choosing the root $\omega_{5,4}$ yields the following approximate bound state and energy as

$$\left\{ \begin{array}{l} \psi_{5,1,1}(\rho, \theta, \phi) = e^{-\frac{\rho^2}{2} + 1.9882\rho} \left(1 + 5.9577\rho + 12.0134\rho^2 + 10.6033\rho^3 \right. \\ \quad \left. + 4.1915\rho^4 + 0.6035\rho^5 \right) \sin \theta e^{i\phi}, \\ E_{5,1,1} = 50.4342, \end{array} \right. \quad (4.67)$$

• **For $n = 6$**

The roots of the coefficient b_7 are

$$\omega_{6,0} = -15.6576, \quad (4.68)$$

$$\omega_{6,1} = -8.6833, \quad (4.69)$$

$$\omega_{6,2} = -1.9157, \quad (4.70)$$

$$\omega_{6,3} = 5.0628, \quad (4.71)$$

$$\omega_{6,4} = 29.6109, \quad (4.72)$$

$$\omega_{6,5} = 12.5781, \quad (4.73)$$

$$\omega_{6,6} = 20.7565, \quad (4.74)$$

choosing the root $\omega_{6,5}$ yields the following approximate bound state and energy as

$$\left\{ \begin{array}{l} \psi_{6,1,1}(\rho, \theta, \phi) = e^{-\frac{\rho^2}{2} + 1.9882\rho} \left(1 + 3.1445\rho + 2.13\rho^2 - 0.7291\rho^3 - 0.7808\rho^4 + \right. \\ \quad \left. 0.0191\rho^5 + 0.0588\rho^6 \right) \sin \theta e^{i\phi}, \\ E_{6,1,1} = 56.7587, \end{array} \right. \quad (4.75)$$

for the following variable $\rho = 5.0297 * 10^{-7} r$.

Comparison

In the absence of the centrifugal term and the generalized Cornell potential, we compare the estimated energy eigenvalues calculated for the generalized Cornell plus Morse potential (4.41) with alternative values (for the value $l = 0$).

Let be the nergy levels that are computed in [66] for $l = 0$ are given by

$$E_{n,0,0} = -\frac{\lambda^2}{2M} \left(\frac{\sqrt{2MD}}{\lambda} - n - \frac{1}{2} \right)^2, \quad (4.76)$$

where the approximate energy levels of the generalized Cornell plus Morse potential are written for the parameters of Morse potential in the reference [66] for the following parameters

$$V_0 = De^{2\lambda r_0}, \quad (4.77)$$

$$V_1 = -2De^{\lambda r_0}. \quad (4.78)$$

then, writing the approximate energy eigenvalues in (4.41) in the absence of the terms of the generalized Cornell potential gives

$$E_{n,0,0} = -D + \lambda e^{\lambda r_0} \sqrt{\frac{D}{2M}} (2 + 2n \pm 1). \quad (4.79)$$

By comaring the approximate energy eigenvalues in (4.76) and those in (4.79), we deduce that they are different.

4.4.2 The generalized Pöschl-Teller potential

Pöschl-Teller potential is one of the famous models in quantum mechanics that are exactly solvable, it is a crucial potential that has many application in chemistry and spectroscopy, it can represent the interaction between particles, atoms and molecules, it is a realistic model that is used in

anharmonic molecular vibrations, it allows the prediction of vibrational spectra of molecules, it introduces anharmonicity in the vibrational energy levels, it is a good approximation for the potential energy surface, it can describe potential wells or potential barriers. Many formulas exist for Pöschl-Teller potential that the researchers treated in their papers, where You et al obtained solutions to the Schrödinger equation for the second Pöschl-Teller potential [69], Yahya and Oyewumi obtained approximate l -state solutions to Schrödinger equation for the Pöschl-Teller like potential [70], Assi et al obtained solutions for Schrödinger equation in D-dimension for the hyperbolic Pöschl-Teller potential plus modified ring-shaped term [71].

In this part, we are interested in the generalized Pöschl-Teller potential that is given in [72] where its expression is given by

$$V_e(r) = \frac{V_2}{\sinh^2 \lambda r} - \frac{V_3 \cosh \lambda r}{\sinh^2 \lambda r}, \quad V_2 > V_3, \quad (4.80)$$

in which V_2, V_3, λ are related to the properties of the potential.

to obtain the potential that we resolve the radial equation for, we substitute this exponential potential of Pö in (4.1) to get

$$V(r) = \frac{a_{-2}}{r^2} + \frac{a_{-1}}{r} + a_0 + a_1 r + a_2 r^2 + \frac{V_2}{\sinh^2 \lambda r} - \frac{V_3 \cosh \lambda r}{\sinh^2 \lambda r}, \quad (4.81)$$

then by inserting the central potential (4.81) in the radial equation (4.18) to get

$$-\frac{1}{2M} \frac{d^2 R_{n,l}(r)}{dr^2} + \left(\frac{\frac{l(l+1)}{2M} + a_{-2}}{r^2} + \frac{a_{-1}}{r} + a_0 + a_1 r + a_2 r^2 + \frac{V_2}{\sinh^2 \lambda r} - \frac{V_3 \cosh \lambda r}{\sinh^2 \lambda r} \right) R_{n,l}(r) = E R_{n,l}(r). \quad (4.82)$$

It is clear that the expression of the effective potential in the case of the generalized Cornell plus the generalized Pöschl-Teller potential makes

the solvability of the radial equation (4.82) hard to resolve analytically, for this reason, we use the following approximation scheme [73]

$$\frac{1}{\sinh \lambda r} \approx \frac{1}{\lambda r}, \quad (4.83)$$

where the figure below shows that the curves of the two functions $\frac{1}{\lambda r}$ and $\frac{1}{\sinh \lambda r}$

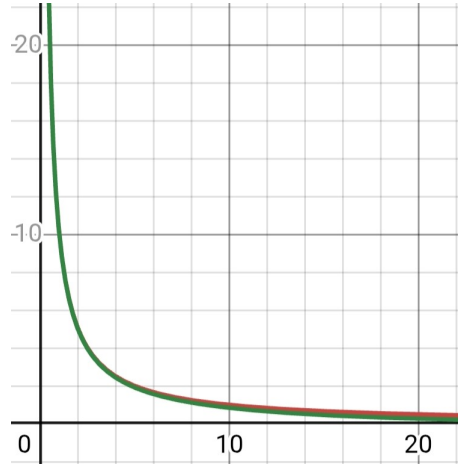


Figure 4.5: The curves of $\frac{1}{\lambda r}$ and $\frac{1}{\sinh \lambda r}$ for $\lambda = 0.1$

and this approximation scheme is used to approximate the effective potential to obtain an equation where the analytic solution are known, this approximation is appropriate for small values of the parameter λ where the left side is a good approximation of the right side.

By taking the term $\frac{1}{\sinh \lambda r}$ and approximating it by the term $\frac{1}{\lambda r}$ in the effective potential of the radial equation (4.82), we obtain the following equation

$$\frac{d^2 R_{n,l}(r)}{dr^2} + \left(\frac{A_2}{r^2} + \frac{B_2}{r} + C_2 + D_2 r + F_2 r^2 \right) R_{n,l}(r) = 0. \quad (4.84)$$

The differential equation (4.84) is the normal form of biconfluent Heun's equation for the following parameters

$$\begin{cases} A_2 = -2M\left(a_{-2} + \frac{V_2 - V_3}{\lambda^2}\right) - l(l+1), \\ B_2 = -2Ma_{-1}, \\ C_2 = 2M\left(E - a_0 + \frac{V_3}{2}\right), \\ D_2 = -2Ma_1, \\ F_2 = 2Ma_2. \end{cases} \quad (4.85)$$

Biconfluent Heun's equation in his normal form is transformed to the following canonical form

$$y \frac{d^2 P(y)}{dy^2} + \left(1 + \alpha_2 - \beta_2 y - 2y^2\right) \frac{dP(y)}{dy} + \left((\gamma_2 - \alpha_2 - 2)y - \frac{1}{2}(\delta_2 + (1 + \alpha_2)\beta_2)\right) P(y) = 0, \quad (4.86)$$

for this set of parameters

$$\begin{cases} \alpha_2 = \sqrt{4\left(l(l+1) + 2M\left(a_{-2} + \frac{V_2 - V_3}{\lambda^2}\right)\right)} + 1, \\ \beta_2 = a_1 \sqrt[4]{\frac{2M}{a_2^3}}, \\ \delta_2 = 2a_{-1} \sqrt[4]{\frac{8M^3}{a_2}}, \\ \gamma_2 = a_1^2 \sqrt{\frac{M}{8a_2^3}} + \left(E - a_0 + \frac{V_3}{2}\right) \sqrt{\frac{2M}{a_2}}. \end{cases} \quad (4.87)$$

The canonical equation 4.86 has polynomial solutions in the following form

$$P(y) = \sum_{k \geq 0}^n \frac{\Gamma(1 + \alpha_2) b_k}{\Gamma(1 + \alpha_2 + k)} \frac{y^k}{k!}, \quad (4.88)$$

where the coefficients b_k are related by the recurrence expression (4.26).

Here, only a finite number of the eigenfunctions can be written in ex-

plicit form, which means that the case here is quasi-exactly solvability of Schrödinger equation.

Now to obtain the energy eigenvalues, we return to the first condition in (4.27) which is given by

$$\gamma_2 - \alpha_2 - 2 = 2n, \quad (4.89)$$

to get the approximate energy values as

$$E_{n,l,m} = -\frac{a_1^2}{4a_2} + a_0 - \frac{V_3}{2} + \sqrt{\frac{a_2}{2M} \left(\sqrt{1 + 4(l(l+1) + 2M(a_{-2} + \frac{V_2 - V_3}{\lambda^2}))} + 2 + 2n \right)}, \quad (4.90)$$

for the condition $1 - 4A_2 \geq 0$ to have real values of the energy besides to the condition $F_2 > 0$.

As a result, the approximate wave function of Schrödinger equation in the case of the central potential: the generalized Cornell plus the generalized Pöschl-Teller potential is given by

$$\psi_{n,l,m}(\rho, \theta, \phi) = \rho^{\frac{\alpha_2-1}{2}} e^{-\frac{\rho^2+\beta_2\rho}{2}} \left(\sum_{k=0}^n \frac{\Gamma(1+\alpha_2)b_k}{\Gamma(1+\alpha_2+k)} \frac{\rho^k}{k!} \right) (1 - \cos^2 \theta)^{\frac{m}{2}} \cdot \frac{d^{l+m}}{d \cos \theta^{l+m}} (1 - \cos^2 \theta)^l e^{im\phi}, \quad (4.91)$$

for the following variable $\rho = \sqrt[4]{F_2}r$.

Numerical application for the approximate bound states of the generalized Pöschl-Teller potential

In order to give some examples of the approximate bound states for the case of the generalized Pöschl-Teller potential, we consider the following

numerical values of the parameters

$$\begin{cases} a_{-2} = a_1 = 0, \\ V_2 = 2, m = -1, \\ a_0 = a_2 = l = V_3 = 1, \lambda = 0.1, M = 0.01 \end{cases} \quad (4.92)$$

• **For $n = 1$**

The roots of the coefficient b_2 are

$$\omega_{1,0} = -2.1641, \quad (4.93)$$

$$\omega_{1,1} = 2.1641, \quad (4.94)$$

choosing the root $\omega_{1,1}$ gives the following approximate wave function and energy value

$$\begin{cases} \psi_{1,1,-1}(\rho, \theta, \phi) = \rho^{1.1708} e^{-\frac{\rho^2}{2}} (1 + 0.9242\rho) \sin \theta e^{-i\phi}, \\ E_{1,1,-1} = 119.9427. \end{cases} \quad (4.95)$$

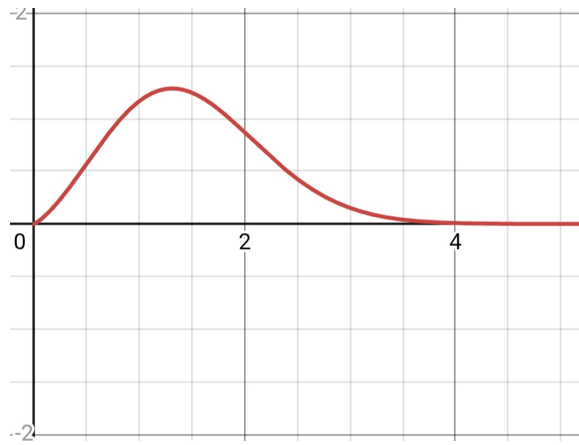


Figure 4.6: The graph of the radial part of $\psi_{1,1,-1}$

- For $n = 2$

The roots of the coefficient b_3 are

$$\omega_{2,0} = -4.7679, \quad (4.96)$$

$$\omega_{2,1} = 0, \quad (4.97)$$

$$\omega_{2,2} = 4.7679, \quad (4.98)$$

choosing the root $\omega_{2,1}$ gives the following approximate wave function and energy value

$$\begin{cases} \psi_{2,1,-1}(\rho, \theta, \phi) = \rho^{1.1708} e^{-\frac{\rho^2}{2}} (1 - 0.5985\rho^2) \sin \theta e^{-i\phi}, \\ E_{2,1,-1} = 164.6641. \end{cases} \quad (4.99)$$

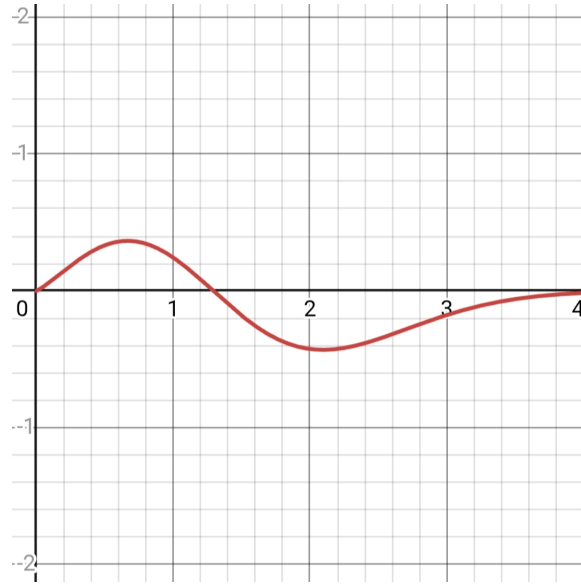


Figure 4.7: The graph of the radial part of $\psi_{2,1,-1}$

- For $n = 3$

The roots of the coefficient b_4 are

$$\omega_{3,0} = -7.7984, \quad (4.100)$$

$$\omega_{3,1} = -2.4532, \quad (4.101)$$

$$\omega_{3,2} = 2.4532, \quad (4.102)$$

$$\omega_{3,3} = 7.7984, \quad (4.103)$$

selecting the root $\omega_{3,2}$ gives the following approximate wave function and energy value

$$\begin{cases} \psi_{3,1,-1}(\rho, \theta, \phi) = \rho^{1.1708} e^{-\frac{\rho^2}{2}} \left(1 + 3.3303\rho + 2.9882\rho^2 + 0.7664\rho^3 \right) \sin \theta e^{-i\phi}, \\ E_{3,1,-1} = 209.3854. \end{cases} \quad (4.104)$$

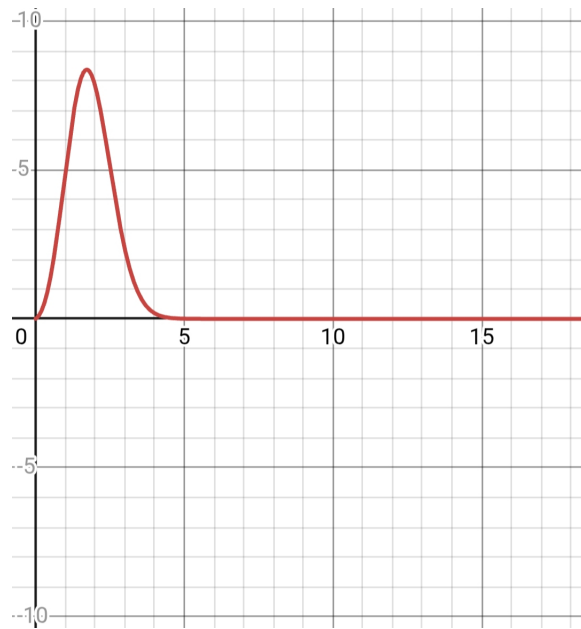


Figure 4.8: The graph of the radial part of $\psi_{3,1,-1}$

• For $n = 4$

The roots of the coefficient b_5 are

$$\omega_{4,0} = -11.2231, \quad (4.105)$$

$$\omega_{4,1} = -5.2639, \quad (4.106)$$

$$\omega_{4,2} = 0, \quad (4.107)$$

$$\omega_{4,3} = 5.2639, \quad (4.108)$$

$$\omega_{4,4} = 11.2231, \quad (4.109)$$

selecting the root $\omega_{4,0}$ gives the following approximate wave function and energy value

$$\begin{cases} \psi_{4,1,-1}(\rho, \theta, \phi) = \rho^{1.1708} e^{-\frac{\rho^2}{2}} \left(1 - 1.197\rho^3 + 0.2241\rho^5\right) \sin \theta e^{-i\phi}, \\ E_{4,1,-1} = 254.1068. \end{cases} \quad (4.110)$$

• **For $n = 5$**

The roots of the coefficient b_6 are

$$\omega_{5,0} = -15.0088, \quad (4.111)$$

$$\omega_{5,1} = -8.4522, \quad (4.112)$$

$$\omega_{5,2} = -2.6854, \quad (4.113)$$

$$\omega_{5,3} = 2.6854, \quad (4.114)$$

$$\omega_{5,4} = 8.4522, \quad (4.115)$$

$$\omega_{5,5} = 15.0088, \quad (4.116)$$

choosing the root $\omega_{5,3}$ gives the following approximate wave function

and energy value

$$\begin{cases} \psi_{5,1,-1}(\rho, \theta, \phi) = \rho^{1.1708} e^{-\frac{\rho^2}{2}} \left(1 + 1.1468\rho - 1.0355\rho^2 - 0.9179\rho^3 + 0.1754\rho^4 \right. \\ \quad \left. + 0.1306\rho^5 \right) \sin \theta e^{-i\phi}, \\ E_{5,1,-1} = 298.8282. \end{cases} \quad (4.117)$$

• **For $n = 6$**

The roots of the coefficient b_7 are

$$\omega_{6,0} = -19.1271, \quad (4.118)$$

$$\omega_{6,1} = -12.0064, \quad (4.119)$$

$$\omega_{6,2} = -5.6801, \quad (4.120)$$

$$\omega_{6,3} = 0, \quad (4.121)$$

$$\omega_{6,4} = 5.6801, \quad (4.122)$$

$$\omega_{6,5} = 12.0064 \quad (4.123)$$

$$\omega_{6,6} = 19.1271, \quad (4.124)$$

choosing the root $\omega_{6,3}$ gives the following approximate wave function and energy value

$$\begin{cases} \psi_{6,1,-1}(\rho, \theta, \phi) = \rho^{1.1708} e^{-\frac{\rho^2}{2}} \left(1 + 2.4257\rho + 0.2661\rho^2 - 1.7463\rho^3 - 0.5639\rho^5 + \right. \\ \quad \left. 0.2294\rho^5 + 0.0808\rho^6 \right) \sin \theta e^{-i\phi}, \\ E_{6,1,-1} = 3.43.5495, \end{cases} \quad (4.125)$$

for the following variable $\rho = 0.0095r$.

Comparison

We compare the approximate energy eigenvalues obtained in the case of the generalized Cornell plus the generalized Pöschl-Teller (4.90) without the generalized Cornell potential with other values obtained for the generalized Pöschl-Teller potential in this section. This means that the term $\frac{1}{\lambda r}$ is substituted with the term $\frac{1}{\sinh \lambda r}$.

Let consider the approximate energy levels that are obtained from the reference [74] as

$$E_{n,l,m} = -\frac{\lambda^2}{8} \left(\frac{1}{2\lambda} \left(\sqrt{8(V_2 + V_3) + \lambda^2} - \sqrt{8(V_2 - V_3) + \lambda^2(2l+1)^2} \right) - 1 - 2n \right), \quad (4.126)$$

at the other hand, the approximate energy levels in (4.90) for $a_{-2} = a_{-1} = a_0 = a_1 = a_2 = 0$ are given by

$$E_{n,l,m} = -\frac{V_3}{2}. \quad (4.127)$$

By comparing the approximate energy levels in (4.126) and the approximate energy levels in (4.127), we deduce that the values are totally different.

4.4.3 Yukawa class potential

One of the well-known exponential type potentials and a well-known model in quantum mechanics is the Yukawa potential. In particular, the Yukawa potential is significant in many different fields, it is a well known potential in many fields such as nuclear physics to describe the strong nuclear force between nucleons, in solid state physics to describe the interaction where the electric field is screened by surrounded charges and in plasma physics to describe the interaction between charged particles

[75]. As the most exponential type potentials, Yukawa potential is not exactly solvable model in non-relativistic quantum mechanics, where approximative techniques had been used to deal with Schrödinger for this potential [76]. When they resolved Schrodinger equation for exponential potentials, the researchers dealt with many classes of Yukawa potential, where Onate and Ojonubah obtained eigenfunctions and eigenvalues for Schrödinger equation using supersymmetric quantum mechanics for a class of Yukawa potential [77], Rajabi and Hamzavi constructed explicit approximate solutions for Schrödinger equation for the perturbed Yukawa potential with a centrifugal term using NU method [78], Okorie et al. obtained approximate solution to the Schrödinger equation for the modified Yukawa potential by transforming the radial equation to Gauss hypergeometric equation [79].

In this part, we are interested in the following Yukawa class [80] which is given by

$$V_e(r) = -\frac{V_4 e^{-2\lambda r}}{r^2} - \frac{V_5 e^{-\lambda r}}{r}. \quad (4.128)$$

In order to obtain the potential that we resolve the radial equation for, we substitute this exponential potential of Yukawa class in (4.1) to get

$$V(r) = \frac{a_{-2}}{r^2} + \frac{a_{-1}}{r} + a_0 + a_1 r + a_2 r^2 - \frac{V_4 e^{-2\lambda r}}{r^2} - \frac{V_5 e^{-\lambda r}}{r}, \quad (4.129)$$

then by inserting the central potential (4.129) in the radial equation (4.18) to get

$$-\frac{1}{2M} \frac{d^2 R_{n,l}(r)}{dr^2} + \left(\frac{\frac{l(l+1)}{2M} + a_{-2}}{r^2} + \frac{a_{-1}}{r} + a_0 + a_1 r + a_2 r^2 - \frac{V_4 e^{-2\lambda r}}{r^2} - \frac{V_5 e^{-\lambda r}}{r} \right) R_{n,l}(r) = E R_{n,l}(r). \quad (4.130)$$

It is clear that the expression of the effective potential in the case of the generalized Cornell plus Yukawa class potential makes the solvability of

the radial equation (4.130) not trivial to resolve analytically due to the combination of exponential terms and polynomial ones, for this reason, we use the following approximation scheme [59]

$$\frac{1}{1 - e^{-\lambda r}} \approx \frac{1}{\lambda r}, \quad (4.131)$$

for approximate the effective potential then obtain an equation where the solutions are known, such that this approximation is accurate for small values of the parameter λ where the left side is good approximation to the right one.

By taking the term $\frac{1}{1 - e^{-\lambda r}}$ and approximate it by the term $\frac{1}{\lambda r}$ in the effective potential of the radial equation (4.130), we obtain the following equation

$$\frac{d^2 R_{n,l}(r)}{dr^2} + \left(\frac{A_3}{r^2} + \frac{B_3}{r} + C_3 + D_3 r + F_3 r^2 \right) R_{n,l}(r) = 0. \quad (4.132)$$

The differential equation (4.132) is the normal form of biconfluent Heun's equation for the following parameters

$$\left\{ \begin{array}{l} A_3 = -2M(V_4 - a_{-2}) - l(l + 1), \\ B_3 = (V_5 - a_{-1} - 2V_4\lambda)2M, \\ C_3 = 2M(E - a_0 - V_5\lambda + V_4\lambda^2), \\ D_3 = -2Ma_1, \\ F_3 = 2Ma_2. \end{array} \right. \quad (4.133)$$

Biconfluent Heun's equation in his normal form is transformed to the following canonical form

$$y \frac{d^2 P(y)}{dy^2} + \left(1 + \alpha_3 - \beta_3 y - 2y^2 \right) \frac{dP(y)}{dy} + \left((\gamma_3 - \alpha_3 - 2)y - \frac{1}{2} \left(\delta_3 + (1 + \alpha_3)\beta_3 \right) \right) P(y) = 0, \quad (4.134)$$

for this set of parameters

$$\begin{cases} \alpha_3 = \sqrt{4(l(l+1) + 2M(a_{-2} - V_4))} + 1, \\ \beta_3 = a_1 \sqrt[4]{\frac{2M}{a_2^3}}, \\ \delta_3 = 2(a_{-1} + 2V_4\lambda - V_5) \sqrt[4]{\frac{8M^3}{a_2}}, \\ \gamma_3 = a_1^2 \sqrt[4]{\frac{M}{8a_2^3}} + \left(E - a_0 - V_5\lambda + V_4\lambda^2\right) \sqrt{\frac{2M}{a_2}}. \end{cases} \quad (4.135)$$

The canonical equation (4.134) has polynomial solutions in the following form

$$P(y) = \sum_{k=0}^n \frac{\Gamma(1 + \alpha_3) b_k}{\Gamma(1 + \alpha_3 + k)} \frac{y^k}{k!}, \quad (4.136)$$

And the recurrence expression (4.26) links the coefficients b_k . Hence only a portion of the eigenfunctions can be written in explicit form, which means that the case here is quasi-exactly solvability of Schrödinger equation.

Now to obtain the energy eigenvalues, we return to the first condition in (4.27) which is given by

$$\gamma_3 - \alpha_3 - 2 = 2n, \quad (4.137)$$

to get the approximate energy values for Yukawa class potential as

$$E_{n,l,m} = \left(\sqrt{1 + 4(l(l+1) + 2M(a_{-2} - V_4))} + 2 + 2n \right) \sqrt{\frac{a_2}{2M}} - \frac{a_1^2}{4a_2} + a_0 + \lambda(V_5 - V_4\lambda), \quad (4.138)$$

for the condition $1 - 4A_3 \geq 0$ to have real values of the energy besides to the condition $F_3 > 0$.

Then, the approximate wave function of Schrödinger equation in the case of the central potential: the generalized Cornell plus Yukawa class

potential is given by

$$\psi_{n,l,m}(\rho, \theta, \phi) = \rho^{\frac{\alpha_3-1}{2}} e^{-\frac{\rho^2+\beta_3\rho}{2}} \left(\sum_{k=0}^n \frac{\Gamma(1+\alpha_3)b_k}{\Gamma(1+\alpha_3+k)} \frac{\rho^k}{k!} \right) (1 - \cos^2 \theta)^{\frac{m}{2}} \cdot \frac{d^{l+m}}{d \cos \theta^{l+m}} (1 - \cos^2 \theta)^l e^{im\phi}, \quad (4.139)$$

for the following variable $\rho = \sqrt[4]{F_3}r$.

Numerical application for the approximate bound states of Yukawa class potential

We take into consideration the following numerical values of the parameters to provide some examples of the estimated bound states for the case of Yukawa class potential

$$\left\{ \begin{array}{l} a_{-2} = \frac{3}{2}, \quad V_5 = \frac{1}{4}, \\ a_1 = 0, \quad l = 3, \\ V_4 = a_2 = m = 2, \\ M = \lambda = a_0 = 1, \lambda = 0.001. \end{array} \right. \quad (4.140)$$

• For $n = 1$

The roots of the coefficient b_2 are

$$\omega_{1,0} = -3.9264, \quad (4.141)$$

$$\omega_{1,1} = 3.9264, \quad (4.142)$$

then, computing the approximate wave function and energy value for the root $\omega_{1,0}$ gives

$$\begin{cases} \psi_{1,3,2}(\rho, \theta, \phi) = \rho^{\frac{3\sqrt{5}-1}{2}} e^{-\frac{\rho^2}{2}} (1 + 0.5094\rho) \sin^2 \theta \cos \theta e^{2i\phi}, \\ E_{1,3,2} = 11.7085. \end{cases} \quad (4.143)$$

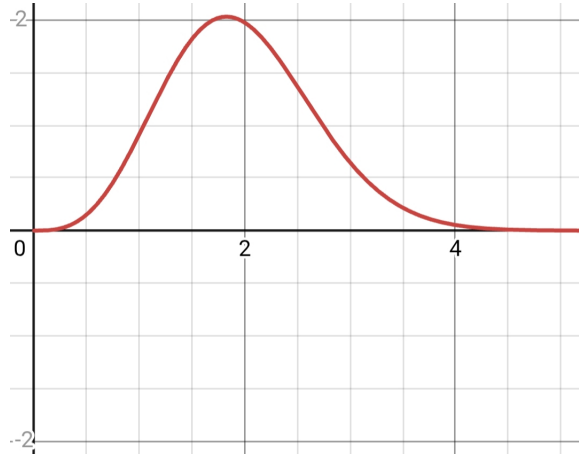


Figure 4.9: The graph of the radial part of $\psi_{1,3,2}$

• **For $n = 2$**

The roots of the coefficient b_3 are

$$\omega_{2,0} = -\sqrt{24\sqrt{5} + 12}, \quad (4.144)$$

$$\omega_{2,1} = 0, \quad (4.145)$$

$$\omega_{2,2} = \sqrt{24\sqrt{5} + 12} \quad (4.146)$$

then, computing the approximate wave function and energy value for the root $\omega_{2,0}$ gives

$$\begin{cases} \psi_{2,3,2}(\rho, \theta, \phi) = \rho^{\frac{3\sqrt{5}-1}{2}} e^{-\frac{\rho^2}{2}} (1 + 1.0513\rho + 0.2595\rho^2) \sin^2 \theta \cos \theta e^{2i\phi}, \\ E_{2,3,2} = 13.7085. \end{cases} \quad (4.147)$$

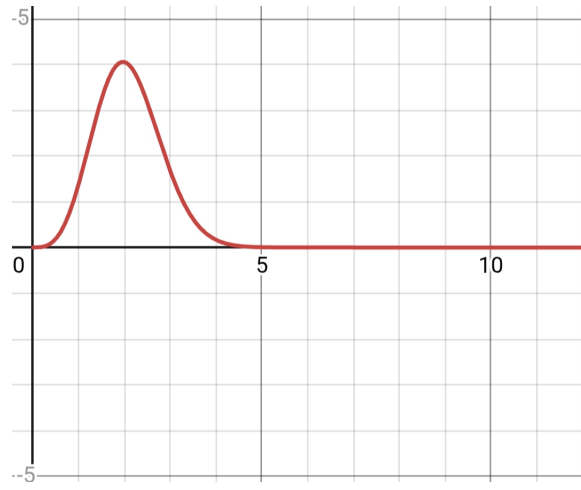


Figure 4.10: The graph of the radial part of $\psi_{2,1,1}$

• **For $n = 3$**

The roots of the coefficient b_4 are

$$\omega_{3,0} = -12.5302, \quad (4.148)$$

$$\omega_{3,1} = -4.1423, \quad (4.149)$$

$$\omega_{3,2} = 4.1423, \quad (4.150)$$

$$\omega_{3,3} = 12.5302 \quad (4.151)$$

then, computing the approximate wave function and energy value for the root $\omega_{3,1}$ gives

$$\begin{cases} \psi_{3,3,2}(\rho, \theta, \phi) = \rho^{\frac{3\sqrt{5}-1}{2}} e^{-\frac{\rho^2}{2}} \left(1 - 0.5374\rho - 0.2167\rho^2 + 0.1046\rho^3\right) \sin^2 \theta \cos \theta e^{2i\phi}, \\ E_{3,3,2} = 15.7085. \end{cases} \quad (4.152)$$

• **For $n = 4$**

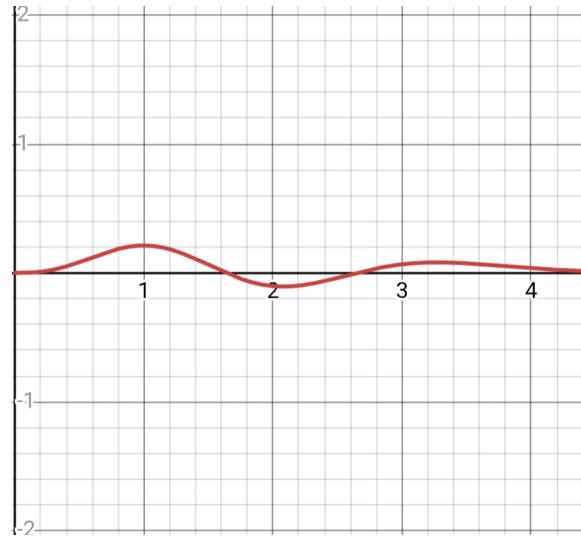


Figure 4.11: The graph of the radial part of $\psi_{3,1,1}$

The roots of the coefficient b_5 are

$$\omega_{4,0} = -17.2034, \quad (4.153)$$

$$\omega_{4,1} = -8.5071, \quad (4.154)$$

$$\omega_{4,2} = 0, \quad (4.155)$$

$$\omega_{4,3} = 8.5071, \quad (4.156)$$

$$\omega_{4,4} = 17.2034, \quad (4.157)$$

then, computing the approximate wave function and energy value for the root $\omega_{4,3}$ gives

$$\left\{ \begin{array}{l} \psi_{4,3,2}(\rho, \theta, \phi) = \rho^{\frac{3\sqrt{5}-1}{2}} e^{-\frac{\rho^2}{2}} \left(1 + 1.1036\rho + 0.0797\rho^2 - 0.2041\rho^3 \right. \\ \quad \left. - 0.048\rho^4 \right) \sin^2 \theta \cos \theta e^{2i\phi}, \\ E_{4,3,2} = 17.7085. \end{array} \right. \quad (4.158)$$

• For $n = 5$

The roots of the coefficient b_6 are

$$\omega_{5,0} = -22.1185, \quad (4.159)$$

$$\omega_{5,1} = -13.0979, \quad (4.160)$$

$$\omega_{5,2} = -4.3348, \quad (4.161)$$

$$\omega_{5,3} = 4.3348, \quad (4.162)$$

$$\omega_{5,4} = 13.0979, \quad (4.163)$$

$$\omega_{5,5} = 22.1185, \quad (4.164)$$

then, computing the approximate wave function and energy value for the root $\omega_{5,4}$ gives

$$\left\{ \begin{array}{l} \psi_{5,3,2}(\rho, \theta, \phi) = \rho^{\frac{3\sqrt{5}-1}{2}} e^{-\frac{\rho^2}{2}} \left(1 + 1.6992\rho + 0.7037\rho^2 - 0.1503\rho^3 - 0.1445\rho^4 - \right. \\ \qquad \qquad \qquad \left. 0.0221\rho^5 \right) \sin^2 \theta \cos \theta e^{2i\phi}, \\ E_{5,3,2} = 19.7085. \end{array} \right. \quad (4.165)$$

• **For $n = 6$**

The roots of the coefficient b_7 are

$$\omega_{6,0} = -27.2699, \quad (4.166)$$

$$\omega_{6,1} = -17.9158, \quad (4.167)$$

$$\omega_{6,2} = -8.8711, \quad (4.168)$$

$$\omega_{6,3} = 0, \quad (4.169)$$

$$\omega_{6,4} = 8.8711, \quad (4.170)$$

$$\omega_{6,5} = 17.9158, \quad (4.171)$$

$$\omega_{6,6} = 27.2699, \quad (4.172)$$

then, computing the approximate wave function and energy value for the root $\omega_{6,2}$ gives

$$\left\{ \begin{array}{l} \psi_{6,3,2}(\rho, \theta, \phi) = \rho^{\frac{3\sqrt{5}-1}{2}} e^{-\frac{\rho^2}{2}} \left(1 + 1.1509\rho - 0.1028\rho^2 - 0.4265\rho^3 - 0.0691\rho^4 \right. \\ \quad \left. + 0.0332\rho^5 + 0.0075\rho^6 \right) \sin^2 \theta \cos \theta e^{2i\phi}, \\ E_{6,3,2} = 21.7085, \end{array} \right. \quad (4.173)$$

for the variable $\rho = 2.8284r$

Comparison

In this part, we compare the approximate energy eigenvalues that are obtained in the case of the generalized Cornell plus Yukawa class potential (4.138) in the absence of the generalized Cornell potential with other values that are taken only for Yukawa class potential, such that the term $\frac{1}{\lambda r}$ is substituted by the term $\frac{1}{1-e^{-\lambda r}}$.

Writing the approximate energy eigenvalues that are obtained in the reference [81] and they are computed for Yukawa class potential using the NU method as follows

$$E_{n,l,m} = -\frac{\lambda^2 \left(-l(l+1) + \frac{MV_5}{2\lambda} - \frac{1}{2} - n(n+1) + 2(n+1) \sqrt{\frac{1}{4} - 2MV_4 + l(l+1)} \right)^2}{8M \left(n + \frac{1}{2} + \sqrt{l(l+1) + \frac{1}{4} - 2MV_4} \right)^2}. \quad (4.174)$$

This is obvious that the approximate energy eigenvalues (4.174) are not derived from the approximate energy levels (4.138) when the parameters $a_{-2} = a_{-1} = a_0 = a_1 = 0$ and $a_2 \rightarrow 0$.

4.4.4 Schiöberg potential

Schiöberg potential is an exponential potential function, it was proposed as a modification to existing potentials to improve the description of different interactions. Although this potential is not a recognized as other potentials like Morse and Yukawa potentials, Schiöberg potential has many applications in laboratory, where it is useful to understand energy levels and bound states of atoms and molecules, it models the vibrational spectra of diatomic molecules, the accuracy predictions for Schiöberg potential is improved for molecular vibrational states compared to other potentials. It helps in understanding the thermodynamic properties of physical systems.

In this part, we are interested in the following Schiöberg potential [82]

$$V_e(r) = K(1 - \sigma \coth \lambda r)^2, \quad \sigma > 0, K > 0. \quad (4.175)$$

In order to obtain the potential that we resolve the radial equation for, we substitute this exponential potential of Schiöberg in the expression

(4.1) to yield the following central potential

$$V(r) = \frac{a_{-2}}{r^2} + \frac{a_{-1}}{r} + a_0 + a_1 r + a_2 r^2 + K(1 - \sigma \coth \lambda r)^2, \quad (4.176)$$

Once the radial equation (4.18) has the central potential (4.176) included, we obtain

$$-\frac{1}{2M} \frac{d^2 R_{n,l}(r)}{dr^2} + \left(\frac{\frac{l(l+1)}{2M} + a_{-2}}{r^2} + \frac{a_{-1}}{r} + a_0 + a_1 r + a_2 r^2 + K(1 - \sigma \coth \lambda r)^2 \right) R_{n,l}(r) = E R_{n,l}(r). \quad (4.177)$$

It is clear that the expression of the effective potential in the case of the generalized Cornell plus Schiöberg potential makes the solvability of the radial equation (4.177) not trivial, hence the analytic solution is hard to obtain due to the combination of exponential terms and polynomial ones, for this reason, we use the following approximation scheme [73]

$$\frac{1}{\sinh \lambda r} \approx \frac{1}{\lambda r}, \quad (4.178)$$

to approximate the effective potential from equation (4.177) then an equation is obtained where the solutions are known, such that this approximation is accurate for small values of the parameter λ where the left side is good approximation to the right one.

By taking the term $\frac{1}{\sinh \lambda r}$ and approximate it by the term $\frac{1}{\lambda r}$ in the effective potential of the radial equation (4.177), we obtain the following equation

$$\frac{d^2 R_{n,l}(r)}{dr^2} + \left(\frac{A_4}{r^2} + \frac{B_4}{r} + C_4 + D_4 r + F_4 r^2 \right) R_{n,l}(r) = 0. \quad (4.179)$$

For the following parameters, Heun's equation in his biconfluent normal form is the differential equation (4.179)

$$\left\{ \begin{array}{l} A_4 = -2M\left(a_{-2} + \frac{\sigma^2 K}{\lambda^2}\right) - l(l+1), \\ B_4 = \left(\frac{2\sigma K}{\lambda} - a_{-1}\right)2M, \\ C_4 = 2M(E - a_0 - K(1 + \sigma^2)), \\ D_4 = 2M(K\sigma\lambda - a_1), \\ F_4 = 2M\left(a_2 + \frac{K\sigma^2\lambda^2}{4}\right). \end{array} \right. \quad (4.180)$$

Heun's equation in his biconfluent normal form is transformed to the following canonical form

$$y \frac{d^2 P(y)}{dy^2} + \left(1 + \alpha_4 - \beta_4 y - 2y^2\right) \frac{dP(y)}{dy} + \left((\gamma_4 - \alpha_4 - 2)y - \frac{1}{2}(\delta_4 + (1 + \alpha_4)\beta_4)\right) P(y) = 0, \quad (4.181)$$

for this set of parameters

$$\left\{ \begin{array}{l} \alpha_4 = \mp \sqrt{4\left(l(l+1) + 2M\left(a_{-2} + \frac{\sigma^2 K}{\lambda^2}\right)\right)} + 1, \\ \beta_4 = \left(a_1 - K\sigma\lambda\right) \sqrt[4]{\frac{2M}{\left(a_2 + \frac{K\sigma^2\lambda^2}{4}\right)^3}}, \\ \delta_4 = 2\left(a_{-1} - \frac{2K\sigma}{\lambda}\right) \sqrt[4]{\frac{8M^3}{a_2 + \frac{K\sigma^2\lambda^2}{4}}}, \\ \gamma_4 = \left(a_1 - K\sigma\lambda\right)^2 \sqrt{\frac{M}{8\left(a_2 + \frac{K\sigma^2\lambda^2}{4}\right)^3}} + \left(E - a_0 - K(1 + \sigma^2)\right) \sqrt{\frac{2M}{a_2 + \frac{K\sigma^2\lambda^2}{4}}}. \end{array} \right. \quad (4.182)$$

The canonical equation (4.181) has polynomial solutions in the following form

$$P(y) = \sum_{k=0}^n \frac{\Gamma(1 + \alpha_4) b_k}{\Gamma(1 + \alpha_4 + k)} \frac{y^k}{k!}, \quad (4.183)$$

And the recurrence expression (4.26) links the coefficients b_k . Here there is only a finite number of the eigenfunctions that can be written in explicit form, which means that the case here is quasi-exactly solvability of Schrödinger equation.

We go back to the first condition in 4.27 to get the energy eigenvalues, which is provided by

$$\gamma_4 - \alpha_4 - 2 = 2n, \quad (4.184)$$

to get the approximate energy values for Schiöberg potential as

$$E_{n,l,m} = \left(\mp \sqrt{4 \left(l(l+1) + 2M \left(a_{-2} + \frac{\sigma^2 K}{\lambda^2} \right) \right) + 1 + 2n + 2} \right) \sqrt{\frac{4a_2 + K\lambda^2\sigma^2}{8M}} - \frac{(K\sigma\lambda - a_1)^2}{4a_2 + K\lambda^2\sigma^2} + a_0 + K(1 + \sigma^2), \quad (4.185)$$

for the condition $1 - 4A_4 \geq 0$ to have real values of the energy besides to the condition $F_4 > 0$.

Then, the approximate wave function of Schrödinger equation in the case of the central potential: the generalized Cornell plus Schiöberg potential is given by

$$\psi_{n,l,m}(\rho, \theta, \phi) = \rho^{\frac{\alpha_4-1}{2}} e^{-\frac{\rho^2 + \beta_4 \rho}{2}} \left(\sum_{k=0}^n \frac{\Gamma(1 + \alpha_4) b_k}{\Gamma(1 + \alpha_4 + k)} \frac{\rho^k}{k!} \right) (1 - \cos^2 \theta)^{\frac{m}{2}} \cdot \frac{d^{l+m}}{d \cos \theta^{l+m}} (1 - \cos^2 \theta)^l e^{im\phi}, \quad (4.186)$$

for the following variable $\rho = \sqrt[4]{F_4} r$.

Numerical application for the approximate bound states of Schiöberg potential

We take into consideration the following numerical values of the parameters to provide some examples of the approximate eigensolutions for Schiöberg potential situation

$$\left\{ \begin{array}{l} K = 4, \quad a_{-2} = -1 \\ a_0 = 1, \lambda = 0.01, M = 0.0001, \\ a_1 = a_2 = l = m = 2, \\ \sigma = \frac{1}{2}. \end{array} \right. \quad (4.187)$$

• For $n = 1$

The roots of the coefficient b_2 are

$$\omega_{1,0} = -3.4047, \quad (4.188)$$

$$\omega_{1,1} = 3.4983, \quad (4.189)$$

then, computing the approximate wave function and energy value for the root $\omega_{1,1}$ gives

$$\left\{ \begin{array}{l} \psi_{1,2,2}(\rho, \theta, \phi) = \rho^{3.004} e^{-0.0636\rho - \frac{\rho^2}{2}} \left(1 - 0.5823\rho\right) \sin^2 \theta e^{2i\phi}, \\ E_{1,2,2} = 906.9497. \end{array} \right. \quad (4.190)$$

• For $n = 2$

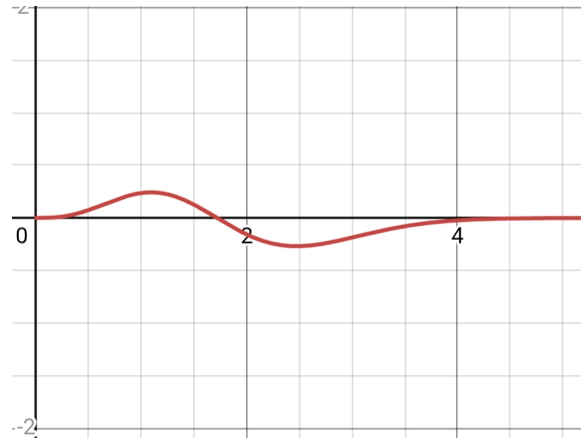


Figure 4.12: The graph of the radial part of $\psi_{1,2,2}$

The roots of the coefficient b_3 are

$$\omega_{2,0} = -7.2818, \quad (4.191)$$

$$\omega_{2,1} = -0.0587, \quad (4.192)$$

$$\omega_{2,2} = 7.1797, \quad (4.193)$$

then, computing the approximate wave function and energy value for the root $\omega_{2,2}$ gives

$$\begin{cases} \psi_{2,2,2}(\rho, \theta, \phi) = \rho^{3.004} e^{-0.0636\rho - \frac{\rho^2}{2}} \left(1 - 1.2120\rho + 0.3388\rho^2\right) \sin^2 \theta e^{2i\phi}, \\ E_{2,2,2} = 1107.1. \end{cases} \quad (4.194)$$

• **For $n = 3$**



Figure 4.13: The graph of the radial part of $\psi_{2,2,2}$

The roots of the coefficient b_4 are

$$\omega_{3,0} = -11.1438, \quad (4.195)$$

$$\omega_{3,1} = -3.7895, \quad (4.196)$$

$$\omega_{3,2} = 3.6123, \quad (4.197)$$

$$\omega_{3,3} = 11.1438, \quad (4.198)$$

then, computing the approximate wave function and energy value for the root $\omega_{3,2}$ gives

$$\begin{cases} \psi_{3,2,2}(\rho, \theta, \phi) = \rho^{3.004} e^{-0.0636\rho - \frac{\rho^2}{2}} \left(1 - 0.6308\rho - 0.2604\rho^2 + 0.1447\rho^3 \right) \sin^2 \theta e^{2i\phi}, \\ E_{3,2,2} = 1307.2. \end{cases} \quad (4.199)$$

• For $n = 4$

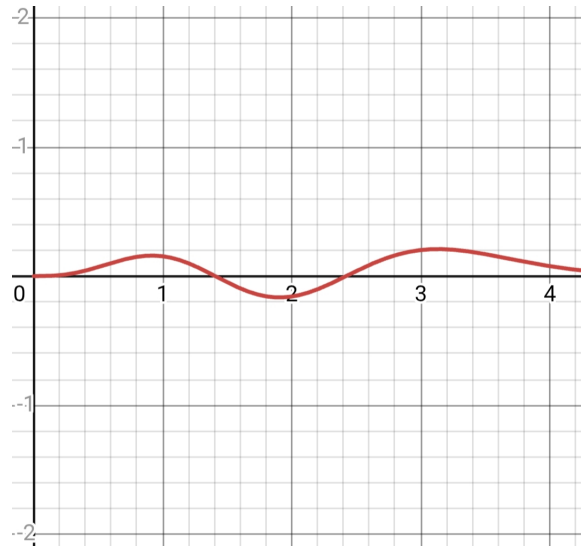


Figure 4.14: The graph of the radial part of $\psi_{3,2,2}$

The roots of the coefficient b_5 are

$$\omega_{4,0} = -15.6913, \quad (4.200)$$

$$\omega_{4,1} = -7.7686, \quad (4.201)$$

$$\omega_{4,2} = -0.1142, \quad (4.202)$$

$$\omega_{4,3} = 7.5263, \quad (4.203)$$

$$\omega_{4,4} = 15.412, \quad (4.204)$$

then, computing the approximate wave function and energy value for the root $\omega_{4,3}$ gives

$$\left\{ \begin{array}{l} \psi_{4,2,2}(\rho, \theta, \phi) = \rho^{3.004} e^{-0.0636\rho - \frac{\rho^2}{2}} \left(1 - 1.2931\rho + 0.1401\rho^2 + 0.2784\rho^3 \right. \\ \quad \left. - 0.0741\rho^4 \right) \sin^2 \theta e^{2i\phi}, \\ E_{4,2,2} = 1507.3. \end{array} \right. \quad (4.205)$$

• For $n = 5$

The roots of the coefficient b_6 are

$$\omega_{5,0} = -20.3034, \quad (4.206)$$

$$\omega_{5,1} = -12.0011, \quad (4.207)$$

$$\omega_{5,2} = -4.0484, \quad (4.208)$$

$$\omega_{5,3} = 3.7628, \quad (4.209)$$

$$\omega_{5,4} = 11.6895, \quad (4.210)$$

$$\omega_{5,5} = 19.947, \quad (4.211)$$

then, computing the approximate wave function and energy value for the root $\omega_{5,4}$ gives

$$\left\{ \begin{array}{l} \psi_{5,2,2}(\rho, \theta, \phi) = \rho^{3.004} e^{-0.0636\rho - \frac{\rho^2}{2}} \left(1 - 1.9976\rho + 0.9879\rho^2 + 0.1769\rho^3 - \right. \\ \quad \left. 0.2225\rho^4 + 0.0381\rho^5 \right) \sin^2 \theta e^{2i\phi}, \\ E_{5,2,2} = 1707.4. \end{array} \right. \quad (4.212)$$

• **For $n = 6$**

The roots of the coefficient b_7 are

$$\omega_{6,0} = -25.7406, \quad (4.213)$$

$$\omega_{6,1} = -16.4877, \quad (4.214)$$

$$\omega_{6,2} = -8.2047, \quad (4.215)$$

$$\omega_{6,3} = -0.1674, \quad (4.216)$$

$$\omega_{6,4} = 7.8564, \quad (4.217)$$

$$\omega_{6,5} = 16.1033, \quad (4.218)$$

$$\omega_{6,6} = 24.7406, \quad (4.219)$$

then, computing the approximate wave function and energy value for the root $\omega_{6,4}$ gives

$$\begin{cases} \psi_{6,2,2}(\rho, \theta, \phi) = \rho^{3.004} e^{-0.0636\rho - \frac{\rho^2}{2}} \left(1 - 1.3656\rho - 0.0629\rho^2 + 0.5896\rho^3 - 0.1172\rho^4 - \right. \\ \quad \left. 0.0521\rho^5 + 0.0133\rho^6 \right) \sin^2 \theta e^{2i\phi}, \\ E_{6,2,2} = 1907.6, \end{cases} \quad (4.220)$$

for the variable $\rho = 0.0028r$

Comparison

In this part, we compare the approximate energy eigenvalues obtained for the generalized Cornell plus Schiöberg potential with other values that were obtained for a situation of Schiöberg potential, where the $\frac{1}{\lambda r}$ is substituted with $\frac{1}{\sinh \lambda r}$.

We write the approximate energy eigenvalues that are obtained in [83]

using the asymptotic iteration method as

$$\begin{aligned}
E_{n,l,m} = & \left(\frac{(1-\sigma)^2 MK}{2\lambda^2} - \left((n+1)^2 + l(l+1) - 2\sigma(1-\sigma) \frac{MK}{\lambda^2} \right. \right. \\
& \left. \left. + (2n+1) \left(-\frac{1}{2} + \sqrt{\frac{1}{4} + 2\frac{MK\sigma^2}{\lambda^2} + l(l+1)} \right) \right)^2 \right. \\
& \left. / \left(4 \left(n + \frac{1}{2} + \sqrt{\frac{1}{4} + 2\frac{MK\sigma^2}{\lambda^2} + l(l+1)} \right)^2 \right) \right) \frac{2\lambda^2}{M}. \quad (4.221)
\end{aligned}$$

Hence the approximate energy levels (4.221) cannot be a limit case of the approximate energy eigenvalues (4.185) when the coefficients $a_{-2} = a_{-1} = a_0 = a_1 = a_2 = 0$.

4.4.5 Manning-Rosen potential

Manning-Rosen function is an exponential potential function, it is a well-known potential in quantum mechanics. In particular Manning-Rosen potential has an important role in physics and related domains, it has several applications in theoretical physics, such that in molecular physics Manning-Rosen potential often used to model the different interactions between diatomic molecules, it is helpful to describe the vibrational energy levels of molecules. Manning-Rosen potential attracted the attention of researchers where Ikhdair and Sever obtained approximate l -state solutions to the Schrödinger equation for Manning-Rosen potential, Qiang and Dong established approximate solutions of Manning-Rosen potential in the presence of the centrifugal term [85], Dong and García-Ravelo obtained exact solutions to the s -wave Schrödinger equation for the same potential [86].

We are interested in the Manning-Rosen potential that is given by [87]

$$V_e(r) = \frac{\lambda^2}{2M} \left(\frac{\xi(\xi-1)e^{-2\lambda r}}{(1-e^{-\lambda r})^2} - \frac{K_1 e^{-\lambda r}}{1-e^{-\lambda r}} \right). \quad (4.222)$$

To obtain the central potential that we resolve the radial equation for, we replace the exponential potential of Manning-Rosen in the expression (4.1) to have

$$V(r) = \frac{a_{-2}}{r^2} + \frac{a_{-1}}{r} + a_0 + a_1 r + a_2 r^2 + \frac{\lambda^2}{2M} \left(\frac{\xi(\xi-1)e^{-2\lambda r}}{(1-e^{-\lambda r})^2} - \frac{K_1 e^{-\lambda r}}{1-e^{-\lambda r}} \right), \quad (4.223)$$

then by inserting the central potential (4.223) in the radial equation (4.18) to get

$$-\frac{1}{2M} \frac{d^2 R_{n,l}(r)}{dr^2} + \left(\frac{\frac{l(l+1)}{2M} + a_{-2}}{r^2} + \frac{a_{-1}}{r} + a_0 + a_1 r + a_2 r^2 + \frac{\lambda^2}{2M} \left(\frac{\xi(\xi-1)e^{-2\lambda r}}{(1-e^{-\lambda r})^2} - \frac{K_1 e^{-\lambda r}}{1-e^{-\lambda r}} \right) \right) R_{n,l}(r) = E R_{n,l}(r). \quad (4.224)$$

It is clear that the expression of the effective potential in the case of the generalized Cornell plus Yukawa class potential makes the solvability of the radial equation (4.224) not trivial to resolve analytically due to the combination of exponential terms and polynomial ones, for this reason, we use the following approximation scheme [59]

$$\frac{1}{1-e^{-\lambda r}} \approx \frac{1}{\lambda r}, \quad (4.225)$$

for approximate the effective potential then obtain an equation where the solutions are known, such that this approximation is accurate when the values of λ are tiny where the left side is accurate approximation to the right one.

By taking the term $\frac{1}{1-e^{-\lambda r}}$ and approximate it by the term $\frac{1}{\lambda r}$ in the effective potential of the radial equation (4.224), we obtain the following equation

$$\frac{d^2 R_{n,l}(r)}{dr^2} + \left(\frac{A_5}{r^2} + \frac{B_5}{r} + C_5 + D_5 r + F_5 r^2 \right) R_{n,l}(r) = 0. \quad (4.226)$$

Heun's differential equation in its biconfluent normal form for the following parameters is the differential equation (4.226)

$$\begin{cases} A_5 = -2Ma_{-2} - l(l+1) + \xi(1-\xi), \\ B_5 = \lambda(K_1 + 2\xi(\xi-1)) - 2Ma_{-1}, \\ C_5 = 2M(E - a_0) + \lambda^2(\xi(1-\xi) - K_1), \\ D_5 = -2Ma_1, \\ F_5 = 2Ma_2. \end{cases} \quad (4.227)$$

The normal form is transformed to the following canonical form

$$y \frac{d^2 P(y)}{dy^2} + \left(1 + \alpha_5 - \beta_5 y - 2y^2\right) \frac{dP(y)}{dy} + \left((\gamma_5 - \alpha_5 - 2)y - \frac{1}{2}(\delta_5 + (1 + \alpha_5)\beta_5)\right) P(y) = 0, \quad (4.228)$$

for this set of parameters

$$\begin{cases} \alpha_5 = \sqrt{4(l(l+1) + \xi(\xi-1) + 2Ma_{-2}) + 1}, \\ \beta_5 = a_1 \sqrt[4]{\frac{2M}{a_2^3}}, \\ \delta_5 = 2\left(a_{-1} - \lambda \frac{2\xi(\xi-1) + K_1}{2M}\right) \sqrt[4]{\frac{8M^3}{a_2}}, \\ \gamma_5 = a_1^2 \sqrt{\frac{M}{8a_2^3}} + \left(E - a_0 + \lambda^2 \frac{\xi(1-\xi) - K_1}{2M}\right) \sqrt{\frac{2M}{a_2}}. \end{cases} \quad (4.229)$$

The canonical equation (4.228) has polynomial solutions in the following form

$$P(y) = \sum_{k=0}^n \frac{\Gamma(1 + \alpha_5) b_k}{\Gamma(1 + \alpha_5 + k)} \frac{y^k}{k!}, \quad (4.230)$$

And the recurrence expression (4.26) links the coefficients b_k . Hence only a portion of the eigenfunctions can be written in explicit form,

which means that the case here is quasi-exactly solvability of Schrödinger equation.

We go back to the first condition in (4.27) to get the energy eigenvalues, which are provided by

$$\gamma_5 - \alpha_5 - 2 = 2n, \quad (4.231)$$

to get the approximate energies of Manning-Rosen potential as

$$E_{n,l,m} = \left(\sqrt{4(l(l+1) + \xi(\xi-1) + 2Ma_{-2} + 1)} + 2 + 2n \right) \sqrt{\frac{a_2}{2M}} - \frac{a_1^2}{4a_2} + a_0 + \lambda^2 \frac{\xi(\xi-1) + K_1}{2M}, \quad (4.232)$$

for the condition $1 - 4A_5 \geq 0$ to have real values of the energy besides to the condition $F_5 > 0$.

Then, the approximate wave function of Schrödinger equation in the case of the central potential: the generalized Cornell plus Manning-Rosen potential is given by

$$\psi_{n,l,m}(\rho, \theta, \phi) = \rho^{\frac{\alpha_5-1}{2}} e^{-\frac{\rho^2+\beta_5\rho}{2}} \left(\sum_{k=0}^n \frac{\Gamma(1+\alpha_5)b_k}{\Gamma(1+\alpha_5+k)} \frac{\rho^k}{k!} \right) (1 - \cos^2 \theta)^{\frac{m}{2}} \cdot \frac{d^{l+m}}{d \cos \theta^{l+m}} (1 - \cos^2 \theta)^l e^{im\phi}, \quad (4.233)$$

for the following variable $\rho = \sqrt[4]{F_5}r$.

Numerical application for the approximate bound states of Manning-Rosen potential

We take into consideration the following numerical values of the parameters to provide some examples of the estimated bound states for the

Manning-Rosen potential case

$$\begin{cases} a_{-2} = \xi = \frac{1}{2}, \\ a_0 = \frac{1}{3}, a_2 = 2, \\ a_1 = K_1 = M = m = l = 1, \lambda = 0.01. \end{cases} \quad (4.234)$$

• For $n = 1$

The roots of the coefficient b_2 are

$$\omega_{1,0} = -\frac{1}{2\sqrt{2}} - \sqrt{\frac{17}{8} + 4\sqrt{3}}, \quad (4.235)$$

$$\omega_{1,1} = -\frac{1}{2\sqrt{2}} + \sqrt{\frac{17}{8} + 4\sqrt{3}}, \quad (4.236)$$

then, computing the approximate wave function and energy value for the root $\omega_{1,1}$ yields

$$\begin{cases} \psi_{1,1,1}(\rho, \theta, \phi) = \rho^{\sqrt{3}-\frac{1}{2}} e^{-\frac{\rho^2}{2}} (1 + 0.5948\rho) \sin \theta e^{i\phi}, \\ E_{1,1,1} = 7.6725. \end{cases}$$

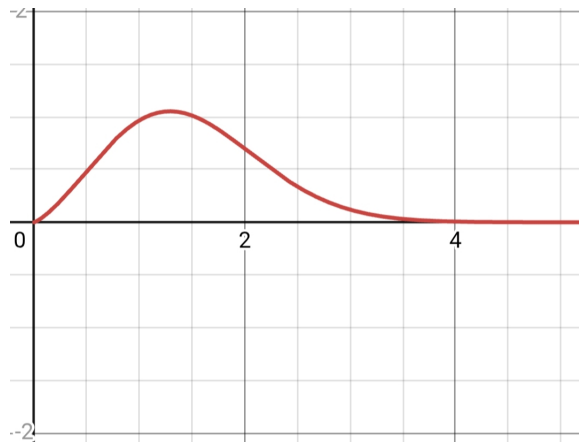


Figure 4.15: The graph of the radial part of $\psi_{1,1,1}$

(4.237)

- **For $n = 2$**

The roots of the coefficient b_3 are

$$\omega_{2,0} = -7.0833, \quad (4.238)$$

$$\omega_{2,1} = -0.6358, \quad (4.239)$$

$$\omega_{2,2} = 5.5988, \quad (4.240)$$

then, computing the approximate wave function and energy value for the root $\omega_{2,1}$ gives

$$\begin{cases} \psi_{2,1,1}(\rho, \theta, \phi) = \rho^{\sqrt{3}-\frac{1}{2}} e^{-\frac{\rho^2}{2}} \left(1 - 0.1426\rho - 0.3669\rho^2\right) \sin \theta e^{i\phi}, \\ E_{2,1,1} = 9.7625. \end{cases} \quad (4.241)$$

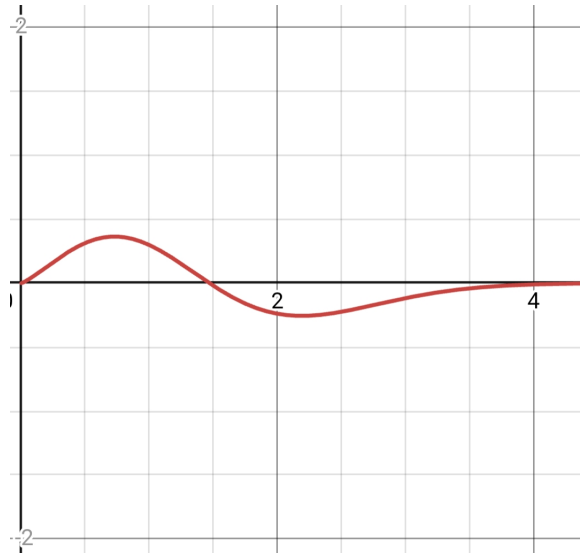


Figure 4.16: The graph of the radial part of $\psi_{2,1,1}$

- **For $n = 3$**

The roots of the coefficient b_4 are

$$\omega_{3,0} = -11.1484, \quad (4.242)$$

$$\omega_{3,1} = -4.2307, \quad (4.243)$$

$$\omega_{3,2} = 2.2996, \quad (4.244)$$

$$\omega_{3,3} = 8.8368, \quad (4.245)$$

then, computing the approximate wave function and energy value for the root $\omega_{3,2}$ gives

$$\begin{cases} \psi_{3,1,1}(\rho, \theta, \phi) = \rho^{\sqrt{3}-\frac{1}{2}} e^{-\frac{\rho^2}{2}} \left(1 + 0.5151\rho - 0.4073\rho^2 - 0.1843\rho^3 \right) \sin \theta e^{i\phi}, \\ E_{3,1,1} = 11.7625. \end{cases} \quad (4.246)$$

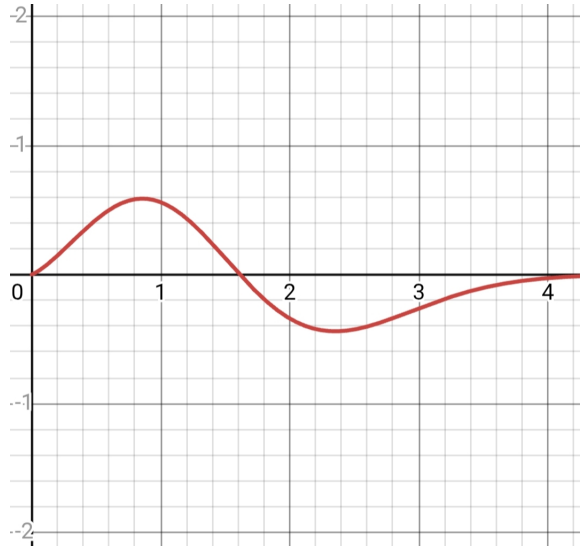


Figure 4.17: The graph of the radial part of $\psi_{3,1,1}$

- **For $n = 4$**

The roots of the coefficient b_5 are

$$\omega_{4,0} = -15.5398, \quad (4.247)$$

$$\omega_{4,1} = -8.1377, \quad (4.248)$$

$$\omega_{4,2} = -1.2326, \quad (4.249)$$

$$\omega_{4,3} = 5.4713, \quad (4.250)$$

$$\omega_{4,4} = 13.7625, \quad (4.251)$$

then, computing the approximate wave function and energy value for the root $\omega_{4,3}$ gives

$$\begin{cases} \psi_{4,1,1}(\rho, \theta, \phi) = \rho^{\sqrt{3}-\frac{1}{2}} e^{-\frac{\rho^2}{2}} \left(1 + 1.2256\rho - 0.0391\rho^2 - 0.3931\rho^3 \right. \\ \quad \left. - 0.0947\rho^4 \right) \sin \theta e^{i\phi}, \\ E_{4,1,1} = 15.7625. \end{cases} \quad (4.252)$$

• **For $n = 5$**

The roots of the coefficient b_6 are

$$\omega_{5,0} = -20.1851, \quad (4.253)$$

$$\omega_{5,1} = -12.3568, \quad (4.254)$$

$$\omega_{5,2} = -5.0292, \quad (4.255)$$

$$\omega_{5,3} = 1.9385, \quad (4.256)$$

$$\omega_{5,4} = 8.8955, \quad (4.257)$$

$$\omega_{5,4} = 16.1851, \quad (4.258)$$

then, computing the approximate wave function and energy value for the root $\omega_{5,4}$ gives

$$\begin{cases} \psi_{5,1,1}(\rho, \theta, \phi) = \rho^{\sqrt{3}-\frac{1}{2}} e^{-\frac{\rho^2}{2}} \left(1 + 1.9927\rho + 0.8359\rho^2 - 0.3776\rho^3 \right. \\ \quad \left. - 0.3073\rho^4 - 0.0494\rho^5 \right) \sin \theta e^{i\phi}, \\ E_{5,1,1} = 17.7625. \end{cases} \quad (4.259)$$

• **For $n = 6$**

The roots of the coefficient b_7 are

$$\omega_{6,0} = -25.2314, \quad (4.260)$$

$$\omega_{6,1} = -16.8794, \quad (4.261)$$

$$\omega_{6,2} = -9.1079, \quad (4.262)$$

$$\omega_{6,3} = -1.8008, \quad (4.263)$$

$$\omega_{6,4} = 5.31, \quad (4.264)$$

$$\omega_{6,4} = 12.5811, \quad (4.265)$$

$$\omega_{6,4} = 20.2792, \quad (4.266)$$

then, computing the approximate wave function and energy value for the root $\omega_{6,4}$ gives

$$\begin{cases} \psi_{6,1,1}(\rho, \theta, \phi) = \rho^{\sqrt{3}-\frac{1}{2}} e^{-\frac{\rho^2}{2}} \left(1 + 2.8183\rho + 2.3288\rho^2 + 0.2274\rho^3 - 0.512\rho^4 \right. \\ \quad \left. - 0.2187\rho^5 - 0.026\rho^6 \right) \sin \theta e^{i\phi}, \\ E_{6,1,1} = 19.7625, \end{cases} \quad (4.267)$$

for the variable $\rho = 2.8284r$.

Comparison

The energy eigenvalues obtained for the generalized Cornell plus Manning-Rosen potential are compared with other values obtained in the case of Manning-Rosen potential only in this section, where in the radial equation, the term $\frac{1}{\lambda r}$ is substituted with the term $\frac{1}{1-e^{-\lambda r}}$.

We write the approximate energy eigenvalues that are obtained in [red81] using Nikiforov-Uvarov method as

$$E_{n,l,m} = -\frac{\lambda^2}{8M} \frac{\left(K_1 - l(l+1) - \frac{1}{2} - n(n+1) + 2(n+1) \sqrt{\frac{1}{4} + \xi(\xi-1) + l(l+1)} \right)^2}{\left(n + \frac{1}{2} + \sqrt{\frac{1}{4} + \xi(\xi-1) + l(l+1)} \right)^2}. \quad (4.268)$$

It is clear that the values (blue4.268) are not a limit case

of the values (blue4.232) when $a_{-2} = a_{-1} = a_0 = a_1 = 0$
and $a_2 \rightarrow 0$.

CONCLUSION

The aim of this work is to establish approximate bound state of Schrödinger equation for some central potentials, where each potential is in the form the generalized Cornell potential plus an exponential potential, and in order to be more precise, the exponential potentials that we treated in this work are Manning-Rosen, Pöschl-Teller, Yukawa class, Morse and Schiöberg in the framework of quasi-exactly solvable problems. At the first place, we started by giving some mathematical notions that are the basis of quantum mechanics, then we introduced Schrödinger equation with some related properties and results such as the probabilistic interpretation of the wave function and the postulates of quantum mechanics, then we resolved approximately Schrodinger equation for some central potentials, for each potential, solving the radial equation is not trivial due to the combination of polynomial terms besides to exponential terms that appeared in the effective potential, hence, finding the exact solutions is not an easy task, for this reason we used for each case an approximation scheme that allowed us to transform the radial equation to the Heun's equation in his biconfluent normal, then the approximate eigenfunctions and the approximate energy levels are put in closed-form, at last for numerical values of the parameters, we computed some approximate eigenfunctions and energy eigenvalues.

For other works, we will try to resolve Schrödinger equation for other type of potentials central and non-central ones and we will try to extend the proposed method to treat other equations such as Dirac and Klein-Gordon

equations.

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