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## Contribution to the improvement of the semiinverse variational method

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## **Dedicate**

This piece of work is dedicated to my parents mam and dad my brothers and sisters, for having contributed a lot in my studies, for the sacrifices they have endured in life. May the Almighty grant them for everything they need. It is also dedicated to my wife and my kids Meriem EL Batoul and Mohamed Ousseyd.

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## Nomenclature

## Most used abbreviations

*ħ* Constant of Planck

 $\vec{\nabla}$  Kinetic energy operator

p the amount of movement

c Speed of light

H Hamiltonian

r The interatomic rayon

au Time

x Deplanement

K Harmonicity constant

 $\omega$  Pulsation

 $a, a^+$  Auxiliary operators

 $f_{nk}$ ,  $g_{nk}(r)$  Wave functions

κ Relativistic quantum number

 $\Delta(r), \Sigma(r)$  Potentials equation

m, M,μ Mass

k Constant of wave function

 $\alpha, \beta$  Dirac matric constants

△ Laplacian

Ec Kinetic energy

 $E_P$  Potential energy

1 Quantum number

 $\theta, \varphi$  Angles

M The mass of particle

S Scalar potential

V Vector potential

 $t, E, \mathcal{E}$  Energy

R Radial wave function

P Polynomial

G LaGrange test function

L Lagrangian

 $\Omega$  Variables

R' first derivation of R

R' Second derivation of R

U Euler equation

g Auxiliary component

Y first part of Euler equation

f determined function.

a, b, f<sub>0</sub> Lagrange equation constants

A, B Potential function

 $\delta$  Strength of Potential

p Constant of power

 $\alpha$  Screening paramater

 $\psi, \varphi, U, Y$  Wave function

 $\lambda$  Constant of perturbation

e Charge of electron

A(r,t) Normalization

 $S(r,t),\emptyset(x)$  Ansatz function

 $\sigma_0, \sigma_1, \sigma_2 \dots$  Wave function parameter

g Polynomial

 $A_1, A_2, B_1, B_2$  Kratzer potential parameter

## **Abstract**

In order to determine the wave functions and accompanying energy, this study is based on the solution of the radial Schrödinger equation. The semi-inverse variational approach, an approximation method, is presented in this work. This approach is applied to different potentials into the most well-known equations which are the Schrödinger, Klein Gordon, and Dirac equations, to determine the solution of the energy eigenvalues and associated wave functions. To demonstrate the accuracy of the computation and the viability of the method, we provided specific instances. Comparing the results of the study with those from other power ways, the information gathered demonstrates the efficacity and precision of the procedure.

**Keywords**: Schrödinger equation, Klein Gordon, Dirac equation, semi-inverse variational approach, eigenvalues

## ملخص

من أجل تحديد وظائف الموجة و مستويات الطاقة ، تستند هذه الدراسة إلى حل معادلة شرودنغر الشعاعية حيث يتم تقديم طريقة التباين شبه العكسي و هي طريقة تقريبية ، في هذا البحث , يتم تطبيق هذا التقريب على حل المعادلات الأكثر شهرة وهي معادلات شرودنجر وكلاين جوردون وديراك بوجود كمونات مختلفة ، لتحديد حل القيم الذاتية للطاقة و دالات الموجة المرتبطة بها. لإثبات دقة الحساب وجدوى الطريقة ، قدمنا حالات محددة و مختلفة و بمقارنة هذه نتائج هذا العمل مع تلك الناتجة عن طرق أخرى فعالة، توضح المعلومات التي تم جمعها عن كفاءة ودقة الإجراءات المتبعة .

الكلمات المفتاحية: معادلة شرودنغر، كلاين جوردون، معادلة ديراك، طريقة التباين شبه العكسي، القيم الذاتية للطاقة

## Resumé

Afin de déterminer les fonctions d'onde et l'énergie qui les accompagne, cette étude est basée sur la solution de l'équation radiale de Schrödinger. L'approche variationnelle semi-inverse, une méthode d'approximation, est présentée dans ce travail. Cette approche est appliquée à différents potentiels dans les équations les plus connues que sont les équations de Schrödinger, Klein Gordon et Dirac, pour déterminer la solution des valeurs propres de l'énergie et des fonctions d'onde associées. Pour démontrer la précision du calcul et la viabilité de la méthode, nous avons fourni des instances spécifiques. En comparant les résultats du travail avec ceux d'autres méthodes de puissance, les informations recueillies démontrent l'efficacité et la précision de la procédure.

**Mots clés** : équation de Schrödinger, Klein Gordon, équation de Dirac, approche variationnelle semi-inverse, valeurs propres

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# General Introduction

## **GENERAL INTRODUCTION**

Schrödinger's theory was tremendously influential in the development of quantum physics. Erwin Schrödinger proposed it for the first time in 1926, just after Heisenberg invented matrix mechanics. These two ideas were the first to formulate some quantum mechanics concepts [1-3].

We shall concentrate our efforts at the start of this work on the formulation of the Schrödinger equation for a specific physical condition, because studying a physical system consists primarily in solving its Schrödinger equation. In particular, the eigenvalues equation, which arises directly in various quantum physics issues, such as determining the energy levels of bound states.

In this thesis, we will look at the problem of bound states [4]. However, the symmetry features of the Hamiltonian can aid in its resolution. We picked a pompous and modern approach for this purpose: the semi-inverse variation method.

The resolution of the Schrödinger equation associated with a physical system is the foundation of quantum analysis [5-9]. This resolution is only possible in very specific instances where the Hamiltonian is sufficiently simple to be easily diagonalizable. In general, the Schrödinger equation is too difficult to find analytical solutions to. In this work, we employ one of the many approximations approaches available in quantum physics. These approximation approaches allow for the generation of analytically approximate solutions that are near to the genuine answers depending on the quality of the approximations and computations. Several approximation approaches for calculating the energy spectrum of the Schrödinger equation for numerous potential functions have been emerged in recent years [10-15].

Schrödinger employed variational theory as an approximation technique in his early research, which began at the very beginning of the establishment of quantum theory. Several researchers have utilized and developed variational approaches for bound state and diffusion issues since then.

In recent years, a considerable number of chemists and physicists have expressed an interest in contributing to the quest for approximate variational solutions to the Schrödinger equation. Hylleraas was the first to apply the variational principle to quantum systems about 70 years ago [16]. Since then, other advances have been reported in the literature.

In recent years, there has been a lot of interest in finding an exact solution to the Schrodinger equation for multiple potentials. Many researchers attempted to solve this equation using various potentials, including Yukawa [17], Morse [18], Rosen-Morse [19], Woods-Saxon [20], and anharmonic [21], with applications in nuclear structure, quantum chemistry, and quark confinement.

Professor He. Jihuan devised the semi-inverse approach in 1997 [22]. This approach was utilized for the first time to create variant formulations for fluid mechanics field equations. This approach is based on variation calculations. The semi-inverse variational approach is an effective mathematical tool for developing a variation formulation for a wave type differential equation. So far, this method provides an effective and best strategy for establishing variational principles for a wide range of physical issues.

Many strategies, such as factorization [23], were initially proposed by Schrödinger to tackle the algebraic issue of hydrogen atoms. Later, other approaches, such as Nikivorov-Uvarov [24], WKB [25], and Ansatz [26], were expanded to generate a broad class of soluble potentials.

The semi-inverse approach is thoroughly investigated, and several examples are provided to demonstrate how to develop a variational formulation for a nonlinear problem. We found that it is difficult to identify a variational principle for nonlinear evolution equations with nonlinear variables of any order based on the examples provided [27].

The goal of this study is to solve the Schrödinger equation using the semi-inverse variation approach, which is based on physical quantity variation to derive the Eigen functions and Eigen value.

The current thesis is divided into four sections. We shall start with an introduction chapter that will provide a quick summary of the Schrödinger equation in a central potential.

The second chapter directly covers the calculation of Schrödinger equation bound states using simple potentials such as the harmonic oscillator and hydrogen atom, then more complicated potentials using the semi-inverse variation approach.

In the third chapter, the same approach is used to determine the bound states of the Klein Gordon equation with other potentials, such as the Colombian and Kratzer potentials.

In the fourth chapter, we immediately present the determination of bound states of the Dirac equation using basic potentials such as the harmonic oscillator and the coulomb one, utilizing the two separate situations spin symmetry limit case and pseudo symmetry case.

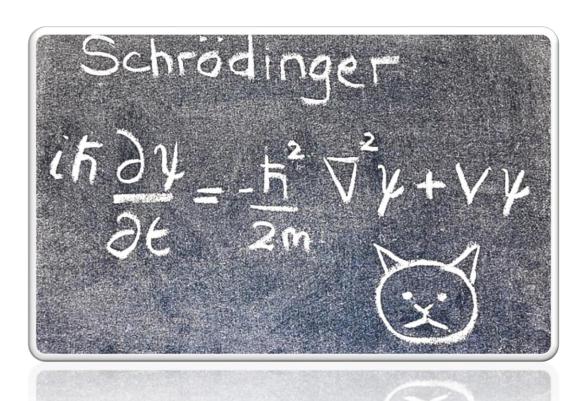
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## Chapter 01

Schrödinger equation in a central potential



## Chapter 1

## SCHRODINGER EQUATION IN CENTRAL POTENTIAL

## 1.1. Schrodinger equation:

Quantum mechanics is a well-known study having applications in atomic and molecular physics, light-matter interaction, solid and liquid state physics, materials science, and other fields. It substitutes observables for classical mechanics notions, which are represented by Hermitian linear operators operating on the wave function. Schrödinger's equation: the basic equation of quantum mechanics, defines the system's stationary states and temporal development. Schrödinger's equation is used in a variety of mathematical contexts, including partial differential equations, geometry, spectrum and scattering theory, and integral systems. It may be stated in two ways: the time-dependent Schrödinger equation and the time-independent Schrödinger equation, as illustrated in equation.

$$ih\frac{\partial\psi}{\partial t} = H(\vec{r},t)\psi(\vec{r},\tau) \tag{1.1}$$

With  $H = \frac{p^2}{2m} + V(\vec{r}, \tau)$  is the energy operation; and  $p = -i\hbar \vec{\nabla}$ 

The resolution of this equation gives us  $\psi(\vec{r}, \tau)$  which is the moment of the system, and we know  $\psi(\vec{r}, \tau)$  knows all its system.

The issue at hand is that we know how to solve the Schrödinger equation in extremely basic circumstances and in particular cases, such as the harmonic oscillator and the hydrogen atom.

To find solutions to the Schrödinger equation, we require approximation methods such as the perturbation method, variational, canonical transformation, and WKB is named after physicists Gregor Wentzel, Hendrik Anthony Kramers, and Léon Brillouin, who all developed it.

Consequently, the following are the wave functions, additionally referred to as eigenfunctions, that make up the solutions to equation (1.1):

$$\psi = \psi_0 e^{-\frac{iE\tau}{\hbar}} \tag{1.2}$$

Whither  $\psi_0$  is the amplitude.

The Schrödinger equation becomes the stationary Schrödinger equation for stationary states that exist independently of time.

$$H\psi(\vec{r}) = E\psi(\vec{r}) \tag{1.3}$$

Where E is the total energy of the system which bears the name of the eigenvalues.

The quantum operator representing the system's overall energy is called the Hamiltonian operator H:

$$H = E_c + V(r) = -\frac{\hbar^2}{2m} \triangle + V(r)$$
(1.4)

Whither V is the potential energy,  $E_c$  is the kinetic energy and  $\triangle$  is the Laplacian.

## 1.1.1. The stationary Schrödinger equation in one dimension

To determine the energy states and associated wave functions for a mass particle moving down an axis and bound by potential, we must solve the one-dimensional Schrödinger equation [2].

$$\left[ -\frac{\hbar^2}{2m} \frac{d^2}{d^2 x} + V(x) \right] \psi(x) = E\psi(x) \tag{1.5}$$

With  $-\infty < x < +\infty$ 

## 1.1.2. The stationary Schrödinger equation in two dimensions

The Schrödinger equation is stated as follows since the potential in this situation is dependent on two dimensions [3]:

$$\left[ -\frac{\hbar^2}{2m} \left( \frac{d^2}{d^2 x} + \frac{d^2}{d^2 y} \right) + V(x, y) \right] \psi(x, y) = E \psi(x, y)$$
 (1.6)

This particle is moving in a potential that is dependent on  $\vec{r}$  and  $V(\vec{r})$ , which may or may not be central. The spherical coordinates, which are more suited to the Laplacian  $\triangle$ , should be used instead, and they are denoted as follows:

$$\triangle = \frac{1}{r^2} \frac{\partial}{\partial r} \left( r^2 \frac{\partial}{\partial r} \right) - \frac{L^2}{\hbar^2 r^2} \tag{1.7}$$

With

$$l^{2} = -\hbar^{2} \left[ \frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \left( \sin \theta \frac{\partial}{\partial \theta} \right) + \frac{1}{\sin^{2} \theta} \frac{\partial^{2}}{\partial^{2} \varphi} \right]$$
 (1.8)

which makes it possible to write the Schrödinger equation for a central potential under the form:

$$\left\{ -\frac{\hbar^2}{2m} \left( \frac{1}{r^2} \frac{\partial}{\partial r} \left( r^2 \frac{\partial}{\partial r} \right) - \frac{L^2}{\hbar^2 r^2} \right) + \frac{-\hbar^2}{2m} \left[ \frac{1}{r^2 \sin \theta} \frac{\partial}{\partial \theta} \left( \sin \theta \frac{\partial}{\partial \theta} \right) + \frac{1}{r^2 \sin^2 \theta} \frac{\partial^2}{\partial^2 \varphi} \right] \right.$$

$$+ V(r) \left\{ \psi(r, \theta, \varphi) = E \psi(r, \theta, \varphi) \right\}$$
(1.9)

## **1.1.2.1.** Separation of variables:

The expression (1.9) shows that all the dependence on  $\theta$ ,  $\varphi$  is contained in the operator  $L^2$  With

$$[H, L^2] = 0 (1.10)$$

And

$$[H, L_z] = 0 (1.11)$$

The three observables  $H,\,L^2,L_z$  admit a complete system of proper functions so that we have

$$H\psi(r,\theta,\varphi) = E\psi(r,\theta,\varphi) \tag{1.12a}$$

$$L^{2}\psi(r,\theta,\varphi) = l(l+1)\hbar^{2}\psi(r,\theta,\varphi)$$
(1.12b)

$$L_{z}\psi(r,\theta,\varphi) = m\hbar\psi(r,\theta,\varphi) \tag{1.12c}$$

The specific functions common to  $L^2$ ,  $L_z$  corresponding to the values l and m of and fixed are the spherical harmonics  $Y_l^m(\theta, \varphi)$ . The functions  $\psi(r, \theta, \varphi)$  are therefore necessarily the product of a radial function R(r) by the spherical harmonic  $Y_l^m(\theta, \varphi)$ , that to say:

$$\psi(r,\theta,\varphi) = R(r)Y_l^m(\theta,\varphi) \tag{1.13}$$

using the fact that

$$L^{2}\psi(r,\theta,\varphi) = L^{2}R(r)Y_{l}^{m}(\theta,\varphi)$$
(1.14a)

$$= R(r)L^2Y_l^m(\theta, \varphi) \tag{1.14b}$$

$$= l(l+1)\hbar^2 R(r) Y_l^m(\theta, \varphi)$$
(1.15)

we end up with the following radial equation.

$$\left[ -\frac{\hbar^2}{2m} \left( \frac{1}{r^2} \frac{\partial}{\partial r} \left( r^2 \frac{\partial}{\partial r} \right) \right) + \frac{l(l+1)\hbar^2}{2mr^2} + V(r) \right] R(r) = ER(r)$$
 (1.15)

With l is the orbital quantum number

## 1.2. Schrödinger's equation in a central potential:

The velocity of a particle submerged in a central potential V(r), which relies solely on the coordinates' distance from the origin, is invariant for any rotation and hence exhibits spherical symmetry.

We have shown that the shape of the Laplacian in spherical dimensions is:

$$\triangle = \frac{1}{r^2} \frac{\partial}{\partial r} \left( r^2 \frac{\partial}{\partial r} \right) + -\frac{L^2}{\hbar^2 r^2}$$
 (1.15)

With

$$L_{x} = \frac{\hbar}{i} \left( \sin\varphi \frac{\partial}{\partial\theta} - \cot\theta \cos\varphi \frac{\partial}{\partial\varphi} \right)$$
 (1.16a)

$$L_{y} = \frac{\hbar}{i} \left( -\cos\varphi \frac{\partial}{\partial\theta} - \cot\theta \sin\varphi \frac{\partial}{\partial\varphi} \right)$$
 (1.16b)

$$L_z = \frac{\hbar}{i} \frac{\partial}{\partial \varphi} \tag{1.16c}$$

Wither  $L^2 = L_x^2 + L_y^2 + L_z^2$ 

The parameter I from equation (1.15) affects the radial functions. On the other hand, these functions have an eigenvalue  $E_{n,l}$  attached to them. Therefore,  $R_{n,l}$  may be used to represent the radial functions. The major quantum number and the quantum number, represented by the indices n, l, and  $n \ge l + 1$ , respectively,

The Schrödinger equation is revised to read:

$$\left[ -\frac{\hbar^2}{2m} \left( \frac{1}{r^2} \frac{\partial}{\partial r} \left( r^2 \frac{\partial}{\partial r} \right) + \frac{l(l+1)}{r^2} \right) + V(r) \right] R_{n,l} = E_{n,l} R_{n,l}$$
 (1.18)

Posing  $R_{n,l} = \frac{U_{n,l}}{r}$  and by multiplying the two sides of the equation by r, after some simplification, we obtain for  $U_{n,l}$  the following differential equation:

$$\left[ -\frac{\hbar^2}{2mr} \left( \frac{1}{r^2} \frac{\partial}{\partial r} \left( r^2 \frac{\partial}{\partial r} \right) + \frac{l(l+1)}{r^2} \right) + \frac{V(r)}{r} \right] U_{n,l} = \frac{E_{n,l}}{r} U_{n,l}$$
 (1.19)

By multiplying the two sides of the equation by r we find:

$$\left[ -\frac{\hbar^2}{2m} \left( \frac{\partial^2}{\partial r^2} + \frac{l(l+1)}{r^2} \right) + V(r) \right] U_{n,l} = E_{n,l} U_{n,l}$$
 (1.20)

We revise Schrödinger's equation. We see that for a particle with an effective potential as, Eq. (1.1), the Schrödinger equation in one dimension is entirely comparable to this equation.

$$V_{eff} = V(r) + \frac{\hbar^2 l(l+1)}{2mr^2}$$
 (1.21)

- The quantity is the centrifugal potential (the force tends to move the particle away from the centre of force O).
- This potential is zero for l=0 the particle can then come to O: we can see that  $R_{n,l} \neq 0$  for r=0.
- If  $l \neq 0$  this potential tends to infinity when r tends to zero:

$$V_{eff}(r) \rightarrow \infty$$
 when  $r \rightarrow 0$ 

The figure 1 represent the variation of coulomb and effective potential and their difference between them:

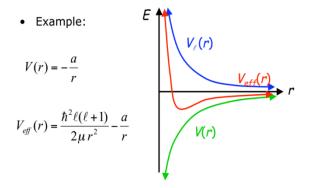


Fig.1.1: example of a potential

and prevents the particle from coming to O. We can see that:

$$R_{n,l} = 0$$
 for  $r = 0$  if  $l \neq 0$ 

In the following we will study the general characteristics of the solutions of the Schrödinger equation [4].

## 1.2.1. Behaviour at the origin of the solutions $(r \rightarrow 0)$ :

We know that, for r tending towards zero, the potential V(r) remains finite neither, or at least does not tend towards to infinity nor faster than  $\frac{1}{r}$ , where V(r) must satisfy the following condition [8]:

$$\lim r^2 V(r) = 0 \to V(r \to 0) = \frac{1}{r^\alpha} \text{ with } \alpha < 2$$
 (1.22)

Consider a solution of equation (1.20) and assume that it originally behaves like  $r^p$ :

$$U_{n,l}(r)_{r\to 0} = \alpha r^p \tag{1.23}$$

where  $\alpha$  is an arbitrary constant and p a power to be determined.

By deferring (1.23) in equation (1.20), and by equalling the coefficient of the dominant term to zero, we obtain the following equation:

$$-p(p-1) = l(l+1)$$
 (1.24)

this equality is verified for:

$$p = -l \tag{1.25a}$$

$$p = p = (l+1) (1.25b)$$

For a given value of  $E_{n,l}$ , we can therefore find two linearly independent solutions of the equation. The acceptable solutions of the equation cancel each other out regardless of l, as:

$$U_{n,l}(r)_{r\to 0} = \alpha r^{l+1} \tag{1.26}$$

Therefore, we must add to equation (1.20) the condition:

$$U_{n,l}(r) = 0 (1.27)$$

Therefore, we must retain the regular solutions which perform the function  $\psi_{n,l,m}(r,\theta,\varphi)$  that is to say a solution of the Schrödinger equation everywhere, including the origin.

## 1.2.2. Asymptotic behaviour

Suppose that the potential V(r) tends asymptotically towards zero faster than  $\frac{1}{r}$ 

$$\lim rV(r)_{r\to\infty} = 0 \tag{1.28}$$

equation (1.20) reduces to:

$$\frac{\partial^2}{\partial r^2} U_{n,l}(r) + k^2 U_{n,l_{r \to \infty}} = 0 \tag{1.29}$$

Whither  $k = \sqrt{\frac{2mE}{\hbar}}$  and because V(r) is cancelled at infinity and  $\frac{l(l+1)}{r^2}$  tends to zero, the energy spectrum has two parts:

If 
$$E < 0$$
:  $U_{n,l}(r) = exp(\pm kr)$ 

If 
$$E > 0$$
:  $U_{n,l}(r) = exp(\pm ikr)$ 

In the first case, we have  $R_{n,l}(r) = \frac{exp(\pm kr)}{r}$ , energy is quantified; it is a bound state and the exponential solution of the positive argument is to be rejected, but in the second case, we have  $R_{n,l}(r) = \frac{exp(\pm ikr)}{r}$ , and we find a divergent spherical wave expressing a well at the origin and the energy is continuous, we are then in a state of diffusion.

## **1.3.** Perturbation theory:

Most quantum mechanics issues have no analytic solution; only a few idealized situations have an accurate solution to the Schrodinger equation. As a result, developing approximation approaches is critical. The theory of disturbances deals with circumstances in which a slight variation from an ideal (solvent) system might explain the real physical system. The actual system's Hamiltonian H is thus expressed as [5]:

$$H = H_0 + V \tag{1.30}$$

or H and  $H_0$  differ little.  $H_0$  denote Hamiltonian of the non-disturbed system, while V represents a small perturbance.

a- We divide the operator H in two parts one  $H_0$  "simple" and independent of time, and verified the equation to  $V_{\alpha}$ 

$$H_0|\psi_{\alpha}\rangle = \mathcal{E}|\psi_{\alpha}\rangle \tag{1.31}$$

the second "small" part called perturbation.

b- We substitute in the Schrödinger equation and E we look for  $|\varphi(\vec{r},t)\rangle$  in terms of  $|\psi_{\alpha}(\vec{r},t)\rangle$  and the matrix elements of V

consider a physical system described by the energy operator.

$$H = \frac{P^2}{2m} + E_P(\vec{r}, \tau) \tag{1.32}$$

We divide H in two parts  $H=H_0+V$ , with  $H_0|\psi_{\alpha}\rangle=\mathcal{E}_{\alpha}|\psi_{\alpha}\rangle$  such that  $\mathcal{E}_{\alpha}$ ,  $|\psi_{\alpha}\rangle$  are known.

So, we resolve the equation:

$$H|\psi_{\alpha}\rangle = E_{\alpha}|\psi_{\alpha}\rangle \tag{1.33}$$

## 1.3.1. Rayleigh -Schrodinger method:

We write  $E_{\alpha}$  and  $|\varphi_{\alpha}\rangle$  as a series.

$$E_{\alpha} = E_{\alpha}^{(0)} + \lambda E_{\alpha}^{(1)} + \lambda^2 E_{\alpha}^{(2)} + \cdots$$
 (1.34)

$$\varphi_{\alpha} = \varphi_{\alpha}^{(0)} + \lambda \, \varphi_{\alpha}^{(1)} + \lambda^2 \, \varphi_{\alpha}^{(2)} + \cdots \tag{1.35}$$

With  $\lambda$  is a constant, in the end of calculation, we tend  $\lambda$  to 1

replacing in (1.34) and (1.35) equation (1.33)

$$H|\varphi_{\alpha}\rangle = E_{\alpha}|\varphi_{\alpha}\rangle \tag{1.36}$$

$$(H_0 + V)|\varphi_{\alpha}\rangle = E_{\alpha}|\varphi_{\alpha}\rangle \tag{1.37}$$

$$(H_0 + V) \Big( \varphi_{\alpha}^{(0)} + \lambda \, \varphi_{\alpha}^{(1)} + \lambda^2 \, \varphi_{\alpha}^{(2)} + \cdots \Big)$$

$$= \Big( E_{\alpha}^{(0)} + \lambda \, E_{\alpha}^{(1)} + \lambda^2 \, E_{\alpha}^{(2)} + \cdots \Big) \Big( \varphi_{\alpha}^{(0)} + \lambda \, \varphi_{\alpha}^{(1)} + \lambda^2 \, \varphi_{\alpha}^{(2)} + \cdots \Big)$$

$$(1.38)$$

by using the terms which have the same power of  $\lambda$  we will have:

$$\lambda^0 \to H_0 |\varphi_\alpha^{(0)}\rangle = E_\alpha^{(0)} |\varphi_\alpha^{(0)}\rangle \tag{1.39a}$$

$$\lambda^{1} \to H_{0} |\varphi_{\alpha}^{(1)}\rangle + V |\varphi_{\alpha}^{(0)}\rangle = E_{\alpha}^{(0)} |\varphi_{\alpha}^{(1)}\rangle + E_{\alpha}^{(1)} |\varphi_{\alpha}^{(0)}\rangle$$
 (1.39b)

$$\lambda^{2} \to H_{0} |\varphi_{\alpha}^{(2)}\rangle + V |\varphi_{\alpha}^{(1)}\rangle = E_{\alpha}^{(0)} |\varphi_{\alpha}^{(2)}\rangle + E_{\alpha}^{(1)} |\varphi_{\alpha}^{(1)}\rangle + E_{\alpha}^{(2)} |\varphi_{\alpha}^{(0)}\rangle$$
(1.39c)

$$\lambda^{n} \to H_{0}|\varphi_{\alpha}^{(n)}\rangle + V|\varphi_{\alpha}^{(n-1)}\rangle = E_{\alpha}^{(0)}|\varphi_{\alpha}^{(n)}\rangle + E_{\alpha}^{(1)}|\varphi_{\alpha}^{(n-1)}\rangle + \cdots E_{\alpha}^{(n)}|\varphi_{\alpha}^{(0)}\rangle$$
(1.39d)

by solving systems of equations, we will have  $E_{\alpha}^{(0)}$ ,  $E_{\alpha}^{(1)}$ , ...  $E_{\alpha}^{(n)}$  and  $|\varphi_{\alpha}^{(0)}\rangle$ ,  $|\varphi_{\alpha}^{(1)}\rangle$ , ...  $|\varphi_{\alpha}^{(n)}\rangle$  in terms of  $\mathcal{E}_{\alpha}$  and  $V_{\alpha\beta}$ 

we multiply on the left by  $\langle \psi_{\alpha} |$  , we find

$$E_{\alpha}^{(0)} = \mathcal{E}_{\alpha}^{0} = \langle \psi_{\alpha} | H_{0} | \psi_{\alpha} \rangle \tag{1.40a}$$

$$E_{\alpha}^{(1)} = \langle \psi_{\alpha} | V | \psi_{\alpha} \rangle \tag{1.40b}$$

$$E_{\alpha}^{(2)} = \left\langle \psi_{\alpha} \middle| V \middle| \varphi_{\alpha}^{(1)} \right\rangle \tag{1.40c}$$

perturbed order energy n

$$E_{\alpha}^{(n)} = \left\langle \psi_{\alpha} \middle| V \middle| \varphi_{\alpha}^{(n-1)} \right\rangle \tag{1.40d}$$

but

$$E_{\alpha} = E_{\alpha}^{(0)} + \lambda E_{\alpha}^{(1)} + \lambda^{2} E_{\alpha}^{(2)} + \cdots$$

$$= \mathcal{E}_{\alpha} + \lambda \langle \psi_{\alpha} | H_{0} | \psi_{\alpha} \rangle + \lambda^{2} \langle \psi_{\alpha} | V | \varphi_{\alpha}^{(1)} \rangle + \cdots \lambda^{n} \langle \psi_{\alpha} | V | \varphi_{\alpha}^{(n-1)} \rangle$$

$$= \mathcal{E}_{\alpha} + \lambda \langle \psi_{\alpha} | V | \left\{ \left| \varphi_{\alpha}^{(0)} \right\rangle + \lambda \left| \varphi_{\alpha}^{(1)} \right\rangle + \lambda^{2} | \varphi_{\alpha}^{(1)} \rangle + \cdots \lambda^{n-1} | \varphi_{\alpha}^{(n-1)} \rangle \right\}$$

$$= \mathcal{E}_{\alpha} + \lambda \langle \psi_{\alpha} | V | \varphi_{\alpha} \rangle \quad \lambda = 1$$

So

$$E_{\alpha} = \mathcal{E}_{\alpha} + \langle \psi_{\alpha} | V | \varphi_{\alpha} \rangle \tag{1.41}$$

## 1.3.2. Determining the perturbed states:

We have  $|\varphi_{\alpha}^{(0)}\rangle \equiv |\psi_{\alpha}\rangle$  then we develop  $|\varphi_{\alpha}^{(1)}\rangle$  in base of  $\{|\psi_{\alpha}\rangle\}$ 

$$|\varphi_{\alpha}^{(1)}\rangle = \sum_{l} |\psi_{l}\rangle \langle \psi_{\alpha} | \varphi_{\alpha}^{(1)}\rangle \tag{1.42a}$$

$$|\varphi_{\alpha}^{(1)}\rangle = \sum_{l} C_{l}^{(1)} |\psi_{l}\rangle \tag{1.42b}$$

by substituting (1.42b) in the  $2^{nd}$  equation of the previous system of equation (1.43):

$$H_0|\varphi_{\alpha}^{(1)}\rangle + V|\psi_{\alpha}\rangle = \mathcal{E}_{\alpha}|\varphi_{\alpha}^{(1)}\rangle + E_{\alpha}^{(1)}|\psi_{\alpha}\rangle \tag{1.43}$$

$$\sum_{l} C_{l}^{(1)} H_{0} |\psi_{l}\rangle + V |\psi_{\alpha}\rangle = \mathcal{E}_{\alpha} \sum_{l} C_{l}^{(1)} H_{0} |\psi_{l}\rangle + E_{\alpha}^{(1)} |\psi_{\alpha}\rangle \tag{1.44}$$

We multiply on the left by  $\langle \psi_{\beta} |$  , we find:

$$\sum_{l} C_{l}^{(1)} \mathcal{E}_{l} \delta_{\beta l} + \langle \psi_{\beta} | V | \psi_{\alpha} \rangle = \mathcal{E}_{\alpha} \sum_{l} C_{l}^{(1)} \delta_{\beta l} + E_{\alpha}^{(1)} \delta_{\beta \alpha}$$
(1.45)

$$C_{\beta}^{(1)} \mathcal{E}_{\beta} + V_{\beta \alpha} = \mathcal{E}_{\alpha} C_{\beta}^{(1)} + E_{\beta}^{(1)}$$
(1.46)

$$C_{\beta}^{(1)}(\mathcal{E}_{\alpha} - \mathcal{E}_{\beta}) = V_{\beta\alpha} \to C_{\beta}^{(1)} = \frac{V_{\beta\alpha}}{(\mathcal{E}_{\alpha} - \mathcal{E}_{\beta})}$$
(1.47)

Where

$$|\varphi_{\alpha}^{(1)}\rangle = \sum_{l} C_{l}^{(1)} |\psi_{l}\rangle \tag{1.48a}$$

$$|\varphi_{\alpha}^{(1)}\rangle = \sum_{l} \frac{V_{l\alpha}}{(\varepsilon_{\alpha} - \varepsilon_{l})} |\psi_{l}\rangle$$
 (1.48b)

therefore, the wave function of operator H is known to the order.

$$|\varphi_{\alpha}\rangle = |\psi_{\alpha}\rangle + \sum_{l} \frac{V_{l\alpha}}{(\varepsilon_{\alpha} - \varepsilon_{l})} |\psi_{l}\rangle$$
 (1.49)

to evaluate the energy of order 2 we substitute  $\varphi_{\alpha}$  in  $E_{\alpha}^{(2)}$ 

$$E_{\alpha}^{(2)} = \left\langle \psi_{\alpha} \middle| V \middle| \varphi_{\alpha}^{(1)} \right\rangle = \left\langle \psi_{\alpha} \middle| V \middle| \left\{ \sum_{l} \frac{V_{l\alpha}}{(\mathcal{E}_{\alpha} - \mathcal{E}_{l})} \middle| \psi_{l} \right\rangle \right\}$$
(1.50a)

$$E_{\alpha}^{(2)} = \sum_{l} \frac{V_{l\alpha} \langle \psi_{\alpha} | V | \psi_{l} \rangle}{(\mathcal{E}_{\alpha} - \mathcal{E}_{l})} \to E_{\alpha}^{(2)} = \sum_{l \neq \alpha} \frac{|V_{l\alpha}|^{2}}{(\mathcal{E}_{\alpha} - \mathcal{E}_{l})}$$
(1.50b)

So, we can determine  $|\varphi_{\alpha}^{(2)}\rangle$ 

$$|\varphi_{\alpha}^{(2)}\rangle = \sum_{l} C_{l}^{(2)} |\psi_{l}\rangle \tag{1.51}$$

Replacing  $|\varphi_{\alpha}^{(2)}\rangle$  by its value in equation (1.51) of equation system

$$H_0|\varphi_{\alpha}^{(2)}\rangle + V|\varphi_{\alpha}^{(1)}\rangle = E_{\alpha}^{(0)}|\varphi_{\alpha}^{(2)}\rangle + E_{\alpha}^{(1)}|\varphi_{\alpha}^{(1)}\rangle + E_{\alpha}^{(2)}|\varphi_{\alpha}^{(0)}\rangle$$
(1.52)

$$H_{0} \sum_{l} C_{l}^{(2)} |\psi_{l}\rangle + V \sum_{l} \frac{V_{l\alpha}}{(\varepsilon_{\alpha} - \varepsilon_{l})} |\psi_{l}\rangle$$

$$= \varepsilon_{\alpha} \sum_{l} C_{l}^{(2)} |\psi_{l}\rangle + V_{\alpha\alpha} \sum_{l} \frac{V_{l\alpha}}{(\varepsilon_{\alpha} - \varepsilon_{l})} |\psi_{l}\rangle + E_{\alpha}^{(2)} |\psi_{\alpha}\rangle$$
(1.53)

Multiplying by  $\langle \psi_{\beta} |$ 

$$\sum_{l} C_{l}^{(2)} \mathcal{E}_{\beta} \delta_{\beta l} + \sum_{l} \frac{V_{l\alpha} V_{\beta l}}{(\mathcal{E}_{\alpha} - \mathcal{E}_{l})} = \mathcal{E}_{\alpha} \sum_{l} \frac{V_{\alpha \alpha} V_{l\alpha} V_{\beta l}}{(\mathcal{E}_{\alpha} - \mathcal{E}_{l})} + \cdots$$
(1.54)

$$E_{\alpha}: \mathcal{E}_{\alpha} + V_{\alpha\alpha} + \sum_{l \neq \alpha} \frac{|V_{l\alpha}|^2}{(\mathcal{E}_{\alpha} - \mathcal{E}_l)} + \sum_{l} \frac{V_{\alpha l} V_{ll'} V_{l'\alpha}}{(\mathcal{E}_{\alpha} - \mathcal{E}_l)(\mathcal{E}_{\alpha} - \mathcal{E}_l)} + \cdots$$
(1.55)

$$|\varphi_{\alpha}\rangle = |\psi_{\alpha}\rangle + \sum_{l\neq\alpha} \frac{V_{l\alpha}}{(\varepsilon_{\alpha} - \varepsilon_{l})} |\psi_{l}\rangle + \sum_{l} \frac{V_{ll'}V_{l'\alpha}}{(\varepsilon_{\alpha} - \varepsilon_{l'})(\varepsilon_{\alpha} - \varepsilon_{l})} + |\psi_{l}\rangle \dots$$
(1.56)

## 1.3.3. Wigner – Brillouin (w-b) method:

We expose here a second method called (w-b) and is different from the previous one ,where H is energy operator with:  $H|\varphi_{\alpha}\rangle = E_{\alpha}|\varphi_{\alpha}\rangle$ 

We write *H* in the form  $H = H_0 + V$ 

With:  $H_0|\varphi_{\alpha}\rangle = E_{\alpha}|\varphi_{\alpha}\rangle$ ,  $\{|\psi_{\alpha}\rangle\}$  complete base

We search  $|\phi_{\alpha}\rangle$  with the form serial base  $\{|\psi_{\alpha}\rangle\}$ :

$$|\varphi_{\alpha}\rangle = C_{\alpha}|\psi_{\alpha}\rangle + \sum_{l\neq\alpha} C_{l}|\psi_{l}\rangle$$

We remark.

$$\left\langle \psi_{\alpha} \middle| \sum_{l \neq \alpha} C_l |\psi_l\rangle \middle| \varphi_{\alpha}^{(1)} \right\rangle = 0 = \sum_{l \neq \alpha} C_l \delta_{l\alpha}$$
 (1.57)

We suppose:  $C_{\alpha} = \langle \psi_{\alpha} | \varphi_{\alpha} \rangle = 1$ 

i.e., 
$$|\varphi_{\alpha}\rangle = |\psi_{\alpha}\rangle + \sum_{l\neq\alpha} C_l |\psi_l\rangle \dots (*)$$

back to the eigenvalue equation:

$$H|\varphi_{\alpha}\rangle = E_{\alpha}|\varphi_{\alpha}\rangle \tag{1.57}$$

$$(H_0 + V)|\varphi_{\alpha}\rangle = E_{\alpha}|\varphi_{\alpha}\rangle \tag{1.58}$$

$$V|\varphi_{\alpha}\rangle = (E_{\alpha} - H_0)|\varphi_{\alpha}\rangle \tag{1.59}$$

Multiplying in the left by  $\langle \psi_{\beta} |$ :

$$C_{\beta}^{(2)} \mathcal{E}_{\beta} + \sum_{l} \frac{V_{l\alpha} V_{\beta l}}{(\mathcal{E}_{\alpha} - \mathcal{E}_{l})} = C_{\beta}^{(2)} \mathcal{E}_{\alpha} + \frac{V_{\alpha \alpha} V_{\beta \alpha}}{(\mathcal{E}_{\alpha} - \mathcal{E}_{\beta})}$$
(1.60)

$$C_{\beta}^{(2)}(\mathcal{E}_{\alpha} - \mathcal{E}_{\beta}) = \sum_{l} \frac{V_{l\alpha}V_{\beta l}}{(\mathcal{E}_{\alpha} - \mathcal{E}_{l})} - \frac{V_{\alpha\alpha}V_{\beta\alpha}}{(\mathcal{E}_{\alpha} - \mathcal{E}_{\beta})}$$
(1.61)

Where

$$C_{\beta}^{(2)} = \sum_{l} \frac{V_{l\alpha}V_{\beta l}}{(\mathcal{E}_{\alpha} - \mathcal{E}_{l})(\mathcal{E}_{\alpha} - \mathcal{E}_{\beta})} - \frac{V_{\alpha\alpha}V_{\beta\alpha}}{(\mathcal{E}_{\alpha} - \mathcal{E}_{\beta})}$$
(1.62)

$$|\varphi_{\alpha}^{(2)}\rangle = \sum_{n} C_{n}^{(2)} |\psi_{n}\rangle = \left[\sum_{l} \frac{V_{l\alpha}V_{nl}}{(\varepsilon_{\alpha} - \varepsilon_{l})(\varepsilon_{\alpha} - \varepsilon_{n})} - \frac{V_{\alpha\alpha}V_{n\alpha}}{(\varepsilon_{\alpha} - \varepsilon_{n})^{2}}\right] |\psi_{n}\rangle$$
(1.63)

$$\langle \psi_{\beta} | V | \varphi_{\alpha} \rangle = [E_{\alpha} - \mathcal{E}_{\beta}] \langle \psi_{\beta} | \varphi_{\alpha} \rangle \tag{1.64}$$

Where

$$\langle \psi_{\beta} | \psi_{\beta} \rangle = \frac{1}{(E_{\alpha} - \mathcal{E}_{\beta})} \langle \psi_{\beta} | V | \varphi_{\alpha} \rangle = C_{\beta}$$
 (1.65)

And the expression \* decry

$$|\varphi_{\alpha}\rangle = |\psi_{\alpha}\rangle + \sum_{l \neq \alpha} \frac{1}{E_{\alpha} - \mathcal{E}_{\beta}} \langle \psi_{l} | V | \varphi_{\alpha} \rangle |\psi_{l}\rangle \tag{1.66}$$

We remark  $|\varphi_{\alpha}\rangle$  appears in both members:

to have all the terms of the series we successively substitute

$$|\varphi_{\alpha}\rangle = |\psi_{\alpha}\rangle + \sum_{l\neq\alpha} |\psi_{l}\rangle \frac{1}{(E_{\alpha} - E_{l})} \left\langle \psi_{l} \middle| V \middle| \left\{ |\psi_{\alpha}\rangle + \sum_{l'} |\psi_{l'}\rangle \frac{1}{(E_{\alpha} - E_{l'})} \langle \psi_{l'} | V | \varphi_{\alpha}\rangle \right\} \right\rangle$$
(1.67a)

$$|\varphi_{\alpha}\rangle = |\psi_{\alpha}\rangle + \sum_{l \neq \alpha} |\psi_{l}\rangle \frac{V_{l\alpha}}{E_{\alpha} - \mathcal{E}_{l}} + \sum_{l,l' \neq \alpha} |\psi_{l}\rangle \frac{V_{ll'}\langle\psi_{l}|V|\varphi_{\alpha}\rangle}{(E_{\alpha} - \mathcal{E}_{l'})(E_{\alpha} - \mathcal{E}_{l})}$$
(1.67b)

$$|\varphi_{\alpha}\rangle = |\psi_{\alpha}\rangle + \sum_{l \neq \alpha} |\psi_{l}\rangle \frac{1}{E_{\alpha} - \varepsilon_{l}} \left[ V_{l\alpha} + \sum_{l' \neq \alpha} \frac{V_{ll'}V_{l'\alpha}}{(E_{\alpha} - \varepsilon_{l'})} + \sum_{l,l'} \frac{V_{\alpha l'}V_{ll'}V_{l'\alpha}}{(E_{\alpha} - \varepsilon_{l'})(E_{\alpha} - \varepsilon_{l'})} \right]$$
(1.67c)

And eigenvalue of H,  $E_{\alpha}$  is written.

$$E_{\alpha} = \langle \psi_{\alpha} | H | \varphi_{\alpha} \rangle = \langle \psi_{\alpha} | H_{0} | \varphi_{\alpha} \rangle + \langle \psi_{\alpha} | V | \varphi_{\alpha} \rangle \tag{1.68a}$$

$$E_{\alpha} = \mathcal{E}_{\alpha} + \langle \psi_{\alpha} | V | \varphi_{\alpha} \rangle \tag{1.68b}$$

$$E_{\alpha} = \mathcal{E}_{\alpha} + V_{\alpha\alpha} + \sum_{l \neq \alpha} \frac{V_{\alpha l} V_{l\alpha}}{(E_{\alpha} - \mathcal{E}_{l})} + \sum_{l \neq \alpha} \frac{V_{\alpha l'} V_{ll'} V_{l'\alpha}}{(E_{\alpha} - \mathcal{E}_{l})(E_{\alpha} - \mathcal{E}_{l'})} + \cdots$$
(1.68c)

$$\langle \psi_{\beta} | V | \varphi_{\alpha} \rangle = (E_{\alpha} - \mathcal{E}_{l}) \langle \psi_{\beta} | \varphi_{\alpha} \rangle \tag{1.69}$$

With

$$\langle \psi_{\beta} | \varphi_{\alpha} \rangle = \frac{1}{(E_{\alpha} - \mathcal{E}_{\beta})} \langle \psi_{\beta} | V | \varphi_{\alpha} \rangle = C_{\beta}$$
 (1.70)

## **1.3.4.** Exact solution of equation of proper values:

the secularly equation  $H|\phi_{lpha}\rangle=E_{lpha}|\phi_{lpha}\rangle$  , we develop the solution  $|\phi_{lpha}\rangle$  on known base

$$|\varphi_{\alpha}\rangle = \sum_{l} C_{l} |\psi_{l}\rangle$$

With

$$H\sum_{l} C_{l} |\psi_{l}\rangle = E_{\alpha} C_{l} |\psi_{l}\rangle \tag{1.71}$$

$$\sum_{l} \langle \psi_k | HC_l | \psi_l \rangle = E_\alpha \sum_{l} C_l \langle \psi_k | \psi_l \rangle$$
 (1.72)

$$\sum_{l} C_{l} H_{kl} = E_{\alpha} \sum_{l} C_{l} \delta_{kl} \tag{1.74}$$

$$\sum_{l} (H_{kl} - E_{\alpha} \delta_{kl}) C_l = 0 \rightarrow \text{secularly. eq}$$
 (1.75)

the explicit form of this equation is:

$$k = x \dots \longrightarrow (H_{x1} - E_{\alpha})C_1 + (H_{x2} - E_{\alpha})C_2 + (H_{x3} - E)_{\alpha}C_{3+\dots+}(H_{xx} - E_{\alpha})C_x = 0$$

$$det(H - IE_{\alpha}) = \begin{bmatrix} (H_{11} - E_{\alpha}) & H_{12} \dots & H_{1x} \\ H_{21} & (H_{22} - E_{\alpha}) \dots & H_{2x} \\ \vdots & \dots & (H_{xx} - E_{\alpha}) \end{bmatrix}$$
(1.77)

$$P_n(E_\alpha) = a_n + E_\alpha^n + a_{n-1}E_\alpha^{n-1} + \dots + a_1E_\alpha^1 + a_0 = 0$$
(1.78)

## 1.3.5. Perturbed harmonic oscillator:

The harmonic oscillator's Hamiltonian equation is represented by the following notation: [6]:

$$\frac{P^2}{2m} + \frac{1}{2}kx^2\tag{1.79}$$

We consider that the oscillator is perturbed by the value:  $V = bx^2$ 

We try to calculate the first two perturbed states.

The energy operator is

$$H = H_0 + V \tag{1.80}$$

We get

$$\frac{P^2}{2m} + \frac{1}{2}kx^2 + bx^2 \tag{1.81}$$

We know

$$\frac{\hbar\omega}{2}(aa^+ + a^+a)P_x = \sqrt{\frac{m\omega\hbar}{2}}(a+a^+)$$
(1.82)

$$x = i\sqrt{\frac{\hbar}{2m\omega}} \ (a-a^+) \tag{1.83}$$

$$V = b \left( i \sqrt{\frac{\hbar}{2m\omega}} (a - a^{+}) \right)^{2} = -b \frac{\hbar}{2m\omega} (a^{2} + a^{+2} - aa^{+} - a^{+}a)$$
 (1.84)

$$V = \frac{\hbar b}{2m\omega} \left[ \frac{2H_0}{\hbar \omega} - \alpha^2 - \alpha^{+2} \right] \tag{1.85}$$

$$E_{\alpha}^{(1)} = \langle \alpha | V | \alpha \rangle = \langle \psi_0 | V | \psi_0 \rangle \tag{1.86}$$

$$\left\langle \psi_0 \middle| \frac{\hbar b}{2m\omega} \left[ \frac{2H_0}{\hbar \omega} - a^2 - a^{+2} \right] \middle| \psi_0 \right\rangle = \frac{2\hbar b}{2m\omega^2 \hbar} \left( \frac{\hbar \omega}{2} \right) \tag{1.87}$$

$$E_0^{(1)} = \frac{\hbar b}{2m\omega} \tag{1.88}$$

The second one

$$E_0^{(1)} = \left\langle \psi_0 \middle| V \middle| \varphi_\alpha^{(1)} \right\rangle = \sum_{l \neq \alpha} \frac{|V_{l\alpha}|^2}{(\mathcal{E}_\alpha - \mathcal{E}_l)} \tag{1.89}$$

We calculate first the value of  $V_{l\alpha}$ 

$$V_{l\alpha} = \langle l|V|\alpha \rangle = \frac{\hbar b}{2m\omega} \left\langle l \left| \frac{\hbar b}{2m\omega} \left[ \frac{2H_0}{\hbar \omega} - \alpha^2 - \alpha^{+2} \right] \right| \alpha \right\rangle$$
 (1.90)

$$V_{l\alpha} = \frac{\hbar b}{2m\omega} \left\{ \frac{2}{\hbar\omega} \mathcal{E}_{\alpha} \delta_{l\alpha} - \langle l | a^2 | \alpha \rangle - \langle l | a^{+2} | \alpha \rangle \right\}$$
 (1.91)

We write

$$a|\alpha\rangle = \sqrt{\alpha}|\alpha - 1\rangle \to a^2|\alpha\rangle = \sqrt{\alpha(\alpha - 1)}|\alpha - 2\rangle$$
 (1.92)

$$a^{+}|\alpha\rangle = \sqrt{(\alpha+1)}|\alpha+1\rangle \to a^{+2}|\alpha\rangle = \sqrt{(\alpha+1)(\alpha+2)}|\alpha+2\rangle \tag{1.93}$$

$$V_{l\alpha} = \frac{\hbar b}{2m\omega} \left\{ \frac{2}{\hbar \omega} \mathcal{E}_{\alpha} \delta_{l\alpha} - \sqrt{\alpha(\alpha - 1)} \langle l | \alpha - 2 \rangle \delta_{l,\alpha - 2} - \sqrt{(\alpha + 1)(\alpha + 2)} \delta_{l,\alpha + 2} \right\}$$
(1.94)

So

$$E_0^{(2)} = \sum_{l \neq \alpha} \left(\frac{\hbar b}{2m\omega}\right)^2 \left[ \frac{4}{\left((\alpha - 1)\right)^2} \frac{{\mathcal{E}_{\alpha}}^2}{{\mathcal{E}_l - \mathcal{E}_{\alpha}}} \delta_{l,\alpha} - \frac{\sqrt{\alpha(\alpha - 1)}^2}{{\mathcal{E}_l - \mathcal{E}_{\alpha}}} \delta_{l,\alpha-2} - \frac{\sqrt{(\alpha + 1)(\alpha + 2)}^2}{{\mathcal{E}_l - \mathcal{E}_{\alpha}}} \delta_{l,\alpha+2} \right]$$

$$(1.95a)$$

$$E_0^{(2)} = \left(\frac{\hbar b}{2m\omega}\right)^2 \left[ -\frac{\alpha(\alpha - 1)}{\varepsilon_{\alpha - 2} - \varepsilon_{\alpha}} - \frac{(\alpha + 1)(\alpha + 2)}{\varepsilon_{\alpha + 2} - \varepsilon_{\alpha}} \right]$$
(1.95b)

We know

$$E_n = \hbar\omega \left( n + \frac{1}{2} \right) \tag{1.96}$$

$$\mathcal{E}_{\alpha-2} - \mathcal{E}_{\alpha} = \hbar\omega(\alpha - 2 - \alpha) = -2\hbar\omega \tag{1.97}$$

$$\mathcal{E}_{\alpha+2} - \mathcal{E}_{\alpha} = \hbar\omega(\alpha + 2 - \alpha) = 2\hbar\omega \tag{1.98}$$

$$\to E_0^{(2)} = \frac{\hbar^2 b^2}{4m^2 \omega^2} \left[ \frac{-\alpha(\alpha - 1)}{-2\hbar\omega} - \frac{(\alpha + 1)(\alpha + 2)}{2\hbar\omega} \right]$$
(1.99)

$$E_0^{(2)} = \frac{\hbar^2 b^2}{4m^2 \omega^2} \frac{1}{2\hbar \omega} [\alpha(\alpha - 1) - (\alpha + 1)(\alpha + 2)]$$

$$= \frac{\hbar b^2}{8m^2 \omega^3} [\alpha^2 - \alpha - \alpha^2 - 3\alpha - 2]$$
(1.100)

$$\frac{-\hbar b^2}{2m^2\omega^3} \left[ \alpha + \frac{1}{2} \right] \to E_0^{(2)} = \frac{-b^2}{2m^2\omega^4} \hbar \omega \left[ \alpha + \frac{1}{2} \right]$$
 (1.101)

$$E_0^{(2)} = \frac{-b^2\hbar\omega}{4m^2\omega^4} \tag{1.102}$$

So, the perturbation became:

$$E = \mathcal{E}_{\alpha} + E_0^{(1)} + E_0^{(2)} = \frac{\hbar\omega}{2} + \frac{\hbar b}{2m\omega} - \frac{b^2\hbar\omega}{4m^2\omega^4}$$
(1.103a)

$$E = \frac{\hbar\omega}{2} \left( 1 + \frac{b}{2m\omega^2} - \frac{b^2}{2m\omega^2} \right) \tag{1.103b}$$

Another way for solution

$$H = H_0 + bx^2 = \frac{P_x^2}{2m} + \frac{1}{2}kx^2 + bx^2$$
 (1.104)

$$= \frac{{P_x}^2}{2m} + \left[ \frac{m\omega^2}{2} + b \right] x^2 = \frac{{P_x}^2}{2m} + \frac{1}{2}m \left[ \omega^2 + \frac{2b}{m} \right] x^2 = \frac{{P_x}^2}{2m} + \frac{1}{2}m\Omega^2 x^2$$
 (1.105)

$$\rightarrow E = \frac{\hbar\Omega}{2} = \frac{\hbar}{2} \sqrt{\omega^2 + \frac{2b}{m}} = \frac{\hbar\omega}{2} \sqrt{1 + \frac{2b}{m\omega^2}} \approx \frac{\hbar\omega}{2} \left(1 + \frac{b}{2m\omega^2} - \frac{b^2}{2m^2\omega^4} \dots\right) \tag{1.106}$$

$$|\varphi_{\alpha}^{(1)}\rangle = \sum_{l \neq \alpha} \frac{V_{l\alpha}}{(\varepsilon_l - \varepsilon_{\alpha})} |\psi_l\rangle = \sum_{l \neq \alpha} \frac{\langle l | V | \alpha \rangle}{(\varepsilon_l - \varepsilon_{\alpha})} |\psi_l\rangle$$

$$V = \frac{\hbar b}{2m\omega} \left\{ \frac{2H_0}{\hbar \omega} - a^2 - a^{+2} \right\}$$
 (1.107)

$$V_{l\alpha} = \frac{\hbar b}{2m\omega} \left\{ \left\langle l \left| \frac{2H_0}{\hbar \omega} \right| \alpha \right\rangle - \left\langle l \left| \alpha^2 \right| \alpha \right\rangle - \left\langle l \left| \alpha^{+^2} \right| \alpha \right\rangle \right\}$$
 (1.108)

$$= \frac{\hbar b}{2m\omega} \left\{ \frac{2}{\hbar \omega} \sum_{l \neq \alpha} \mathcal{E}_{\alpha} \delta_{l\alpha} - \sum_{l \neq \alpha} \sqrt{\alpha(\alpha - 1)} \langle l | \alpha - 2 | \psi_{l} \rangle - \sum_{l \neq \alpha} \sqrt{(\alpha + 1)(\alpha + 2)} \langle l | \alpha + 2 | \psi_{l} \rangle \right\}$$
(1.109)

$$= \frac{\hbar b}{2m\omega} \left[ -\frac{\sqrt{\alpha(\alpha-1)}}{\varepsilon_{\alpha-2} - \varepsilon_{\alpha}} |\psi_{\alpha-2}\rangle - \frac{\sqrt{\alpha(\alpha-1)}}{\varepsilon_{\alpha+2} - \varepsilon_{\alpha}} |\psi_{\alpha+2}\rangle \right]$$
(1.110)

For  $\alpha = 0$  we have:

$$|\varphi_{\alpha}^{(1)}\rangle = \frac{-\hbar b}{2m\omega} \sqrt{2} |\psi_{2}\rangle / 2\hbar\omega = \frac{\sqrt{2}\hbar b}{2m\omega} |\psi_{2}\rangle / 2\hbar\omega$$
 (1.111)

$$|\varphi_{\alpha}^{(1)}\rangle = \frac{\sqrt{2}}{4} \frac{b}{m\omega^2} |\psi_2\rangle \tag{1.112}$$

### 1.4. Variational method:

We are aware that the undisturbed Hamiltonian H\_0's associated eigenvalues and eigenvectors must be known in order to use the stationary perturbation method, but we are unable to divide the total Hamiltonian H of the system into the principal part H\_0 and the disturbance W, making it very challenging to solve the equation for the values H.

Since solving this problem involves knowing the energy of the ground state, we must instead apply the variational approach, a straightforward approximation technique that is extremely helpful in many quantum physics situations. or finding the precise solution is quite tough. It is based on a series of mathematical operations that we shall list here briefly [7].

### 1.4.1. Principle of the method

Using test state and the parameters  $a = \{a_1, a_2, ...\}$  the variational approach may be used to approximate the energy of the ground state of a quantum system defined by a Hamiltonian H. The method's applicability for any state results from the inequality, which makes it legitimate. [8]

$$\frac{\langle a|H|a\rangle}{\langle a|a\rangle} \ge E_0 \tag{1.112}$$

Where  $E_0$  is the energy of the ground state  $|\psi_0\rangle$ . Indeed, if the kets  $\psi_n$  form a basis of eigenvectors of H.

Moreover, we show that any function a such as  $E_{[a]}$  is stationary, is a proper function of H,

i.e.,

if  $a = \psi_n + \delta a$  , so  $\delta E = 0$  (at the first order of energy)  $E_n$ 

or again  $E = E_n + \delta E \approx E_n$ 

$$\delta(E_{[a]}\langle a|a\rangle) = \delta(\langle a|a\rangle) \tag{1.113}$$

$$= \delta(E_{[a]})\langle a|a\rangle + E_{[a]}\delta(\langle a|)|a\rangle + E_{[a]}\langle a|\delta(|a\rangle)$$
(1.114)

$$= \delta(\langle a|)H|a\rangle + \langle a|\delta H|a\rangle + \langle a|H(\delta|a\rangle) \tag{1.115}$$

$$\leftrightarrow \delta\{\langle a|\}(H-E)|a\rangle + \langle a|(H-E)\delta\{|a\rangle\} = 0 \tag{1.116}$$

In integral form, we have:

$$\int \delta a^* (H - E) a \, d\tau = 0 \text{ and, } \int a^* (H - E) \delta a \, d\tau = 0 \tag{1.117}$$

$$(H - E_{[a]})a = 0 (1.118)$$

which is equivalent to:

Thus, any function  $a \approx \psi_n$  , such as  $E_{[a]}$  is stationary, is a proper function of H

### **Remark:**

- the equation of  $E_{[a]}$  is independent of  $\langle a|a\rangle$  and the phase of a.
- the result is found in the particular case  $\langle a | a \rangle = 1$ .

The equation of  $E_{[a]}$  gives a superior limit of energy  $(E_0)$  of the ground state. We suppose, in fact, that we can develop

$$|a\rangle = \sum a_n |n\rangle, \langle a|H|a\rangle = \sum |a_n|^2 E_n \ge E_0 \sum |a_n|^2 = E_0 \langle a|a\rangle$$
 (1.119)

Always with

$$H|n\rangle = E_n|n\rangle \tag{1.120}$$

where we took use of the fact that, by definition, the energy levels  $E_n$  are greater than the ground state,  $E_n \ge E_0$ . The wave function  $\psi(x)$  can be written with the parameter a as:

$$\psi(x) = \psi_a(x) = \langle x | a \rangle \tag{1.121}$$

depends on whatever option is selected to most closely approach  $\langle x|0\rangle$ , the ground state's actual wave function, which is itself unknown. Therefore, by doing a straightforward reduction on all

the parameters, we may obtain a decent approximation of the energy of the ground state depending on the physics of the issue and the shape of the function  $\psi = \psi_a$ :

$$E = \min_{a} \frac{\langle \psi_a | H | \psi_a \rangle}{\langle \psi_a | \psi_a \rangle} \ge E_0 \tag{1.122}$$

The variational approach, commonly known as the Rayleigh-Ritz method, entails determining  $E_{[a]}$  from a test function that relies on a few variables. (These factors also affect  $E_{[a]}$ ...)

To get the closest possible value of E\_0 for this combination of parameters and this function a, we minimize  $E_{[a]}$ .

Thus, the selection of a depends on the entire question!

The original circumstances of the issue being examined are attempted to be respected, and the system's symmetry features are utilized.

Select a ground state test function that is affected by one or more variational factors  $\alpha_i$ :

$$\psi_{\alpha} = \psi(\alpha_1, \alpha_2, \alpha_3, \dots) \tag{1.123}$$

Let's start by calculating

$$E(\alpha_1, \alpha_2, \alpha_3, \dots) = \frac{\langle \psi_a | H | \psi_a \rangle}{\langle \psi_a | \psi_a \rangle}$$
(1.124)

then use the set of equations to find the values of the variational parameters  $\alpha_i$  that minimize the energy:

$$\frac{\partial E(\alpha_1, \alpha_2, \alpha_3, \dots)}{\partial \alpha_i} = 0 \tag{1.125}$$

The minimal value of  $E(\alpha_1, \alpha_2, \alpha_3, ...)$  so produced provides the best approximation, by excess, of the basic energy as acquired with the test function (1.121), and the equation (1.122) appears as a minimization or extremization principle (stationarity requirement).

The search for excited states takes a somewhat different approach. We already know that the function  $\psi_1$ , which represents the excited level, is orthogonal to the function  $\psi_0$ , which represents the ground state.

As a result, E approaches

$$E = \frac{\sum_{n} |C_{n}|^{2} E_{n}}{\sum_{n} |C_{n}|^{2}} \ge \frac{\sum_{n} |C_{n}|^{2} E_{1}}{\sum_{n} |C_{n}|^{2}} = E_{1}$$
(1.126)

The inequality becomes an equality in the only case where all  $C_n$  are zero, except  $C_1$  which is equal to 1, in which  $|\psi\rangle$  is only the exact state of  $|E_1\rangle$ .

### 1.4.2. Variational Method for the Hydrogen Atom:

According to the following, the hydrogen atoms Hamiltonian [9]

$$\widehat{H} = \frac{\hbar}{2m} \nabla^2 - \frac{e^2}{r} \tag{1.127}$$

Where indicates the proton-electron pair's decreased mass ( $m \approx 1$  for the hydrogen atom) and the inter-particle spacing. We can now make an informed approximation for our wavefunction shape by considering what occurs when the electron is separated from the proton. Because the electron is linked to the proton, we would expect  $\psi \to 0$  asymptotically, hence the chance of it being an infinite distance away from the proton will trend to zero. A reasonable wavefunction ansatz may be a negative exponential function of the kind[10].

$$\psi_1 = Ae^{-cr} \tag{1.128}$$

With c is a single parameter of variation. We can now operate on the wavefunction using our Hamiltonian from equation (1.5) by constructing the time independent Schrödinger equation shown in equation (1.1). To give our Laplacian operator in the Hamiltonian the proper form, which is where the math gets a bit more difficult, we must follow a number of small, simple steps. It is preferable to depict the Laplacian using spherical polar coordinates because of the spherical symmetry.

$$\nabla^2 = \frac{\partial^2}{\partial r^2} + \frac{e}{r} + \frac{1}{r^2} \left( \frac{\partial^2}{\partial \theta^2} + \frac{1}{\tan \theta} \frac{\partial}{\partial \theta} + \frac{1}{\sin^2 \theta} + \frac{\partial^2}{\partial \varphi^2} \right)$$
(1.129)

We can make this simpler by realizing that our wavefunction only needs the radial solution since we are only interested in the spherically symmetric ground state of the hydrogen atom. This means that our wavefunction has no angular components. The current form of the Laplacian is

$$\nabla^2 = \frac{\partial^2}{\partial r^2} + \frac{2}{r} \frac{\partial}{\partial r} \tag{1.130}$$

$$\nabla^2 \psi_1 = \left(C^2 - \frac{2C}{r}\right) e^{-Cr} \tag{1.131}$$

We can now construct an energy expression using equation (4) and equation (8)

$$E(C) = \int \frac{\psi_1 \hat{H} \psi_1 d\tau}{\psi_1 \psi_1 d\tau} = \frac{\frac{(C\hbar^2 - 2e^2)\pi}{2C^2}}{\frac{\pi}{C^3}}$$
(1.132)

$$=\frac{\hbar^2 c^2}{2} - e^2 C \tag{1.133}$$

By recasting the problem into atomic units, we can dispose of the annoying  $\hbar$  and e giving

$$E(C) = \frac{C^2}{2} - C \tag{1.134}$$

A plot of E(C) is seen below

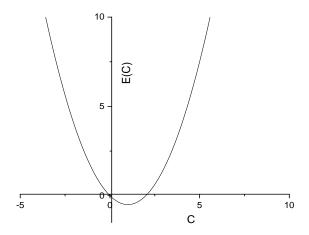


Fig.1.2: the ground state energy variation as function C

The final result from our minimization is

$$E = -0.5 \, Hartrees \tag{1.135}$$

### 1.5. Wentzel – Kramers – Brillouin (WKB) Approximation:

The BKW Brillouin, Kramers, and Wentzel equations in physics Approximation is a technique created in 1926 that enables the analysis of a quantum device's semi-classical regime. The wave function increases asymptotically to the power of the quantum of action's first order  $\hbar$ .

The Schrödinger equation is obtained from the wave propagation equation according to the BKW method's fundamental tenet. Therefore, we must discover classical mechanics in the limit  $\hbar \to 0$  just as we discover geometric optics in the theory of wave optics when the wavelength is  $\lambda \to 0$  right arrow.

The WKB approach is most commonly used for 1D issues, but it may also be used for 3D spherically symmetric problems.

The wave function is often expressed as ansatz:

$$\psi(\vec{r},t) = A(\vec{r},t)exp\left(\frac{i}{\hbar}S(\vec{r},t)\right)$$
(1.136)

The amplitude A and the action S are the two unknown functions; one of these two variables is typically regarded as "slowly varying." In fact, we shall only examine this problem here for the one-dimensional example when  $\vec{r} = R$  is utilized [14].

### 1.5.1. WKB Approximation formula:

Denote by  $\psi$  the wave function, stationary solution of the Schrödinger equation, of a particle of mass m moving in the potential V(r) [15]:

$$\left[ -\frac{\hbar^2}{2m} \frac{d^2}{dR^2} + V(r) \right] \psi(R) = E\psi(R) \tag{1.137}$$

The WKB approximation consists in writing the wave function in the form:

$$\psi^{WKB}(R) = \frac{C_{+}}{\sqrt{p(R)}} e^{\frac{i}{\hbar} \int p} + \frac{C_{-}}{\sqrt{p(R)}} e^{-\frac{i}{\hbar} \int p}$$
(1.138)

Where  $p(R) = \sqrt{2m(E - V(R))}$  is the local impulse of the particle.

### 1.5.1.1. Physical meaning

Note the simple physical meaning:

1- In the conventionally allowed region, the faster the particle, the more its probability of presence decreases. Indeed, at the place where E > V(R), the probability of presence  $|\psi|^2$  will be proportional to  $\frac{1}{n}$ .

2- In the classically forbidden region the probability of presence  $|\psi|^2$  will be exponentially decreasing in  $e^{-\frac{1}{\hbar}\int |p|}$ . Indeed, at the place where E < V(R), we then have  $p(R) = i\sqrt{2m(E-V(R))}$  and the exponentially increasing term will generally be divergent and therefore not physical, the normalization of the wave function then imposes  $C_+ = 0$ .

### **Demonstration**

By showing the different orders of the power development of  $\hbar$  we set

$$\psi(R) = e^{\frac{i}{\hbar} \left[ \sigma_0(R) + \frac{\hbar}{i} \sigma_1(R) + \left(\frac{\hbar}{i}\right)^2 \sigma_2(R) + \dots \right]}$$
(1.139)

*Ordre 0:* 

By using only  $\sigma_0$  in  $\psi$  we immediately obtain

$$-\sigma_0^{\prime 2}(R) + i\hbar\sigma_1^{\prime\prime}(R) + p^2(R) \tag{1.140}$$

The order 0, which is called the classical approximation, consists in not keeping any term in  $\hbar$ . We obtain

$$\sigma_0(R) = \mp \int p \operatorname{so} \psi(R) \approx e^{\frac{i}{\hbar} \int p}$$
 (1.141)

### Ordre 1:

The following order is the B. K. W. approximation itself.

Using the previous formula, with  $\sigma_0 + \frac{\hbar}{i}\sigma_1(R)$  instead of  $\sigma_0$ , and keeping only the terms in  $\hbar$  we get immediately  $2\sigma_0' + \sigma_0'' = 0$ 

Using the value of  $\sigma_0(R) = \pm \int p(R)$ , we can deduce  $\sigma_1(R) = cte + \frac{1}{2} \ln|p(R)|$  and

$$\psi^{WKB}(R) = \frac{C_1'}{\sqrt{|p(R)|}} e^{\frac{i}{\hbar} \int p} + \frac{C_2'}{\sqrt{|p(R)|}} e^{-\frac{i}{\hbar} \int p}$$
(1.141)

### 1.5.2. Stationary phase WKB method

The wave function therefore generalizes the free motion of a particle. However, it is not satisfactory at the cusps  $x_0$  and  $-x_0$  where p=0 and where therefore the wave function diverges. MASLOV, a Russian physicist of the XXth century circumvented this problem by noting that one could remove the singularity by carrying out the connection of the wave function in phase space (p, s). [16]

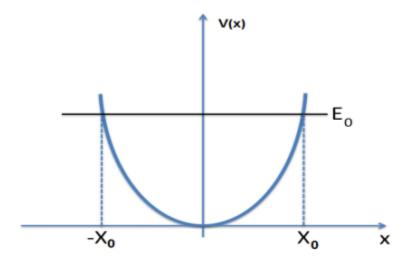


Fig.1.3: Harmonic potential well

To switch from one representation to another, we give the following two formulas:

$$\widehat{\psi(p)} = \frac{1}{\sqrt{2\pi\hbar}} \int e^{-\frac{i}{\hbar}x \, p} \psi(x) dx \tag{1.142}$$

Where  $\psi(p)$  represents the Fourier transform of  $\psi(x)$ 

$$\psi(x) = \frac{1}{\sqrt{2\pi\hbar}} \int e^{\frac{i}{\hbar}x} p} \widehat{\psi(p)} dx \tag{1.143}$$

Although we frequently are unable to calculate these formulas precisely, we may still obtain an approximation since the WKB wave function is itself an approximation. The stationary phase approach is used to achieve this. In fact, if we have an integral of the following type:

$$I = \int A(x)e^{is\phi(x)} dx \tag{1.144}$$

With s a very large real parameter (in our case:  $\frac{1}{\hbar}$ ), the phase of the function oscillates very quickly. The notable contributions for the integral are therefore close to the points  $x_0$  where  $\phi_0(x_0)=0$  (Which correspond to the places where the phase oscillates less quickly). We can therefore carry out a limited expansion of  $\phi$  around  $x_0$ , and we obtain:

$$I \approx \int A(x)e^{is\left(\phi(x_0) + \frac{1}{2}\phi''(x_0)\delta x^2\right)} dx \tag{1.145}$$

With  $\delta x \cdot \phi'(x_0) = 0$ 

If in the neighbourhood of  $x_0$ , the amplitude A(x) varies slowly with respect to the exponential, we can approximate A(x) by  $A(x_0)$  and thus get it out of the previous integral. This becomes

so:

$$I \approx A(x_0)e^{is\phi(x)} \int A(x)e^{\frac{1}{2}is\phi''(x_0)(x-x_0)^2} dx$$
 (1.146)

Using the Fresnel integral formula:

$$\frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} e^{-\frac{x^2}{2ia}} dx = \sqrt{ia} = |a|^2 e^{i\frac{\pi a}{4|a|}}$$
 (1.147)

Finally, we got

$$I \approx A(x_0) \left| \frac{2\pi}{s\phi''(x_0)} \right|^{\frac{1}{2}} e^{is\phi(x_0) \pm i\frac{\pi}{4}}$$
 (1.148)

Where  $\pm$  corresponds to the sign of phase  $s\phi''(x_0)$ 

Now let's apply this method to equation (1.142):

$$\widehat{\psi(p)} = \frac{C}{\sqrt{2\pi\hbar}} \int \frac{dx}{|p(x)|^{\frac{1}{2}}} e^{\frac{i}{\hbar} \left( \int_{x}^{x_0} p dx - px \right)}$$
(1.149)

We identify:

$$A(x) = \frac{1}{|p(x)|^{\frac{1}{2}}} \tag{1.150}$$

Then:

$$\phi(x) = \int_{x}^{x_0} p dx - px \tag{1.151}$$

We have:

$$A(x_0) = \frac{1}{|p(x_0)|^{\frac{1}{2}}}$$
 (1.152)

$$\phi''(x_0) = p'(x_0) \tag{1.153}$$

Thus, using equation (27), we finally obtain:

$$\widehat{\psi(p)} = \frac{C}{|p(x_0)p(x_0)'|^{\frac{1}{2}}} \int e^{\frac{i}{\hbar}\phi(x_0) + i\frac{\pi}{4}sgn[\phi''(x_0)]}$$
(1.154)

In the representation p, the passage from A to B does not pose a problem, there is no singularity. According to the expression of  $\widehat{\psi(p)}$ , we have  $\widehat{\psi(p_B)} = \widehat{\psi(p_A)} e^{\pm i\frac{\pi}{2}}$  (at e and, the second derivative changes sign at x0). By performing the inverse Fourier transform, we go back to the x representation, we have  $\psi_B(x) = \psi_A(x)e^{\pm i\frac{\pi}{2}}$ . The wave function, at the cusp, therefore, undergoes a phase shift of  $\pm \frac{\pi}{2}$ . This is independent of the shape of the potential. [17]

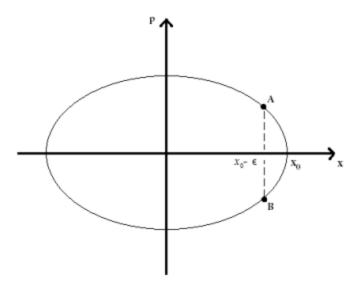


Fig.1.4: Representation of p as function of x

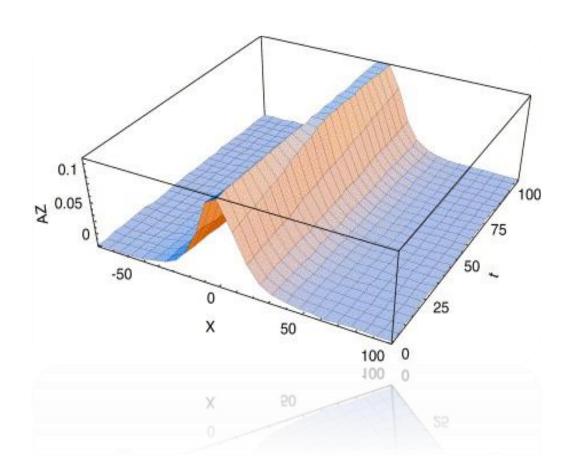
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## Chapter 02

### THE RESOLUTION OF SCHRODINGER EQUATION WITH THE SEMI INVERSE VARIATIONAL METHOD



### Chapter 2

# THE RESOLUTION OF SCHRODINGER EQUATION WITH THE SEMI INVERSE VARIATIONAL METHOD

### 2.1. The Semi-inverse variational method:

Professor He. Jihuan proposed the semi-inverse approach in 1997 [1]. For the first time, this strategy was utilized to provide variational formulations for field equations in fluid mechanics. This approach is based on variation calculations. Before we go into the details of this technique, remember the Schrödinger equation radial for a potential with spherical symmetry.

Several notable researchers, including Abdelouahab Zerarka [2-4], Zhou Xin-Wei [5,6], and Liu Hong-Mei [7,8], have calculated the eigenvalues of the Schrodinger equation. Several earlier research on this strategy [9-25] have recently been published. The implementation of this approach in many systems produced good results when compared to other methods such as ,Nikiforv-Uvarov method ,WKB approximation and factorization method etc., and this technique is highly significant in dynamic theory, indicating the efficacy of this methodology.

The major goal of this study is to provide a variational framework for searching solutions in the quantum domain using the semi-inverse variational approach [26], which is based on resolving the Schrodinger equation and therefore finding the wave function and energy eigenvalues. This approach used the radial component of the Schrodinger equation with various potentials such as the Yukawa potential, screened coulomb potential, and anharmonic one. The option of this possibility is to compare the findings obtained by the semi-inverse variational approach with other methods to see how precise it is.

The expression for the radial Schrödinger's equation is:

$$\left[\frac{\hbar^2}{2m}\left(-\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) + \frac{l(l+1)}{r^2}\right) + V(r)\right]R(r) = ER(r)$$
 (2.1)

This equation may be rewritten in the form of

$$\frac{-\hbar^2}{2m} \frac{1}{r^2} \frac{\partial}{\partial r} \left( r^2 \frac{\partial}{\partial r} \right) + (w(r) - E)R = 0$$
 (2.2)

w(r) the effective potential is provided using the form:

$$w(r) = V(r) + \frac{\hbar^2}{2m} \frac{l(l+1)}{r^2}$$
 (2.3)

l is the quantum number, and  $\hbar$  the Planck constant and m is the mass of the particle. We can write the equation 1 in the form of

$$U(r;R;R';R'') = \frac{-\hbar^2}{2m} \frac{d^2R}{dr^2} - \frac{-\hbar^2}{2m} \frac{dR}{dr} + (w(r) - E)R = 0$$
 (2.4)

And so:

$$U(r;R;R';R'') = \frac{-\hbar^2}{2m}R'' - \frac{-\hbar^2}{2m}R' + (w(r) - E)R = 0$$
 (2.5)

Where exhibitors' ' and " are the partial derivatives with respect to r

### 2.1.1. Euler's equation:

$$\frac{\partial U}{\partial R'} = \frac{d}{dr} \left( \frac{\partial U}{\partial R''} \right) \tag{2.6}$$

It is simple to confirm that this requirement is not met when we apply the consistency condition (2.6) to the equation (2.5). Therefore, we recast the equation using an auxiliary factor called g(r). [27,28]:

$$Y(r; R; R'; R'') = g(r)U(r; R; R'; R'') = 0$$
(2.7)

And in the equation. (2.3), U is replaced by Y. Now the consistency condition is satisfied provided that.  $g(r) = r^2$ 

$$Y(r;R;R';R'') = r^2 U(r;R;R';R'') \equiv \frac{-\hbar^2}{2m} r^2 \frac{d^2 R}{dr^2} - \frac{\hbar^2}{m} \frac{dR}{dr} + (w(r) - E)r^2 R = 0$$
 (2.8)

So, this equation can be derived from a specific function as a stationary condition.

Now, using a particular function as a stationary condition, the differential equation (2.6) may be obtained. We use the semi-inverse approach, which is currently the best way for deriving variation principles for many physical issues, to determine this functional. The semi-inverse method's fundamental concept is demonstrated in. We create a broad functional procedure for the equation in an alternate form as:

$$J(r) = \int_0^{+\infty} L(r; R; R'; R'') dr$$
 (2.9)

Which L(r; R; R'; R'') is the function of lagrange (where lagrangian) depends on and its derivatives, guise reads:

$$L = \frac{\alpha \hbar^2}{2m} \left( r \frac{dR}{dr} \right)^2 + b(w(r) - E)(rR)^2 + F$$
 (2.10)

is an unknown function depending on R or of its derivatives.

 $\alpha$  and b are arbitrary constants to be determined.

The goal is to look for the wave function R(r) which minimizes the integral of the relation (2.10). This is done by calculating the variations  $\delta j = 0$  (the stationarity condition). The stationary condition is satisfied if the Euler-Lagrange equation is satisfied.

$$\frac{\partial L}{\partial R} - \frac{d}{dr} \left( \frac{\partial L}{\partial R'} \right) = 0$$

$$\frac{\partial L}{\partial R} - \frac{d}{dr} \left( \frac{\partial L}{\partial R'} \right) = 0 \tag{2.11}$$

By applying this equation to the previous Lagrangian, we obtain the following equation:

$$\frac{\alpha\hbar^2}{2m}r^2\frac{d^2R}{dr^2} - 2\alpha\frac{\hbar^2}{m}\frac{dR}{dr} + 2b(w(r) - E)r^2R + \frac{\delta F}{\delta R}$$
 (2.12)

We refer to  $\frac{\delta F}{\delta R}$  as the variation derivative of F with respect to R, expressed by:

$$\frac{\delta F}{\delta R} = \frac{\partial F}{\partial R} - \frac{d}{dr} \left( \frac{\partial F}{\partial R'} \right) + \frac{d}{dr} \left( \frac{\partial^2 F}{\partial R''} \right) - \cdots$$
 (2.13)

We look for the quantities F,  $\alpha$  and b so that equation (5) identifies with the equation original.

So, we found  $\alpha = b = \frac{1}{2}$  and F = 0

$$L = \frac{1}{2} \left[ \frac{\hbar^2}{2m} \left( \frac{dR}{dr} \right)^2 + (w(r) - E)R^2 \right] r^2 dr$$
 (2.14)

So, the Lagrangian of the problem can be written as:

$$J(r) = \int_0^{+\infty} \frac{1}{2} \left[ \frac{\hbar^2}{2m} \left( \frac{dR}{dr} \right)^2 + (w(r) - E)R^2 \right] r^2 dr$$
 (2.15)

Now the theory is ready to use. For application, we will propose the anharmonic potential potential:

$$V_T(r) = \frac{1}{2}m\omega r^2 + \frac{1}{2}\rho\hbar\omega r^2 \tag{2.16}$$

So, we write functional test:

$$J(r) = \int_0^{+\infty} L(r; R; R_r) dr$$
 (2.17)

Where  $L(r; R; R_r) = \frac{\hbar^2}{4m} \left(r \frac{dR}{dr}\right)^2 + F(R)$ 

We use the stationary form

$$\delta R : \frac{\hbar^2}{2m} \frac{d}{dr} \left( r^2 \frac{dR}{dr} \right)^2 + \frac{\delta F}{\delta R} = \frac{\hbar^2}{2m} \frac{d}{dr} \left( r^2 \frac{dR}{dr} \right)^2 + (w(r) - E)r^2 R^2$$
 (2.18)

it follows that  $\frac{\delta F}{\delta R} = (w(r) - E)r^2R^2$  then we can find F with:

 $F = \frac{1}{2}(w(r) - E)r^2R^2 + F_0$ , with  $F_0$  is a constant equal 0. Finally we can write the Lagrangian

Like

$$L(r;R;R_r) = \frac{\hbar^2}{4m} \left(r\frac{dR}{dr}\right)^2 + \frac{1}{2}(w(r) - E)r^2R^2$$
 (2.19)

We find

$$L = \frac{1}{2} \left[ \frac{\hbar^2}{2m} \left( \frac{dR}{dr} \right)^2 + (w'(r) - E)R^2 \right] r^2 dr$$
 (2.20)

So, the Lagrangian of the problem can be written as:

$$J(r) = \int_0^{+\infty} \frac{1}{2} \left[ \frac{\hbar^2}{2m} \left( \frac{dR}{dr} \right)^2 + (w'(r) - E)R^2 \right] r^2 dr$$
 (2.21)

The theory is now prepared for use. We will use the radial isotropic harmonic oscillator, which is denoted as follows:

$$w'(r) = V(r) + \frac{\hbar^2}{2m} \frac{l(l+1)}{r^2} + \frac{1}{2}\rho\hbar\omega r^2$$
 (2.22)

Therefore, we create a functional test:

$$J(r) = \int_0^{+\infty} L(r; R; R_r) dr$$
 (2.23)

$$L(r;R;R_r) = \frac{1}{2} \left[ \frac{\hbar^2}{2m} \left( \frac{dR}{dr} \right)^2 + \left( \frac{\hbar^2 l(l+1)}{2mr^2} + \frac{1}{2} m \omega r^2 + \frac{1}{2} \rho \hbar \omega r^2 - E \right) R^2 \right]$$
(2.24)

$$J(r) = \int_0^{+\infty} \frac{1}{2} \left[ \frac{\hbar^2}{2m} \left( \frac{dR}{dr} \right)^2 + \left( \frac{\hbar^2 l(l+1)}{2mr^2} + \frac{1}{2} m \omega r^2 + \frac{1}{2} \rho \hbar \omega r^2 - E \right) R^2 \right] r^2 dr \tag{2.25}$$

Before doing numerical testing, we employ the atomic unit system, where  $\hbar = 2m = 1$ , and we have the analytical solution of the used potential.

Harmonic oscillator with perturbation by a quadratic un potential:

We propose W with form

$$W = \frac{1}{2}\rho\hbar\omega r^2 \tag{2.26}$$

Ou  $\rho$  is a real parameter, without dimension with  $\rho < 1$ . H S'écrit alors :

$$H = H_0 + W = \frac{P^2}{2m} + \frac{1}{2}m\omega^2 r^2 + \frac{1}{2}\rho\hbar\omega r^2$$
 (2.27)

In this situation, the disturbance effect is just changing the Harmonic oscillator's recall constant.

$${\omega'}^2 = \omega^2 (1 + \rho) \tag{2.28}$$

We see that H is always a Hamiltonian, the Harmonic oscillator, whose pulse has become  $\omega''$ 

The study of the value of the eigenvalues of H. They are simply written according to (2) et (3):

$$E_n = \left(n + \frac{1}{2}\right)\hbar\omega' = \left(n + \frac{1}{2}\right)\hbar\omega\sqrt{(1+\rho)}$$
 (2.29)

That is to say again, when we develop the radial:

$$E_n = \left(n + \frac{1}{2}\right)\hbar\omega \left[1 + \frac{\rho}{2} + \frac{\rho^2}{8} + \cdots\right]$$
 (2.30)

### 2.1.2. Test functions:

$$1-R = ae^{-kr^2}$$

We substitute the wave function  $R = ae^{-kr^2}$  in equation (2.25) we get:

For the simplification calculus in Mathematica [29] we replace the value of energy E by the symbol t, we found J(a,k) the results in terms of a and:

$$J(a,k) = \frac{a^2 \sqrt{\frac{\pi}{2}} (12k^2 - 8kt + 3(1+p)w^2)}{64k^{5/2}}$$
(2.31a)

The stationary condition provides the following expressions.

$$\frac{\partial J(a,k)}{\partial a} = \frac{a\sqrt{\frac{\pi}{2}}(12k^2 - 8kt + 3(1+p)w^2)}{32k^{5/2}}$$
(2.31b)

$$\frac{\partial J(a,k)}{\partial k} = -\frac{3a^2\sqrt{\frac{\pi}{2}}(4k^2 - 8kt + 5(1+p)w^2)}{128k^{7/2}}$$
(2.31c)

The resolution of the algebraic system provides the values of k and the constant a can be determined via the normalization condition  $\int_0^{\infty} |R|^2 r^2 dr$ 

Always with Mathematica we get:

$$k = \frac{\omega\sqrt{\rho+1}}{2} = \frac{\omega'}{2}$$
 And  $E = \frac{3\omega\sqrt{\rho+1}}{2} = \frac{3\omega'}{2}$ 

The resolution of the algebraic system provides the values of k and the constant a can be determined via the normalization condition  $\int_0^{\infty} |R|^2 r^2 dr$ 

We deduce that this result corresponds to the configuration: n = 1, l = 0 (state 1s), since the wave function  $R_{nl}$  is given by:

$$R_{10} = \frac{2}{\sqrt{\sqrt{\pi}}} \omega'^{\frac{3}{4}} r e^{-\frac{\omega'}{2}r^2} or \frac{2}{\sqrt{\sqrt{\pi}}} (\omega \sqrt{\rho + 1})^{\frac{3}{4}} r e^{-\frac{(\omega \sqrt{\rho + 1})}{2}r^2}$$

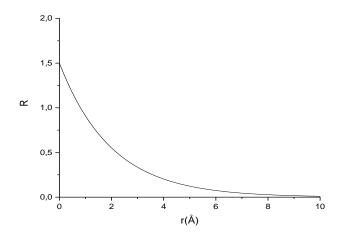


Fig.2.1. The wave function  $R_{10}$  for  $\omega = 1$  and  $\rho = 10^{-3}$ 

$$2-R = are^{-kr^2}$$

With the same method and by Mathematica we found J(a, k) the results in terms of a and:

$$J(a,k) = \frac{3a^2\sqrt{\frac{\pi}{2}}(-8ek + 20k^2 + 5(1+p)w^2)}{512k^{7/2}}$$
 (2.32a)

The stationary condition provides the following expressions.

$$\frac{\partial J(a,k)}{\partial a} = \frac{3a\sqrt{\frac{\pi}{2}}(-8ek + 20k^2 + 5(1+p)w^2)}{256k^{7/2}}$$
(2.32b)

$$\frac{\partial J(a,k)}{\partial k} = -\frac{15a\sqrt{\frac{\pi}{2}}(-8ek + 12k^2 + 7(1+p)w^2)}{512k^{9/2}}$$
(2.32c)

The resolution of the algebraic system provides the values of k and the constant a can be determined via the normalization condition  $\int_0^{\infty} |R|^2 r^2 dr$ 

Always with Mathematica we get:

$$k = \frac{\omega\sqrt{\rho+1}}{2} = \frac{\omega'}{2}$$
 And  $E = \frac{5\omega\sqrt{\rho+1}}{2} = \frac{5\omega'}{2}$ 

The resolution of the algebraic system provides the values of k and the constant a can be determined via the normalization condition  $\int_0^{\infty} |R|^2 r^2 dr$ 

We deduce that this result corresponds to the configuration: n = 1, l = 1 (state 1p), since the wave function  $R_{nl}$  is given by:

$$R_{11} = \frac{2\sqrt{2}}{\sqrt{3\sqrt{\pi}}}\omega' \ re^{-\frac{\omega'}{2}r^2} \ ou \frac{2\sqrt{2}}{\sqrt{3\sqrt{\pi}}} (\omega\sqrt{\rho+1})^{\frac{5}{4}} re^{-\frac{(\omega\sqrt{\rho+1})}{2}r^2}$$

The wave function graph  $R_{11}$  for  $\omega=1$  and  $\rho=10^{-3}$  is shown in the figure 2.2

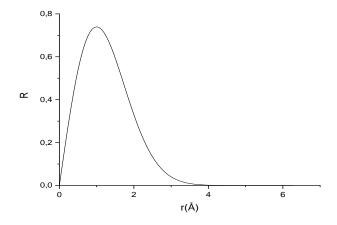


Fig.2.2. The wave function  $R_{11}$  for  $\omega = 1$  and  $\rho = 10^{-3}$ 

$$3-R = ar^2 e^{-kr^2}$$

With the same method and By Mathematica we found I(a, k) the results in terms of a and:

$$J(a,k) = \frac{15a^2\sqrt{\frac{\pi}{2}}(-8ek + 28k^2 + 7(1+p)w^2)}{2048k^{9/2}}$$
(2.33a)

The stationary condition provides the following expressions.

$$\frac{\partial J(a,k)}{\partial a} = \frac{15a\sqrt{\frac{\pi}{2}}(-8ek + 28k^2 + 7(1+p)w^2)}{1024k^{9/2}}$$
(2.33b)

$$\frac{\partial J(a,k)}{\partial k} = -\frac{105a^2\sqrt{\frac{\pi}{2}}(-8ek + 20k^2 + 9(1+p)w^2)}{4096k^{11/2}}$$
(2.33c)

The resolution of the algebraic system provides the values of k and the constant a can be determined via the normalization condition  $\int_0^{\infty} |R|^2 r^2 dr$ 

Always with Mathematica we get:

$$k = \frac{\omega\sqrt{\rho+1}}{2} = \frac{\omega'}{2}$$
 And  $E = \frac{7\omega\sqrt{\rho+1}}{2} = \frac{5\omega'}{2}$ 

The resolution of the algebraic system provides the values of k and the constant a can be determined via the normalization condition  $\int_0^{\infty} |R|^2 r^2 dr$ 

We deduce that this result corresponds to the configuration: n = 2, l = 1 (state 2p), since the wave function  $R_{nl}$  is given by:

$$R_{21} = \frac{4}{\sqrt{15\sqrt{\pi}}} \omega' \, r^2 e^{-\frac{\omega'}{2}r^2} \, ou \, \frac{4}{\sqrt{15\sqrt{\pi}}} \left(\omega \sqrt{\rho + 1}\right)^{\frac{7}{4}} r^2 e^{-\frac{(\omega \sqrt{\rho + 1})}{2}r^2}$$

The wave function graph  $R_{21}$  for  $\omega=1$  and  $\rho=10^{-3}$  is shown in the figure 2.3

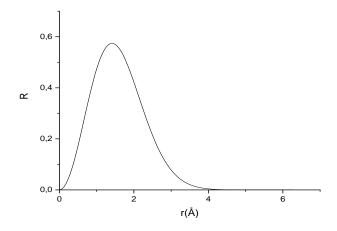


Fig.2.3. The wave function  $R_{21}$  for  $\omega=1$  and  $\rho=10^{-3}$ 

$$2-R = (ar^2 + b)e^{-kr^2}$$

By Mathematica we found J(a, b, k) the results in terms of a and k:

$$J(a,b,k) = \frac{1}{2048k^{9/2}} \sqrt{\frac{\pi}{2}} \left( 4k(24abk(-2e+k) + 16b^2k^2(-2e+3k) + a^2(-30e+33k)) + 3(35a^2 + 40abk + 16b^2k^2)(1+p)w^2 \right)$$
(2.34a)

The stationary condition provides the following expressions.

$$\frac{\partial J(a,k)}{\partial a} = \frac{1}{2048k^{9/2}} \left( \sqrt{\frac{\pi}{2}} \left( 4k(24bk(-2e+k) + 2a(-30e+33k)) + 3(70a+40bk)(1+p)w^2 \right) \right)$$
(2.34b)

$$\frac{\partial J(a,k)}{\partial b} = \frac{\sqrt{\frac{\pi}{2}} (4k(24ak(-2e+k) + 32bk^2(-2e+3k)) + 3(40ak+32bk^2)(1+p)w^2)}{2048k^{9/2}}$$

$$\frac{\partial J(a,k)}{\partial b} = \frac{1}{2048k^{9/2}} \left( \sqrt{\frac{\pi}{2}} \left( 4k(24ak(-2e+k) + 32bk^2(-2e+3k)) + 3(40ak+32bk^2)(1+p)w^2 \right) \right)$$
(2.34c)

$$\frac{\partial J(a,k)}{\partial k} = -\frac{1}{4096k^{11/2}} 3\sqrt{\frac{\pi}{2}} \left(-5a^2(56ek - 44k^2 - 63(1+p)w^2) + 16b^2k^2(-8ek + 4k^2 + 5(1+p)w^2) + 8abk(-40ek + 12k^2 + 35(1+p)w^2)\right)$$
(2.34d)

The resolution of the algebraic system provides the values of k and the constant a can be determined via the normalization condition  $\int_0^{\infty} |R|^2 r^2 dr$ 

Always with Mathematica we get:

$$a = -\frac{2b\omega\sqrt{\rho+1}}{3}$$
,  $k = \frac{\omega\sqrt{\rho+1}}{2} = \frac{\omega'}{2}$  And  $E = \frac{7\omega\sqrt{\rho+1}}{2} = \frac{5\omega'}{2}$ 

The resolution of the algebraic system provides the values of k and the constant a can be determined via the normalization condition  $\int_0^{\infty} |R|^2 r^2 dr$ 

We deduce that this result corresponds to the configuration: n = 2, l = 0 (state 2s), since the wave function  $R_{nl}$  is given by:

$$R_{20} = \frac{2\sqrt{3}}{\sqrt{5\sqrt{\pi}}} \left(1 - \frac{2\omega'}{3}\right) r^2 e^{-\frac{\omega'}{2}r^2} ou \frac{2\sqrt{3}}{\sqrt{5\sqrt{\pi}}} \left(1 - \frac{2\omega\sqrt{\rho+1}}{3}r^2\right) e^{-\frac{\omega\sqrt{\rho+1}}{2}r^2}$$

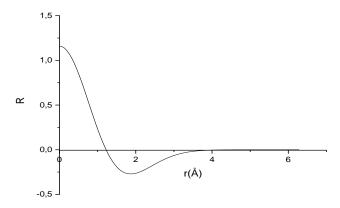


Fig.2.4. The wave function  $R_{20}$  for  $\omega = 1$  and  $\rho = 10^{-3}$ 

$$2-R = ar^3e^{-kr^2}$$

By Mathematica we found J(a, k) the results in terms of a and:

$$J(a,k) = \frac{105a^2\sqrt{\frac{\pi}{2}}(-8ek + 36k^2 + 9(1+p)w^2)}{8192k^{11/2}}$$
(2.35a)

The stationary condition provides the following expressions.

$$\frac{\partial J(a,k)}{\partial a} = \frac{105a\sqrt{\frac{\pi}{2}}(-8ek + 36k^2 + 9(1+p)w^2)}{4096k^{11/2}}$$

$$\frac{\partial J(a,k)}{\partial k} = -\frac{945a^2\sqrt{\frac{\pi}{2}}(-8ek + 28k^2 + 11(1+p)w^2)}{16384k^{13/2}}$$
(2.35b)

$$\frac{\partial J(a,k)}{\partial k} = -\frac{945a^2\sqrt{\frac{\pi}{2}}(-8ek + 28k^2 + 11(1+p)w^2)}{16384k^{13/2}}$$
(2.35c)

The resolution of the algebraic system provides the values of k and the constant a can be determined via the normalization condition  $\int_0^{\infty} |R|^2 r^2 dr$ 

Always with Mathematica we get:

$$k = \frac{\omega\sqrt{\rho+1}}{2} = \frac{\omega'}{2}$$
 And  $E = \frac{9\omega\sqrt{\rho+1}}{2} = \frac{9\omega'}{2}$ 

The resolution of the algebraic system provides the values of k and the constant a can be determined via the normalization condition  $\int_0^{\infty} |R|^2 r^2 dr$ 

We deduce that this result corresponds to the configuration: n = 3, l = 0 (state 3s), since the wave function  $R_{nl}$  is given by:

$$R_{30} = \frac{4\sqrt{2}}{\sqrt{105\sqrt{\pi}}} \omega' \, r^3 e^{-\frac{\omega'}{2}r^2} \, ou \frac{4\sqrt{2}}{\sqrt{105\sqrt{\pi}}} (\omega\sqrt{\rho+1})^{\frac{7}{4}} r^3 e^{-\frac{(\omega\sqrt{\rho+1})}{2}r^2}$$

The wave function graph  $R_{30}$  for  $\omega=1$  and  $\rho=10^{-3}$  is shown in the figure.

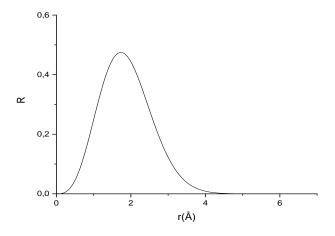


Fig.2.5. The wave function  $R_{30}$  for  $\omega = 1$  and  $\rho = 10^{-3}$ 

$$2-R = (ar^2 + b)e^{-kr^2}$$

By Mathematica we found J(a, b, k) the results in terms of a and:

$$J(a,b,k) = \frac{1}{8192k^{11/2}} 3\sqrt{\frac{\pi}{2}} \left(4k(40abk(-2e+3k) + 16b^2k^2(-2e+5k) + a^2(-70e+115k)\right) + 5(63a^2 + 56abk + 16b^2k^2)(1+p)w^2\right)$$
(2.36a)

The stationary condition provides the following expressions.

$$\frac{\partial J(a,k)}{\partial a} = \frac{1}{8192k^{11/2}} \left( 3\sqrt{\frac{\pi}{2}} \left( 4k(40bk(-2e+3k) + 2a(-70e+115k)) + 5(126a+56bk)(1+p)w^2) \right)$$
(2.36b)

$$\frac{\partial J(a,k)}{\partial b} = \frac{1}{8192k^{11/2}} \left( 3\sqrt{\frac{\pi}{2}} \left( 4k(40ak(-2e+3k) + 32bk^2(-2e+5k)) + 5(56ak + 32bk^2)(1+p)w^2 \right) \right)$$
(2.36c)

$$\frac{\partial J(a,k)}{\partial k} = -\frac{1}{16384k^{13/2}} 15 \sqrt{\frac{\pi}{2}} (-7a^2(72ek - 92k^2 - 99(1+p)w^2) 
+ 16b^2k^2(-8ek + 12k^2 + 7(1+p)w^2) + 8abk(-56ek + 60k^2 
+ 63(1+p)w^2))$$
(2.36d)

The resolution of the algebraic system provides the values of k and the constant a can be determined via the normalization condition  $\int_0^{\infty} |R|^2 r^2 dr$ 

Always with Mathematica we get:

• Case1:

$$a=0$$
,  $k=\frac{\omega\sqrt{\rho+1}}{2}=\frac{\omega'}{2}$  And  $E=\frac{5\omega\sqrt{\rho+1}}{2}=\frac{5\omega'}{2}$ 

We deduce that this result corresponds to the configuration: n = 0, l = 0 (state 0s),

• Case 2:

$$a=-\frac{2b\omega\sqrt{\rho+1}}{5}$$
,  $k=\frac{\omega\sqrt{\rho+1}}{2}=\frac{\omega'}{2}$  And  $E=\frac{9\omega\sqrt{\rho+1}}{2}=\frac{9\omega'}{2}$ 

The resolution of the algebraic system provides the values of k and the constant a can be determined via the normalization condition  $\int_0^{\infty} |R|^2 r^2 dr$ 

We deduce that this result corresponds to the configuration: n = 3, l = 1 (state 3p), since the wave function  $R_{nl}$  is given by:

$$R_{31} = \frac{2\sqrt{5}}{\sqrt{3\sqrt{\pi}}} \left( 1 - \frac{2\omega'}{5} r^2 \right) r e^{-\frac{\omega'}{2}r^2} ou \frac{2\sqrt{5}}{\sqrt{3\sqrt{\pi}}} \left( 1 - \frac{2\omega\sqrt{\rho+1}}{5} r^2 \right) r e^{-\frac{\omega\sqrt{\rho+1}}{2}r^2}$$

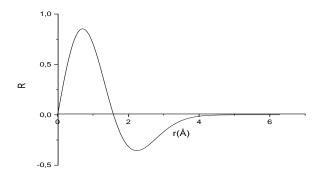


Fig.2.6. The wave function  $R_{31}$  for  $\omega = 1$  and  $\rho = 10^{-3}$ 

### 2.2. Resolution the Schrodinger equation with some different potentials:

### 2.2.1. Yukawa potential:

A Yukawa potential, also known as a screened Coulomb potential, is a potential in particle, atomic, and condensed matter physics named for the Japanese physicist Hideki Yukawa. The potential takes the shape of the form [29]:

$$V_{\text{Yukawa}}(r) = -\delta^2 \frac{e^{-\alpha mr}}{r}$$
 (2.37)

where  $\delta$  is a magnitude scaling constant and the amplitude of potential, m is the mass of the particle, r is the radial distance to the particle, and  $\alpha$  is another scaling constant.

For  $\hbar = m = 1$ , we express: the Lagrangian of the problem as below can be written as:

$$J(r) = \int_0^{+\infty} \frac{1}{2} \left[ \left( \frac{dR}{dr} \right)^2 + \left( \frac{l(l+1)}{2r^2} - V_0 \frac{e^{-\lambda r}}{r} - E \right) R^2 \right] r^2 dr$$
 (2.38)

And as a result, we may utilize values like  $\lambda = \frac{1}{1000}$  and set  $V(r) = -V_0 \frac{e^{-\lambda r}}{r}$  as Yukawa potential in these stages, where  $R(r) = ae^{-kr}$  is the radial trial function. R(r) is substituted in equation (2.38) for this reason, we may express Lagrange's overall functionality as follows:

$$J(a,k) = \frac{1}{16}a^2(\frac{1}{k} - \frac{8}{(\frac{1}{1000} + 2k)^2} - \frac{2t}{k^3})$$
(2.39a)

In this case we use the stationary condition provides by the following expressions:

$$\frac{\partial J(a,k)}{\partial a} = \frac{1}{8}a(\frac{1}{k} - \frac{8}{(\frac{1}{1000} + 2k)^2} - \frac{2t}{k^3})$$
(2.39b)

$$\frac{\partial J(a,k)}{\partial k} = \frac{1}{16}a^2\left(-\frac{1}{k^2} + \frac{32}{(\frac{1}{1000} + 2k)^3} + \frac{6t}{k^4}\right)$$
(2.39c)

For all applications in this study, the k, E, and other variables are determined by solving the nonlinear system of equations  $\partial J$  using the Mathematica package. Noting that E represents the energy value, which has previously been employed in Mathematica, we obtain the following outcomes:  $k \approx 0.999999$ ,  $E \approx 0.499001$  and  $R_{10} = ae^{-0.9999997}$ .

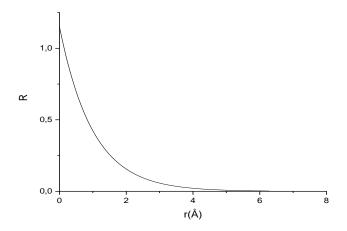


Fig.2.7. The wave function  $R_{10}$  for Yukawa potential (  $V_0=1$  ,  $\lambda=0.0001$  ).

We'll continue with another example,  $\lambda = \frac{1}{100}$  we expressed the general functional of LaGrange as below:

$$J(a,k) = \frac{1}{16}a^2(\frac{1}{k} - \frac{8}{(\frac{1}{100} + 2k)^2} - \frac{2t}{k^3})$$
 (2.40a)

The stationary condition provides the following expressions:

$$\frac{\partial J(a,k)}{\partial a} = \frac{1}{8}a(\frac{1}{k} - \frac{8}{(\frac{1}{100} + 2k)^2} - \frac{2t}{k^3})$$
(2.40b)

$$\frac{\partial J(a,k)}{\partial k} = \frac{1}{16}a^2\left(-\frac{1}{k^2} + \frac{32}{(\frac{1}{100} + 2k)^3} + \frac{6t}{k^4}\right)$$
(2.40c)

Always with our packaging we get,  $k \approx 0.999926$ ,  $E \approx 0.4990075$  and  $R_{10} = ae^{-0.999926r}$ .

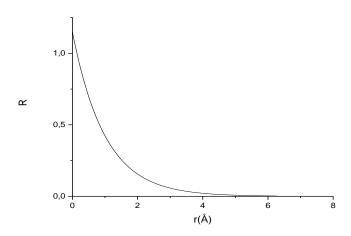


Fig.2.8. The wave function  $R_{10}$  for Yukawa potential (  $V_0=1$  ,  $\lambda=0.001$  ).

In the case,  $\lambda = \frac{1}{100}$  we obtain:

$$J(a,k) = \frac{1}{16}a^2(\frac{1}{k} - \frac{800}{(1+20k)^2} - \frac{2t}{k^3})$$
 (2.41a)

and for the stationary condition provides the following expressions:

$$\frac{\partial J(a,k)}{\partial a} = \frac{1}{8}a(\frac{1}{k} - \frac{800}{(1+20k)^2} - \frac{2t}{k^3})$$
(2.41b)

$$\frac{\partial J(a,k)}{\partial k} = \frac{1}{16}a^2\left(-\frac{1}{k^2} + \frac{32000}{(1+20k)^3} + \frac{6t}{k^4}\right)$$
(2.41c)

For this we get,  $k \approx 0.99333$ ,  $E \approx 0.407051$  and  $R_{10} = ae^{-0.993336r}$ .

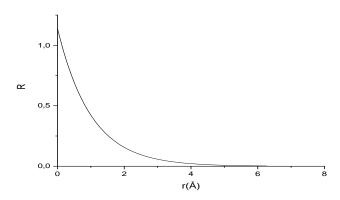


Fig.2.9. The wave function  $R_{10}$  for Yukawa potential (  $V_0=1$  ,  $\lambda=0.01$  ).

**Tab.2.1**. The eigenvalues of Yukawa potential for different values of  $\lambda$  of the state 1s.

λ our results		Ref [30]	<b>Ref</b> [31]
0.001	-0.499000749500547	-0.4990008	
0.002	-0.498002996009470	-0.4980030	-0.4950
0.005	-0.495018687868179	-0.4950187	-0.4901
0.01	-0.490074505845447	-0.4900745	-0.4803
0.02	-0.480296092106669	-0.4802961	-0.4755
0.05	-0.451815942579349	-0.4518164	-0.4518
0.1	-0.407051443942481	-0.4070780	-0.4071
0.2	-0.326729365014589	-0.3268078	-0.3268
0.3	-0.257324659356835	-0.2526452	
0.5	-0.146509393838167	-0.1480844	-0.1881

**Tab.2.2**. The eigenvalues of Yukawa potential for different values of  $\lambda$  of the state 2s.

λ	our results	Ref [30]	Ref [31]
0.001	-0.123585225161263	-0.1240167	
0.002	-0.122592659608282	-0.1230119	-0.1230
0.005	-0.119644376768699	-0.1200743	-0.1201
0.01	-0.114826981119266	-0.1152939	-0.1153
0.02	-0.105542391028958	-0.1061483	-0.1062
0.05	-0.080301645549905	-0.0817711	-0.08175
0.1	-0.046033580447479	-0.0499266	-0.04993

**Tab.2.3.** The energy eigenvalues of the Yukawa potential with different values of g and  $V_0 = 1$  of the state 1s.

δ	our results	Numerical [31]	Supersymmetry [32]
0.002	-0.996005992018941	-0.99600	-0.99601
0.005	-0.990037375736382	-0.99000	-0.99004
0.01	-0.980149011690898	-0.98010	-0.98015
0.02	-0.960592184213339	-0.96060	-0.96059
0.0256	-0.950922321362622	-0.95090	-0.95092
0.05	-0.903631885158696	-0.90360	-0.90363

The next results are for  $\hbar = 2m = 1$ .

**Tab.2.4**. The eigenvalues of Yukawa potential for different values of  $V_0$  of the state 1s.

$V_0$	Our results	Numerical [34]	Analytical [33]	Supersymmetry [33]
4	-3.2564115515398573	-3.2565	-3.2199	-3.2563
8	-14.458110162539146	-14.4571	-14.4199	-14.4581
	-2.5833830563780093	-2.5836	-2.4332	-2.5830
16	-60.85902856720754	-60.8590	-60.8193	-60.8590
	-12.990939538350945	-12.8375	-12.9910	-12.9908
24	-139.25934619091115	-139.2594	-139.2201	-139.2590
	-31.393767390991638	-11.5959	-11.2456	-11.5951
	-11.595667857596096	-11.5959	-11.2456	-11.5951

According to figures 2.7, 2.8 and 2.9 we identify the ground states 1s and the first excited state 2s.

Table 2.1 and Table 2.2 displays the eigenvalues of Yukawa potential for different values of  $\lambda$  of 1s and 2s respectively. It observed that :

- The energy increases when the values of  $\lambda$  increases.
- The outcomes are in good agreement with the results in references [30] and [31].

Table 2.3 shows the energy eigenvalues of the Yukawa potential with different values of g and  $V_0 = 1$  of the state 1s. We note increasing of energy values when the value g rises, and the results are very close with another works mentioned in [31] and [32] with error of 0.0001%.

Table 2.4 The eigenvalues of Yukawa potential for different values of  $V_0$  of the state 1s.We note increasing of energy values when the value  $V_0$  rises, and the results are very close with another works mentioned in [31] and [32] with error of 0.000013%.

The numerical simulations demonstrate the feasibility and accuracy of our semi-inverse variational approach in solving the Yukawa potential problem. Our results align well with known references, showcasing the effectiveness of this method in tackling quantum mechanics challenges.

### 2.2.2. Cornell potential

The known Cornell potential takes the form  $-\frac{\alpha}{r} + \beta r$ . For the case of  $\alpha = 1$  and  $\beta = 1$  we express the Lagrange equation as below:

$$J(r;R;R_r) = \int_{0}^{+\infty} \frac{1}{2} \left[ \left( \frac{dR}{dr} \right)^2 + \left( \frac{l(l+1)}{2r^2} - \frac{1}{r} + r - E \right) R^2 \right] r^2$$
 (2.42)

and as a result, we may employ, for instance, the screened coulomb potential  $V(r) = -\frac{1}{r} + r$  in these stages, where the radial trial function is  $R(r) = (a + br + cd)e^{-kr}$ . To solve for r in equation (2.42), we use R(r). For this reason, we may express Lagrange's overall functionality as follows:

$$J(a,b,d,k) = \frac{1}{32k^8} (2k^2(b^2(15+k(k(-3+2k)-6t)) + 2abk(6+k((-2+k)k) - 3t)) + a^2k^2(3+2k((-1+k)k-t))) + 3d^2(105+2k(k(-5+2k)k) - 15t)) + 12dk(b(15+k((-2+k)k-5t)) - ak(-5+k^2+2kt)))$$
(2.43a)

The stationary condition offered by the following phrases is used in this instance:

$$\frac{\partial J(a,b,c,k)}{\partial a} = \frac{1}{32k^8} (2k^2 (2bk(6+k((-2+k)k-3t)) + 2ak^2 (3+2k((-1+k)k-t))) - 12dk^2 (-5+k^2+2kt))$$

$$\frac{\partial J(a,b,c,k)}{\partial a} = \frac{1}{32k^8} (2k^2(2bk(6+k((-2+k)k-3t)) + 2ak^2(3+2k((-1+k)k-t))) - 12dk^2(-5+k^2+2kt))$$
(2.43b)

$$\frac{\partial J(a,b,d,k)}{\partial b} = \frac{1}{32k^8} (2k^2(2b(15+k(k(-3+2k)-6t)) + 2ak(6+k((-2+k)k-6t))) + 2ak(6+k((-2+k)k-6t)) +$$

$$(3t)$$
)) +  $12dk(15 + k((-2 + k)k - 5t))$ 

$$\frac{\partial J(a,b,d,k)}{\partial d} = \frac{1}{32k^8} (6d(105 + 2k(k(-5+3k) - 15t)) + 12k(b(15+k((-2+3k) - 15t)) + 12k(b$$

$$\frac{\partial J(a,b,d,k)}{\partial k} = -\frac{1}{16k^9} (45d^2(28 - 2k^2 + k^3 - 7kt) + 2k^2(2abk(15 - 3k^2 + k^3 - 6kt) + 3b^2(15 - 2k^2 + k^3 - 5kt) + a^2k^2(6 - 2k^2 + k^3 - 3kt))$$

$$+ 6dk(b(105 - 10k^2 + 4k^3 - 30kt) - 2ak(-15 + 2k^2 + 5kt)))$$
(2.43f)

For all of the applications in this paper, we solve the nonlinear system of equations  $\partial J$  using the Mathematica packaging. We note that t represents the energy value, and that k and t are constants that can be found using the normalization condition  $k \approx 2.08$ ,  $b \approx 1.297a, d \approx 1.413a$  and  $E \approx 1.3987$  and  $R_{00} = a(1 + 1.297r + 1.413r^2) e^{-2.08 r}$ 

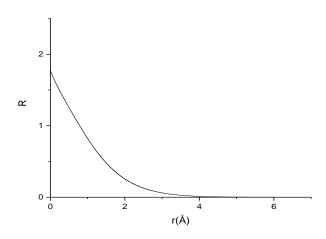


Fig.2.10. The wave function  $R_{00}$  for  $V(r) = -\frac{1}{r} + r$ .

We'll proceed on to examine a further wave function,  $R = (ar^4 + br^2 + d)e^{-kr}$ , which we'll insert in equation (2.42) to represent the generic LaGrange functional as follows:

$$J(a,b,d,k) = \frac{1}{32k^{12}}(315a^2(495 + 2k(k(-9 + 5k) - 45t)) + 3b^2k^4(105 + 2k(k(-5 + 3k) - 15t)) + 2d^2k^8(3 + 2k((-1 + k)k - t)) - 12bdk^6(-5 + k^2 + 2kt) - 30ak^2(dk^2(-21 + 2k(k + k^2 + 3t)) + b(-378 + 3k((7 - 2k)k + 28t))))$$
(2.44a)

and for the stationary condition provides the following expressions:

$$\frac{\partial J(a,b,d,k)}{\partial a} = \frac{1}{32k^{12}} 630a(495 + 2k(k(-9 + 5k) - 45t)) - 30k^{2}(dk^{2}(-21 + 2k(k + k^{2} + 3t)) + b(-378 + 3k((7 - 2k)k + 28t)))$$
(2.44b)

$$\frac{\partial J(a,b,d,k)}{\partial b} = \frac{1}{32k^{12}} 6bk^4 (105 + 2k(k(-5+3k) - 15t)) - 12dk^6 (-5+k^2 + 2kt) - 30ak^2 (-378 + 3k((7-2k)k + 28t))$$
(2.44c)

$$\frac{\partial J(a,b,d,k)}{\partial k} = \frac{1}{16k^{13}} (-14175a^2(66 - 2k^2 + k^3 - 11kt) - 45b^2k^4(28 - 2k^2 + k^3 - 7kt) - 2d^2k^8(6 - 2k^2 + k^3 - 3kt) + 12bck^6(-15 + 2k^2 + 5kt) + 30ak^2(-21b(90 - 4k^2 + k^3 - 18kt) + dk^2(-84 + 6k^2 + 5k^3 + 21kt)))$$
(2.44d)

For this we get k = 2.124, b = -1.834a, d = -0.927a, E = 3.489 and

$$R_{10} = a(r^4 - 1.834r^2 - 0.927)e^{-2.124r}$$
.

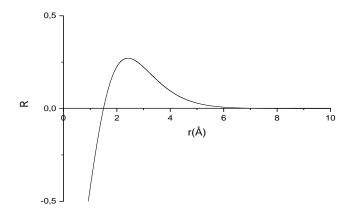


Fig.2.11. The wave function  $R_{10}$  for  $V(r) = -\frac{1}{r} + r$ .

We'll proceed on to examine a further wave function,  $R = (ar^3 + d)e^{-kr}$ , which we'll insert in equation (2.42) to represent the generic LaGrange functional as follows:

$$J(a,d,k) = \frac{1}{32k^{10}} (45a^2(126 + k(k(-7 + 16k) - 28t)) + 12adk^3(15 + k(k(-2 + 16k) - 28t)) + 12adk^3(15 + k(k(-2$$

The stationary condition provides the following expressions.

$$\frac{J(a,d,k)}{\partial a} = \frac{1}{32k^{10}}(90a(126 + k(k(-7 + 16k) - 28t)) + 12dk^{3}(15 + k(k(-2 + 16k) - 28t)) + 12dk^{3}(15 + k(k(-2 + 16k) - 28t)) + 12dk^{3}(15 + k(k(-2 + 16k) - 28t)))$$

$$(2.45b)$$

$$\frac{\partial J(a,d,k)}{\partial d} = \frac{12ak^3(15 + k(k(-2 + 5k) - 5t)) + 4ck^6(3 - 2k^2 + 26k^3 - 2kt)}{32k^{10}}$$
(2.45c)

$$\frac{J(a,d,k)}{\partial k} = \frac{1}{8k^{11}} \left( -315a^2(45 - 2k^2 + 4k^3 - 9kt) - 15adk^3(21 - 2k^2 + 4k^3 - 6kt) + d^2k^6(-6 + 2k^2 - 13k^3 + 3kt) \right)$$
(2.45d)

For this we get k = 0.611, d = -61.345a, E = 8.616 and  $R_{50} = a(r^3 - 61.345)e^{-0.611r}$ .

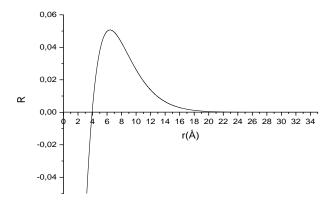


Fig.2.12. The wave function  $R_{50}$  for  $V(r) = -\frac{1}{r} + r$ .

We may describe the generic LaGrange functional as follows for various values of  $\beta$ , for instance  $\beta = 100$  with the same wave function for the basic level energy:

$$J(a,b,d,k) = \frac{1}{16k^8} (k^2(b^2(1500 + k(k(-3 + 2k) - 6t)) + 2abk(600 + k((-2k)k - 3t)) + 2a^2k^2(150 + k((-1 + k)k - t))) + 3d^2(5250 + k(k(-5 + 3k) - 15t)) + 6dk(b(1500 + k((-2 + k)k - 5t)) - ak(-500 + k^2 + 2kt)))$$
(2.46a)

The stationary condition provides the following expressions:

$$\frac{\partial J(a,b,d,k)}{\partial a} = 1/(16k^8) \left( k^2 \left( 2bk(600 + k((-2+k)k - 3t)) + 4a k^2 (150 + k((-1+k)k - t)) \right) - 6dk^2 \left( -500 + k^2 + 2kt \right) \right)$$
(2.46b)

$$\frac{\partial J(a,b,d,k)}{\partial b} = \frac{1}{16k^8} (k^2 (2b(1500 + k(k(-3+2k) - 6t)) + 2ak(600 + k((-2+k)k - 3t))) + 6dk(1500 + k((-2+k)k - 5t)))$$
(2.46c)

$$\frac{\partial J(a,b,d,k)}{\partial d} = \frac{1}{16k^8} \left( 6d(5250 + k(k(-5+3k) - 15t)) + 6k(b(1500 + k((-2 + k)k - 5t)) - ak(-500 + k^2 + 2kt)) \right)$$
(2.46d)

$$\frac{\partial J(a,b,d,k)}{\partial k} = -\frac{1}{16k^9} (45d^2(2800 - 2k^2 + k^3 - 7kt) + 12dk(b(5250 - 5k^2 + 2k^3 - 15kt) + ak(1500 - 2k^2 - 5kt)) + 2k^2(2abk(1500 - 3k^2 + k^3 - 6kt) + 3b^2(1500 - 2k^2 + k^3 - 5kt) + a^2k^2(600 - 2k^2 + k^3 - 3kt)))$$
(2.46e)

For this we get k = 8.905, b = 5.823a, d = 43.301a, E = 46.441

$$R_{00} = a(1 + 5.823r + 43.301r^2) e^{-8.905 r}$$

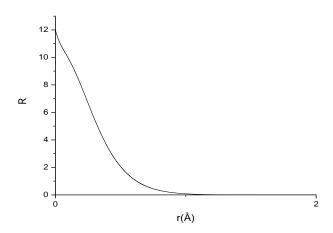


Fig.2.13. The wave function  $R_{00}$  for  $V(r) = -\frac{1}{r} + 100 r$ .

We'll proceed on to examine a further wave function,  $R = (ar^4 + br^2 + d)e^{-kr}$ , which we'll insert in equation (2.42) to represent the generic LaGrange functional as follows:

$$J(a,b,d,k) = \frac{1}{16k^{12}} (315a^2(24750 + k(k(-9 + 5k) - 45t)) + 3b^2k^4(5250 + k(k(-5 + 3k) - 15t)) + 2d^2k^8(150 + k((-1 + k)k - t)) - 6bdk^6(-500 + k^2 + 2kt) - 15ak^2(2dk^2(-1050 + k^2 + k^3 + 3kt) + b(-37800 + 3k((7 - 2k)k + 28t))))$$
(2.47a)

The stationary condition provides the following expressions:

$$\frac{\partial J(a,b,d,k)}{\partial a} = \frac{1}{16k^{12}} (630a(24750 + k(k(-9 + 5k) - 45t)) 
- 15k^{2}(2dk^{2}(-1050 + k^{2} + k^{3} + 3kt) + b(-37800 + 3k((7 - 2k)k + 28t)))) 
\frac{\partial J(a,b,d,k)}{\partial b} = \frac{1}{16k^{12}} (6bk^{4}(5250 + k(k(-5 + 3k) - 15t)) 
- 6dk^{6}(-500 + k^{2} + 2kt) 
- 15ak^{2}(-37800 + 3k((7 - 2k)k + 28t)))$$
(2.47b)

$$\frac{\partial J(a,b,d,k)}{\partial d} = \frac{1}{16k^{12}} (4dk^8 (150 + k((-1+k)k - t)) - 6bk^6 (-500 + k^2 + 2kt) - 30ak^4 (-1050 + k^2 + k^3 + 3kt))$$
(2.47d)

$$\frac{\partial J(a,b,d,k)}{\partial k} = \frac{1}{16k^{13}}(-14175a^{2}(6600 - 2k^{2} + k^{3} - 11kt) - 45b^{2}k^{4}(2800 - 2k^{2} + k^{3} - 7kt) - 2d^{2}k^{8}(600 - 2k^{2} + k^{3} - 3kt) + 12bdk^{6}(-1500 + 2k^{2} + 5kt) + 30ak^{2}(-21b(9000 - 4k^{2} + k^{3} - 18kt) + dk^{2}(-8400 + 6k^{2} + 5k^{3} + 21kt)))$$
(2.47e)

For this we get k = 9.245, b = -0.117a, d = -0.0021a, E = 85.659 and

$$R_{10} = a(r^4 - -0.117r^2 - 0.0021)e^{-9.245r}$$
.

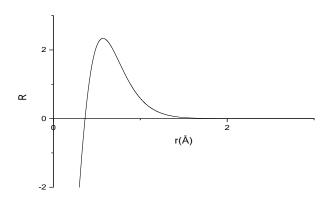


Fig.2.14. The wave function 
$$R_{10}$$
 for  $V(r) = -\frac{1}{r} + 100 r$ .

We'll proceed on to examine a further wave function,  $R = (ar^3 + d)e^{-kr}$ , which we'll insert in equation (2.42) to represent the generic LaGrange functional as follows:

$$J(a,b,d,k) = \frac{1}{32k^{10}} (45a^2(12600 + k(k(-7 + 16k) - 28t)) + 12adk^3(1500 + k(k(-2 + 5k) - 5t)) + 4d^2k^6(150 + k(k(-1 + 13k) - t)))$$
(2.48a)

The stationary condition provides the following expressions:

$$\frac{J(a,b,d,k)}{\partial a} = \frac{1}{32k^{10}}(90a(12600 + k(k(-7 + 16k) - 28t)) + 12dk^{3}(1500 + k(k(-2 + 5k) - 5t)))$$
(2.48b)

$$\frac{J(a,b,d,k)}{\partial d} = \frac{1}{32k^{10}} (12ak^3(1500 + k(k(-2+5k) - 5t)) + 8dk^6(150 + k(k(-1+5k) - 5t)) + 8dk^6(150 + k(k(-1+5k$$

$$\frac{J(a,b,d,k)}{\partial k} = \frac{1}{8k^{11}} (-315a^2(4500 - 2k^2 + 4k^3 - 9kt) - 30ack^3(1050 - k^2 + 2k^3 - 3kt) + d^2k^6(-600 + 2k^2 - 13k^3 + 3kt))$$
(2.48d)

For this we get k = 2.771, d = -0.665a, E = 192.146 and

$$R_{50} = a(r^3 - 0.665)e^{-2.771r}$$
.

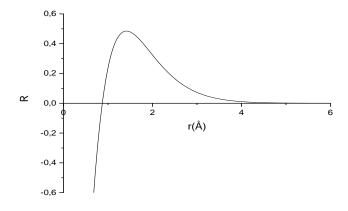


Fig.2.15. The wave function  $R_{50}$  for  $V(r) = -\frac{1}{r} + 100 r$ .

With the same wave function for the basic level energy and different values of  $\beta$ , such as  $\beta = 0.01$ , the generic Lagrange functional may be stated as follows:

$$J(a,b,d,k) = \frac{1}{3200k^8} (2k^2(5b^2(3+20k(k(-3+2k)-6t))+4abk(3+50k((-2+k)k-3t))+a^2k^2(3+200k((-1+k)k-t))) + 15d^2(21+40k(k(-5+3k)-15t))+60dk(b(3+20k((-2+k)k-5t))+ak(1-20k(k+2t))))$$
(2.49a)

The stationary condition provides the following expressions:

$$\frac{\partial J(a,b,d,k)}{\partial a} = \frac{1}{3200k^8} (2k^2(4bk(3+50k((-2+k)k-3t)) + 2ak^2(3 + 200k((-1+k)k-t))) + 60dk^2(1-20k(k+2t)))$$
(2.49b)

$$\frac{\partial J(a,b,d,k)}{\partial b} = \frac{1}{3200k^8} (2k^2 (10b(3+20k(k(-3+2k)-6t)) + 4ak(3 + 50k((-2+k)k-3t))) + 60dk(3+20k((-2+k)k-5t)))$$
(2.49c)

$$\frac{\partial J(a,b,d,k)}{\partial d} = \frac{1}{3200k^8} (30d(21 + 40k(k(-5+3k) - 15t)) + 60k(b(3 + 20k((-2+k)k - 5t)) + ak(1 - 20k(k + 2t))))$$
(2.49d)

$$\frac{\partial J(a,b,d,k)}{\partial k} = \frac{1}{800k^9} (-90d^2(7 - 50k^2 + 25k^3 - 175kt) - 15dk(b(21 - 200k^2 + 80k^3 - 600kt) - 2ak(-3 + 40k^2 + 100kt)) + k^2(-10abk(3 - 60k^2 + 20k^3 - 120kt) - 15b^2(3 - 40k^2 + 20k^3 - 100kt) + 2a^2k^2(-3 + 100k^2 - 50k^3 + 150kt))$$
(2.49e)

For this we get k = 0.447, b - 0.0642a,  $d = 4.593 \times 10^{-8}$  and E = -0.221

$$R_{00} = (1 - 0.0642r + 4.593 \times 10^{-8}r^2)e^{-0.447r}.$$

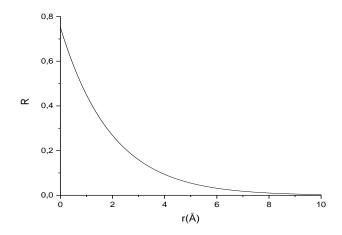


Fig.2.16. The wave function  $R_{00}$  for  $V(r) = -\frac{1}{r} + 0.01 r$ .

We'll proceed on to examine a further wave function,  $(ar^4 + br^2 + c)e^{-kr}$ , which we'll insert in equation (2.42) to represent the generic LaGrange functional as follows:

$$J(a,b,d,k) = \frac{1}{3200k^{12}}(1575a^{2}(99 + 40k(k(-9 + 5k) - 45t)) + 15b^{2}k^{4}(21 + 40k(k(-5 + 3k) - 15t)) + 2d^{2}k^{8}(3 + 200k((-1 + k)k - t)) - 60bdk^{6}(-1 + 20k(k + 2t)) - 30ak^{2}(dk^{2}(-21 + 200k(k + k^{2} + 3t)) + 6b(-63 + 50k((7 - 2k)k + 28t))))$$
(2.50a)

For this we get k = 0.447, b - 0.0642a,  $c = 4.593 \times 10^{-8}$ 

The stationary condition provides the following expressions:

$$\frac{\partial J(a,b,c,k)}{\partial a} = \frac{1}{3200k^{12}} (3150a(99 + 40k(k(-9 + 5k) - 45t)) - 30k^{2}(ck^{2}(-21 + 200k(k + k^{2} + 3t)) + 6b(-63 + 50k((7 - 2k)k + 28t)))) 
+ 200k(k + k^{2} + 3t)) + 6b(-63 + 50k((7 - 2k)k + 28t))))$$

$$\frac{\partial J(a,b,d,k)}{\partial b} = \frac{1}{3200k^{12}} (30bk^{4}(21 + 40k(k(-5 + 3k) - 15t)) - 60cd(-1 + 200k(k(-5 + 3k) - 15t))) - 60cd(-1 + 200k(k(-5 + 3k) - 15t))) - 60cd(-1 + 200k(k(-5 + 3k) - 15t))) - 60cd(-1 + 200k(k(-5 + 3k) - 15t)))$$

+20k(k+2t))  $-180ak^{2}(-63+50k((7-2k)k+28t)))$ 

$$\frac{\partial J(a,b,d,k)}{\partial k} = \frac{1}{800k^{13}} (-14175a^2(33 - 100k^2 + 50k^3 - 550kt) - 3150abk^2(9) 
- 40k^2 + 10k^3 - 180kt) - 90b^2k^4(7 - 50k^2 + 25k^3 - 175kt) 
+ 30bdk^6(-3 + 40k^2 + 100kt) + 2d^2k^8(-3 + 100k^2 - 50k^3) 
+ 150kt) + 60adk^4(-21 + 150k^2 + 125k^3 + 525kt))$$
(2.50d)

For this we get k = 0.497, b 141.61a, d = -1882.37a, E = 0.0358

$$R_{10} = (1 - 0.0642r + 4.593 \times 10^{-8}r^2)e^{-0.447r}$$
.

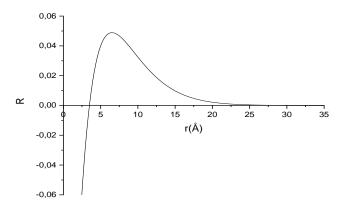


Fig.2.17. The wave function  $R_{10}$  for  $V(r) = -\frac{1}{r} + 0.01 r$ .

We'll continue with another wave function  $R = (ar^3 + b)e^{-kr}$  which we substitute it in the equation (2.42) for this way we can expressed the general functional of LaGrange as below:

$$J(a,b) = \frac{1}{3200k^{12}} (1575a^2(99 + 40k(k(-9 + 5k) - 45t)) + 15b^2k^4(21 + 40k(k(-5 + 3k) - 15t)) + 2b^2k^8(3 + 200k((-1 + k)k - t)) - 60bck^6(-1 + 20k(k + 2t)) - 30ak^2(ck^2(-21 + 200k(k + k^2 + 3t)) + 6b(-63 + 50k((7 - 2k)k + 28t))))$$
(2.51a)

The stationary condition provides the following expressions:

$$\frac{\partial J(a,b,k)}{\partial a} = \frac{1}{1600k^{10}} (45a^2(63+50k(k(-7+16k)-28t)) + 30abk^3(3 + 20k(k(-2+5k)-5t)) + b^2k^6(3+200k(k(-1+13k)-t)))$$
(2.51b)

$$\frac{\partial J(a,b,k)}{\partial b} = \frac{1}{1600k^{10}} (90a(63 + 50k(k(-7 + 16k) - 28t)) + 30bk^{3}(3 + 20k(k(-2 + 5k) - 5t)))$$
(2.51c)

$$\frac{\partial J(a,b,k)}{\partial k} = \frac{1}{800k^{11}} \left( -15abk^3 (21 - 200k^2 + 400k^3 - 600kt) - 1575a^2 (9 - 40k^2 + 80k^3 - 180kt) + 2b^2k^6 (-3 + 100k^2 - 650k^3 + 150kt) \right)$$
(2.51d)

For this we get k = 0.148, b = -4094.7, E = 0.0358 and

$$R_{10} = (1 - 0.0642r + 4.593 \times 10^{-8}r^2)e^{-0.447r}$$

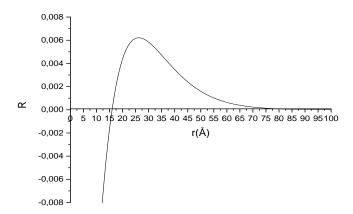


Fig.2.18. The wave function  $R_{50}$  for  $V(r) = -\frac{1}{r} + 0.01 r$ .

The same methodology was used to obtain the findings, which are displayed in the table below and contrasted with reference to energies.

**Tab.2.5**. The eigenvalues for the potential  $V(r) = -\frac{1}{r} + r$ .

1	n	$E_{n0}$	Ref [35]
0	0	1.398693189852505	1.397875641660
	1	3.489277280271818	3.475086545396
	5	8.616348360276358	8.687914590401

**Tab.2.6.** The eigenvalues for the potential  $V(r) = -\frac{1}{r} + 100r$ .

1	n	$E_{n0}$	Ref [35]
	0	46.441191906167891	46.402258652779
0	1	85.659789498307922	85.339271687574
	5	192.14601869818213	192.850291861086

**Tab.2.7.** The eigenvalues for the potential  $V(r) = -\frac{1}{r} + 0.01r$ .

1	n	$E_{n0}$	Ref [35]
0	0	-0.221030225522051	-0.221030563404
	1	0.0348734315973113	0.034722241998
	5	0.3323785244213793	0.344602792592

According to the drawn figures 2.10,2.11 and 2.12 we noticed that the cases:

- n = 0: the curve has no node, so it corresponds to the ground state.
- n = 1:The curve has a node, so it corresponds to the first excited state.
- n = 5: the curve has more than one node, so it corresponds to the fifth excited state the same observations for the other figures.

Table 2.5, Table 2.6 and Table 2.7 displays the eigenvalues of the eigenvalues for the potentials  $V(r)=-\frac{1}{r}+1, V(r)=-\frac{1}{r}+100r$  and  $V(r)=-\frac{1}{r}+0.01r$  respectively. It observed that :

- When the values of  $\beta$  rise, so does the energy.
- A rise in  $\beta$  value corresponds with an increase in energy.
- The outcomes are in good agreement with the results in reference [35] with error of 0.003% to 0.7%.

Additionally, by setting the value of  $\beta$ , we compare the outcomes with fresh values of  $\alpha$ .

We will now begin by substituting the wave function  $R = (a + br + dr^2)e^{-kr}$  for  $\alpha = 0.6$  and the basic level energy n = 0 in the equation (2.42). In this manner, we may express LaGrange's overall functionality as follows:

$$J(a,b,d,k) = \frac{1}{160k^8} (2k^2(b^2(75 + k(k(-9 + 10k) - 30t)) + 2abk(30 + k(k(-6 + 5k) - 15t)) + a^2k^2(15 + 2k(k(-3 + 5k) - 5t))) + 45d^2(35 + 2k((-1 + k)k - 5t)) + 12dk(b(75 + k(k(-6 + 5k) - 25t)) + ak(25 - 3k^2 - 10kt)))$$
(2.52a)

The stationary condition provides the following expressions.

$$\frac{\partial J(a,b,d,k)}{\partial a} = \frac{1}{160k^8} (2k^2(2bk(30 + k(k(-6+5k) - 15t)) + 2ak^2(15 + 2k(k(-3+5k) - 5t))) + 12dk^2(25 - 3k^2 - 10kt))$$
(2.52b)

$$\frac{\partial J(a,b,d,k)}{\partial b} = \frac{1}{160k^8} (2k^2(2b(75 + k(k(-9 + 10k) - 30t)) + 2ak(30 + k(k(-6 + 5k) - 15t))) + 12dk(75 + k(k(-6 + 5k) - 25t)))$$
(2.52c)

$$\frac{\partial J(a,b,d,k)}{\partial d} = \frac{1}{160k^8} (90d(35 + 2k((-1+k)k - 5t)) + 12k(b(75 + k(k(-6 + 5k) - 25t)) + ak(25 - 3k^2 - 10kt)))$$
(2.52d)

$$\frac{\partial J(a,b,d,k)}{\partial k} = -\frac{1}{80k^9} (45d^2(140 - 6k^2 + 5k^3 - 35kt) + 2k^2(2abk(75 - 9k^2 + 5k^3 - 30kt) + 3b^2(75 - 6k^2 + 5k^3 - 25kt) + a^2k^2(30 - 6k^2 + 5k^3 - 15kt)) + 6dk(5b(105 - 6k^2 + 4k^3 - 30kt) - 2ak(-75 + 6k^2 + 25kt)))$$
(2.52e)

We always get this using Mathematica k = 0.753, b = 0.181a,  $d = -3.92 \times 10^{-14} a$ , E = 1.811

**Tab.2.8.** The eigenvalues for the potential  $V(r) = -\frac{\alpha}{r} + \beta r$  for  $\beta = 1$ .

a	$E_{00}$	[37]	а	$E_{00}$	[36]
0.1	2.255685737118077	2.253678	1	1.398693189852503	1.397877
0.2	2.169149258473687	2.167316	1.1	1.291440450127502	1.290709
0.3	2.196094631930914	2.078949	1.2	1.181487676919001	1.180836
0.4	1.990021925905266	1.988504	1.3	1.068754023134303	1.068171
0.5	1.897281086457094	1.895904	1.4	0.953158984773472	0.952644
0.6	1.802319830942286	1.801074	1.5	0.834622612633280	0.834162
0.7	1.705059950548391	1.703935	1.6	0.713065740626510	0.712662
0.8	1.605422270956004	1.60441	1.7	0.588410191334066	0.588049
0.9	1.503326850255253	1.502415	1.8	0.460578976490569	0.460266

In this step, we compare the results with new values of  $\beta$  by fixing the value of  $\beta$ .

<b>Tab.2.9.</b> The eigenvalues for the potential $V(r)$	$=-\frac{\alpha}{r}+\beta r$ for $\alpha=1$ .
--	---

β	$E_{00}$	Ref [37]
0	2.338 107 410 458 750	2.353 435 026 671 857
0.2	2.167 316 208 771 731	2.180 529 351 111 987
0.4	1.988 503 899 749 943	1.992 373 140 519 031
0.6	1.801 073 805 646 145	1.8106755016440432
0.8	1.604 408 543 235 973	1.612 503 175 709 080
1	1.397 875 641 659 578	1.398 693 189 852 505
1.2	1.180 833 939 744 863	1.181 504 444 955 205
1.4	1.180 833 939 744 863	0.957 291 510 592 218
1.6	0.712 657 680 462 421	0.716 473 847 728 527
1.8	0.460 260 113 875 977	0.463377 533 653 339

Table 2.8 displays the eigenvalues for the potential  $V(r) = -\frac{\alpha}{r} + \beta r$  for  $\beta = 1$ . As the value of  $\beta$  increases, we see a decrease in energy levels, and the results are very close with another works mentioned in [31] and [32] with error of 0.0008%.

Table 2.9 displays the eigenvalues for the potential  $V(r) = -\frac{\alpha}{r} + \beta r$  for  $\alpha = 1$ . As the value of  $\beta$  increases, we see a decrease in energy levels, and the results are very close with another works mentioned in [31] and [32] with error of 0.0008%.

The presented table show that the semi-inverse variational method successfully obtains eigenvalues for different potentials. The results are in good agreement with known references, which indicates the accuracy and efficacy of this method in solving quantum mechanics problems involving various potentials. Furthermore, by fixing the value of  $\beta$  and comparing the outcomes with new values of  $\alpha$ , the study explores how the eigenvalues change with different parameters. This analysis provides valuable insights into the behaviour of the system with varying potential parameters, revealing the sensitivity of the quantum states to changes in the potential function. Overall, the tables reinforce the validity of the semi-inverse variational method and its capability to analyse complex quantum potentials. The method's success in obtaining accurate eigenvalues for different potentials makes it a promising tool in the study of quantum mechanics, offering valuable information about the behaviour of quantum systems under various conditions.

### 2.2.3. Anharmonic potential

For  $\hbar = m = 1$ , we express the Lagrange equation as below:

$$J(r;R;R_r) = \int_{0}^{+\infty} \frac{1}{2} \left[ \left( \frac{dR}{dr} \right)^2 + \left( \frac{l(l+1)}{2r^2} - r - \lambda r^{2\mu} - E \right) R^2 \right] r^2 dr$$
 (2.53)

and as a result, we may use, for instance,  $\lambda = \frac{1}{10}$  and  $\mu = 2$ . In these stages, we have established  $V(r) = r + \lambda r^{2\mu}$  as anharmonic potential, where  $(r) = ar^b e^{-kr^2}$  is the radial trial function. In the equation (2.53), R(r) is substituted, and we may formulate the generic LaGrange function as follows:

$$J(a,b,k) = \frac{1}{5} 2^{-\frac{19}{2}-b} a^2 k^{-\frac{7}{2}-b} (15 + 46b + 36b^2 + 8b^3 + 40(3 + 4b(2+b))k + 160(3 + 4b)k^3 - 160k^2(t+2bt))$$
(2.54a)

The stationary condition provides the following expressions:

$$\frac{\partial J(a,b,k)}{\partial a} = \frac{1}{5} 2^{-\frac{17}{2}-b} ak^{-\frac{7}{2}-b} (15 + 46b + 36b^2 + 8b^3 + 40(3 + 4b(2+b))k + 160(3 + 4b)k^3 - 160k^2(t+2bt))$$
(2.54b)

$$\frac{\partial J(a,b,k)}{\partial b} = -\frac{1}{5} 2^{-\frac{19}{2} - b} a^2 k^{-\frac{7}{2} - b} (-46 - 320k - 640k^3 + 320k^2t + 15\text{Log}[2]$$

$$+ 8b^3 \text{Log}[2] + 120k \text{Log}[2] + 480k^3 \text{Log}[2] - 160k^2t \text{Log}[2]$$

$$+ b(-72 + 320k(-1 + \text{Log}[2]) + 46\text{Log}[2] + 640k^3 \text{Log}[2]$$

$$- 320k^2t \text{Log}[2]) + 4b^2(-6 + 40k \text{Log}[2] + \text{Log}[512]) + (8b^3 + 4b^2(9 + 40k) + b(46 + 320k + 640k^3 - 320k^2t) + 5(3 + 24k + 96k^3 - 32k^2t))\text{Log}[k])$$

$$(2.54c)$$

$$\frac{\partial J(a,b,k)}{\partial k} = -\frac{1}{5}2^{-\frac{19}{2}-b}a(1+2b)k^{-\frac{9}{2}-b}(8b^3 + 20b^2(3+8k) + 2b(71+320k + (2.54d)))$$

$$320k^3 - 160k^2t) + 15(7+40k+32k^3 - 32k^2t)$$

For this we get  $k \approx 0.553$ ,  $b \approx -1.009$ ,  $E \approx 1.066$  and  $R_{10} = ar^{-1.009}e^{-0.553r^2}$ .

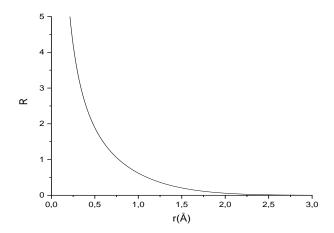


Fig.2.19. The wave function  $R_{00}$  for  $\lambda = 0.1$ .

We'll proceed on to examine a further wave function,  $ae^{-kr^2}$ , which we'll insert in equation (2.53) to represent the generic LaGrange functional as follows:

$$J(a,k) = \frac{a^2 \sqrt{\frac{\pi}{2}} (3 + 8k(3 + 12k^2 - 4kt))}{512k^{7/2}}$$
(2.55a)

The stationary condition provides the following expressions:

$$\frac{\partial J(a,k)}{\partial a} = \frac{a\sqrt{\frac{\pi}{2}}(3 + 8k(3 + 12k^2 - 4kt))}{256k^{7/2}}$$
(2.55b)

$$\frac{\partial J(a,k)}{\partial a} = \frac{a\sqrt{\frac{\pi}{2}}(3+8k(3+12k^2-4kt))}{256k^{7/2}}$$

$$\frac{\partial J(a,k)}{\partial k} = -\frac{3a^2\sqrt{\frac{\pi}{2}}(7+40k+32k^3-32k^2t)}{1024k^{9/2}}$$
(2.55b)

For this we get  $k \approx 0.596$ ,  $E \approx 3.31$  and  $R_{10} = ae^{-0.596r^2}$ .

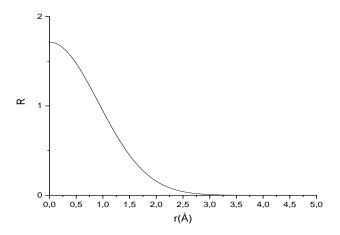


Fig.2.20. The wave function  $R_{10}$  for  $\lambda = 0.1$ .

We'll proceed on to examine a further wave function,  $are^{-kr^2}$ , which we'll insert in equation (2.53) to represent the generic LaGrange functional as follows:

$$J(a,k) = \frac{3a^2\sqrt{\frac{\pi}{2}}(7 + 8k(5 + 20k^2 - 4kt))}{2048k^{9/2}}$$
(2.56a)

The stationary condition provides the following expressions.

$$\frac{\partial J(a,k)}{\partial a} = \frac{3a\sqrt{\frac{\pi}{2}}(7 + 8k(5 + 20k^2 - 4kt))}{1024k^{9/2}}$$
(2.56b)

$$\frac{\partial J(a,k)}{\partial a} = \frac{3a\sqrt{\frac{\pi}{2}}(7 + 8k(5 + 20k^2 - 4kt))}{1024k^{9/2}}$$

$$\frac{\partial J(a,k)}{\partial k} = -\frac{3a^2\sqrt{\frac{\pi}{2}}(63 + 280k + 480k^3 - 160k^2t)}{4096k^{11/2}}$$
(2.56b)

For this we get  $k \approx 0.625, E \approx 5.685$  and  $R_{10} = are^{-0.625r^2}$ .

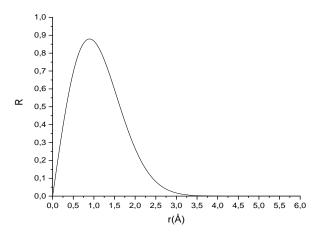


Fig.2.21. The wave function  $R_{20}$  for  $\lambda = 0.1$ .

We'll proceed on to examine a further wave function,  $(ar^2 + b)e^{-kr^2}$ , which we'll insert in equation (2.53) to represent the generic LaGrange functional as follows:

$$J(a,b,k) = \frac{1}{8192k^{11/2}} \left( \sqrt{\frac{\pi}{2}} \left( 24abk(7 + 8k(5 + 4k(k - t))) + 3a^2(63 + 8k(35 + 44k^2 - 20kt)) + 16b^2k^2(3 + 8k(3 + 12k^2 - 4kt))) \right)$$
(2.57a)

The stationary condition provides the following expressions:

$$\frac{\partial J(a,k)}{\partial a} = \frac{\sqrt{\frac{\pi}{2}} \left(24bk(7 + 8k(5 + 4k(k-t))) + 6a(63 + 8k(35 + 44k^2 - 20kt))\right)}{8192k^{11/2}}$$
(2.57b)

$$\frac{\partial J(a,k)}{\partial b} = \frac{\sqrt{\frac{\pi}{2}}(24ak(7+8k(5+4k(k-t)))+32bk^2(3+8k(3+12k^2-4kt)))}{8192k^{11/2}}$$
(2.57c)

$$\frac{\partial J(a,k)}{\partial k} = -\frac{1}{16384k^{13/2}} \left( 3\sqrt{\frac{\pi}{2}} (a^2(693 + 2520k + 1760k^3 - 1120k^2t) + 8abk(63 + 280k + 96k^3 - 160k^2t) + 16b^2k^2(7 + 40k + 32k^3 - 32k^2t)) \right)$$
(2.57d)

For this we get  $k \approx 0.65$ , b = -1.21,  $E \approx 8.36$  and  $R_{30} = a(r^2 - 1.21)e^{-0.65r^2}$ 

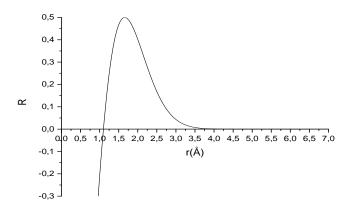


Fig.2.22. The wave function  $R_{30}$  for  $\lambda = 0.1$ .

We'll proceed on to examine a further wave function,  $ar^3e^{-kr^2}$ , which we'll insert in equation (2.53) to represent the generic LaGrange functional as follows:

$$J(a,k) = \frac{21a^2\sqrt{\frac{\pi}{2}}(99 + 40k(9 + 36k^2 - 4kt))}{32768k^{13/2}}$$
(2.58a)

The stationary condition provides the following expressions:

$$\frac{\partial J(a,k)}{\partial a} = \frac{21a\sqrt{\frac{\pi}{2}}(99 + 40k(9 + 36k^2 - 4kt))}{16384k^{13/2}}$$
(2.58b)

$$\frac{\partial J(a,k)}{\partial a} = \frac{21a\sqrt{\frac{\pi}{2}}(99 + 40k(9 + 36k^2 - 4kt))}{16384k^{13/2}}$$

$$\frac{\partial J(a,k)}{\partial k} = -\frac{189a^2\sqrt{\frac{\pi}{2}}(143 + 440k + 1120k^3 - 160k^2t)}{65536k^{15/2}}$$
(2.58c)

For this we get  $k \approx 0.643$ ,  $E \approx 10.766$  and  $R_{40} = ar^3 e^{-0.643r^2}$ 

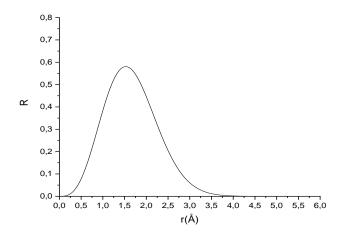


Fig.2.23. The wave function  $R_{40}$  for  $\lambda = 0.1$ .

**Tab.2.10.** The eigenvalues of the quartic anharmonic oscillator  $\mu=2$  for var quantum number n and  $\lambda$  anharmonicity.

λ	n = 0	Ref [38]	n = 1	Ref [38]
0.00001	1	1.00000749987	3.000037499062546	3.000037498969
0.0001	1.00007498937795214	1.00007486926	3.000374906296839	3.000374896936
0.001	1.00074894044248497	1.00074869267	3.003740671569707	3.003739748168
0.01	1.00739660055331098	1.00737367208	3.036606515172337	3.036525304513
0.1	1.06656814715510628	1.06528550954	3.310312805305138	3.306872013152

λ	n = 2	Ref [38]	n = 3	Ref	[38]
0.00001	5.000087496937712	5.000097496157	7.000187490813372	7.000187	490157290
0.0001	5.000874693964177	5.000974615938	7.001882553100586	7.001874	01666766
0.001	5.008719587426195	5.009711872788	7.018658988177776	7.018652	59205752
0.01	5.084634061035908	5.093939132742	7.179090409551282	7.178573	18070050
0.1	5.684998302958418	5.747959268834	8.368186390838924	8.352677	82578575
λ	n = 4		Ref [38]	Ref [38]	
0.00001	9.000247486388995		9.00030747969643		
0.0001	9.002473640245217		9.00307297204461		
0.001	9.024615351112462		9.03054956607471		
0.01	9.235199339552453		9.28947981631189		
0.1	10.766335921616188		11.0985956226	5330	

According to the drawn figures 2.20,2.21,2.22 and 2.23 we noticed that the cases:

- n = 1: the curve has no node, so it corresponds to the ground state.
- n =2:The curve has a node, so it corresponds to the first excited state.
- n = 3: the curve has two nodes, so it corresponds to the second excited state.
- n =4: the curve has more than two node, so it corresponds to the third excited state.

Table 2.10 The eigenvalues of the quartic anharmonic oscillator  $\mu$ =2 for var quantum number n and  $\lambda$  anharmonicity. It pointed out:

- When the values of  $\lambda$  rise, so does the energy.
- A rise in quantum number n corresponds with an increase in energy.
- The outcomes are in good agreement with the results in reference [38] with maximum error of 0.03 %.

Additionally, we may utilize examples like,  $\lambda = \frac{1}{10}$  and  $\mu = 3$ . In these stages, we have established  $V(r) = r + \lambda r^{2\mu}$  as anharmonic potential, where  $R(r) = ar^b e^{-kr^2}$  is the radial trial function. In the equation (2.53), R(r) is substituted, and we may formulate the generic Lagrange function as follows:

$$J(a,b,k) = \frac{1}{5} 2^{-\frac{23}{2}-b} a^2 k^{-\frac{9}{2}-b} (105 + 352b + 344b^2 + 128b^3 + 16b^4 + 160(3 + 4b(2+b))k^2 + 640(3+4b)k^4 - 640k^3(t+2bt))$$
(2.59a)

The stationary condition provides the following expressions.

$$\frac{\partial J(a,b,k)}{\partial a} = \frac{1}{5} 2^{-\frac{21}{2} - b} a k^{-\frac{9}{2} - b} (105 + 352b + 344b^2 + 128b^3 + 16b^4 + 160(3) + 4b(2+b)) k^2 + 640(3+4b) k^4 - 640k^3(t+2bt))$$

$$\frac{\partial J(a,b,k)}{\partial b} = -\frac{1}{5} 2^{-\frac{23}{2} - b} a^2 k^{-\frac{9}{2} - b} (-352 - 1280k^2 - 2560k^4 + 1280k^3t + 105\text{Log}[2] + 16b^4\text{Log}[2] + 480k^2\text{Log}[2] + 1920k^4\text{Log}[2] + 640k^3t\text{Log}[2] + 8b^2(-48 + 43\text{Log}[2] + 80k^2\text{Log}[2]) + 16b(-43) + 80k^2(-1 + \text{Log}[2]) + 22\text{Log}[2] + 160k^4\text{Log}[2] - 80k^3t\text{Log}[2]) + 64b^3(-1 + \text{Log}[4]) + (128b^3 + 16b^4 + 8b^2(43 + 80k^2) + 5(21) + 96k^2 + 384k^4 - 128k^3t) + 32b(11 + 40k^2 + 80k^4) - 40k^3t))\text{Log}[k])$$

$$(2.59b)$$

$$\frac{\partial J(a,b,k)}{\partial k} = -\frac{1}{5} 2^{-\frac{25}{2}-b} a^2 (1+2b) k^{-\frac{11}{2}-b} (192b^3 + 16b^4 + 8b^2 (103+80k^2) + 15(63+160k^2 + 128k^4 - 128k^3t) + 16b(93+160k^2 + 160k^4 - 80k^3t))$$
(2.59d)

For this we get  $k \approx 0.62, b \approx -1.06, E \approx 1.1236$  and  $R_{00} = ar^{-1.06}e^{-0.62r^2}$ .

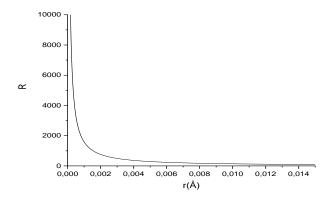


Fig.2.24. The wave function  $R_{00}$  for  $\lambda = 0.1$ .

We'll proceed on to examine a further wave function,  $ae^{-kr^2}$ , which we'll insert in equation (2.53) to represent the generic LaGrange functional as follows:

$$J(a,k) = \frac{a^2 \sqrt{\frac{\pi}{2}} (21 + 32k^2 (3 + 12k^2 - 4kt))}{2048k^{9/2}}$$
(2.60a)

The stationary condition provides the following expressions.

$$\frac{\partial J(a,k)}{\partial a} = \frac{a\sqrt{\frac{\pi}{2}}(21 + 32k^2(3 + 12k^2 - 4kt))}{1024k^{9/2}}$$
(2.60b)

$$\frac{\partial J(a,k)}{\partial k} = \frac{3a^2\sqrt{\frac{\pi}{2}}(63 + 160k^2 + 128k^4 - 128k^3t)}{4096k^{11/2}}$$
(2.60c)

For this we get  $k \approx 0.741$ ,  $E \approx 3.638$  and  $R_{10} = ae^{-0.741r^2}$ .

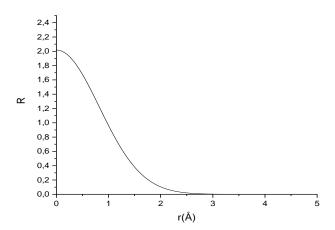


Fig.2.25. The wave function  $R_{10}$  for  $\lambda = 0.1$ .

We'll proceed on to examine a further wave function,  $are^{-kr^2}$ , which we'll insert in equation (2.53) to represent the generic LaGrange functional as follows:

$$J(a,k) = \frac{3a^2\sqrt{\frac{\pi}{2}}(63 + 32k^2(5 + 20k^2 - 4kt))}{8192k^{11/2}}$$
(2.61a)

The stationary condition provides the following expressions.

$$\frac{\partial J(a,k)}{\partial a} = \frac{3a\sqrt{\frac{\pi}{2}}(63 + 32k^2(5 + 20k^2 - 4kt))}{4096k^{11/2}}$$
(2.61b)

$$\frac{\partial J(a,k)}{\partial k} = -\frac{3a^2\sqrt{\frac{\pi}{2}}(693 + 1120k^2 + 1920k^4 - 640k^3t)}{16384k^{13/2}}$$
(2.61c)

For this we get  $k \approx 0.826$  ,  $E \approx 6.517$  and  $R_{20} = are^{-0.826r^2}$ 

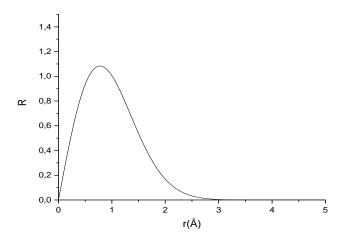


Fig.2.26. The wave function  $R_{20}$  for  $\lambda = 0.1$ .

We'll proceed on to examine a further wave function,  $(ar^2 + b)e^{-kr^2}$ , which we'll insert in equation (2.53) to represent the generic LaGrange functional as follows:

$$J(a,b,k) = \frac{1}{32768k^{13/2}} \left( \sqrt{\frac{\pi}{2}} (24abk(63 + 32k^2(5 + 4k(k - t))) + 3a^2(693 + 32k^2(35 + 44k^2 - 20kt)) + 16b^2k^2(21 + 32k^2(3 + 12k^2 - 4kt))) \right)$$
(2.62a)

The stationary condition provides the following expressions:

$$\frac{\partial J(a,b,k)}{\partial a} = \frac{1}{32768k^{13/2}} \left( \sqrt{\frac{\pi}{2}} \left( 24bk(63 + 32k^2(5 + 4k(k-t))) + 6a(693 + 32k^2(35 + 44k^2 - 20kt)) \right) \right)$$
(2.62b)

$$\frac{\partial J(a,b,k)}{\partial b} = \frac{1}{32768k^{13/2}} \left( \sqrt{\frac{\pi}{2}} \left( 24ak(63 + 32k^2(5 + 4k(k-t))) + 32bk^2(21 + 32k^2(3 + 12k^2 - 4kt)) \right) \right)$$
(2.62c)

$$\frac{\partial J(a,b,k)}{\partial k} = -\frac{1}{65536k^{15/2}} \left( 3\sqrt{\frac{\pi}{2}} \left( a^2(9009 + 10080k^2 + 7040k^4 - 4480k^3t) + 8abk(693 + 1120k^2 + 384k^4 - 640k^3t) + 16b^2k^2(63 + 160k^2 + 128k^4 - 128k^3t) \right)$$
(2.62d)

For this we get  $k \approx 0.91$  ,  $b \approx 0.928$  ,  $E \approx 10.41$  and  $R_{30} = (ar^2 + b)e^{-0.91r^2}$ .

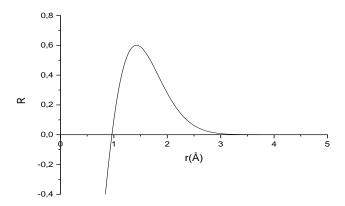


Fig.2.27. The wave function  $R_{30}$  for  $\lambda = 0.1$ .

We'll proceed on to examine a further wave function,  $ar^3e^{-kr^2}$ , which we'll insert in equation (2.53) to represent the generic LaGrange functional as follows:

$$J(a,k) = \frac{21a^2\sqrt{\frac{\pi}{2}}(1287 + 160k^2(9 + 36k^2 - 4kt))}{131072k^{15/2}}$$
(2.63a)

The stationary condition provides the following expressions:

$$\frac{\partial J(a,k)}{\partial a} = \frac{21a\sqrt{\frac{\pi}{2}}(1287 + 160k^2(9 + 36k^2 - 4kt))}{65536k^{15/2}}$$
(2.63b)

$$\frac{\partial J(a,k)}{\partial a} = \frac{21a\sqrt{\frac{\pi}{2}}(1287 + 160k^2(9 + 36k^2 - 4kt))}{65536k^{15/2}}$$

$$\frac{\partial J(a,k)}{\partial k} = -\frac{945a^2\sqrt{\frac{\pi}{2}}(429 + 352k^2 + 896k^4 - 128k^3t)}{262144k^{17/2}}$$
(2.63b)

For this we get  $k \approx 0.976$ ,  $E \approx 13.252$  and  $R_{40} = ar^3 e^{-0.976r^2}$ .

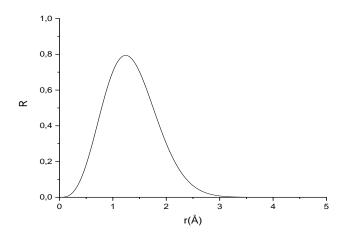


Fig.2.28. The wave function  $R_{40}$  for  $\lambda = 0.1$ .

**Tab.2.11.** The eigenvalues of the quartic anharmonic oscillator  $\mu = 3$  for var quantum number n and  $\lambda$  the anharmonicity.

λ	n = 0	Ref [38]	n = 1	Ref [38]
0.00001	1.000018748607233	1.00001874727074	3.0001312241703073	3.00013121319510
0.0001	1.000187360904953	1.00018722815368	3.001309926137334	3.00013121319510
0.001	1.0014438243267185	1.00184881557231	3.0128762758090533	3.01278096069010
0.01	1.0181884582082556	1.01674136375473	3.1122349397090883	3.10797991274458
0.1	1.1236163008323140	1.10908707846558	3.6383773830539057	3.59603692122046
λ	n = 2	Ref [38]	n = 3	Ref [38]
0.00001	5.000393610563672	5.00046851972698	7.0011935276829105	6.64439170865661
0.0001	5.0039236444618895	5.00466471129998	7.011738450196156	7.01172052372043
0.001	5.038070170954247	5.04479992578458	7.111425622658624	7.11009285586092
0.01	5.307421622580530	5.34742035100854	7.809742553943158	7.77769746656750
0.1	6.516671017926577	6.64439170865661	10.410088890873299	10.2378737214239
λ	n	= 4	Ref [38]	
0.00002	<b>9.001607458039079</b>		9.00241588390908	
0.0001	<b>0.0001</b> 9.015960134684915		9.02390720140850	
0.001	<b>0.001</b> 9.149659768475203		9.21858174873225	
0.01	<b>0.01</b> 10.042636379683646 10.4083375080935		080935	
<b>0.1</b> 13.252289307371183 14.3070400461209		461209		

According to the drawn figures 2.20,2.21,2.22 and 2.23 we noticed that the cases:

- n = 1: the curve has no node, so it corresponds to the ground state.
- n = 2: The curve has a node, so it corresponds to the first excited state.
- n = 3: the curve has two nodes, so it corresponds to the second excited state.
- n =4: the curve has more than two node, so it corresponds to the third excited state.

Table 2.10 The eigenvalues of the quartic anharmonic oscillator  $\mu$ =3 for var quantum number n and  $\lambda$  anharmonicity. It pointed out:

- The energy increases as the values of  $\lambda$  increase.
- An increase in energy is correlated with a rise in quantum number n.
- With a maximum inaccuracy of 0.07 percent, the results are in good agreement with the findings in reference [38].

The numerical simulations demonstrate the feasibility and accuracy of our semi-inverse variational approach in solving the Anharmonic potential problem. Our results align well with known references, showcasing the effectiveness of this method in tackling quantum mechanics challenges.

#### **Conclusion:**

In this work, we applied the semi-inverse variational method to study the nonlinear Schrödinger equations and calculate the bound energies for each potential. The simplicity and effectiveness of this method make it a valuable tool in practice. The technique developed here provides convenient and accurate approximations for solving Schrödinger problems by determining eigenvalues and eigenfunctions. Notably, the precise eigenvalues and eigenfunctions obtained in this study align with those reported in other references, validating the reliability of our approach. The outstanding results achieved through this study suggest that the semi-inverse variational method can find applications beyond our current scope. The potential of this method can be explored in other quantum physics domains, including the Klein-Gordon equation. Further research in this direction will be pursued in upcoming works. The semi-inverse variational method holds promise as a robust and versatile approach for tackling complex quantum mechanics problems. Its success in calculating bound energies for various potentials underscores its significance in quantum physics research. By offering accurate solutions to Schrödinger equations, this method opens new avenues for investigating the behavior of quantum systems and

their interactions in diverse physical scenarios. In conclusion, the findings of this study present a significant contribution to the field of quantum mechanics. The demonstrated efficiency and compatibility with established results affirm the potential of the semi-inverse variational method as an asset for future research in quantum physics and related disciplines.

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# Chapter 03

## THE RESOLUTION OF KLEIN GORDON EQUATION WITH THE SEMI INVERSE VARIATIONAL METHOD

Equation de Klein-Gordon

$$\square \psi(\vec{r},t) = \frac{m_0^2 c^2}{\hbar^2} \psi(\vec{r},t)$$

$$\Box = \nabla^2 - \frac{1}{c^2} \frac{\partial^2}{\partial t^2}$$

### **Chapter 3**

### RESOLUTION OF KLEIN GORDON EQUATION WITH THE SEMI INVERSE VARIATIONAL METHOD

### 3.1. The Klein Gordon equation:

#### 3.1.1. Introduction

It was separately proposed by Swedish physicist O. Klein, Soviet scientist V. A. Fok, and German physicist W. Gordon [1].

The Klein-Gordon equation is expressed for a free particle.

$$\hbar^2 \frac{d^2 \psi}{dt^2} = \hbar^2 c^2 \left( \frac{d^2 \psi}{dx^2} + \frac{d^2 \psi}{dy^2} + \frac{d^2 \psi}{dz^2} \right) - m^2 c^4 \psi$$
 (3.1)

This equation, which goes like this:  $\rho = p^2c^2 + m^2c^4$  where m is the particle's mass and c is the speed of light, describes the relativistic connection between a particle's energy £ and momentum p.

The function  $\psi(x, y, z, t)$ , which is just a function of the coordinates (x, y, z) and the time (t), is the answer to the equation. Since the  $\pi$ -meson and the K-meson fall into this category, the particles represented by this function have no additional internal degrees of independence or are spinless. However, analysis of the equation revealed that its solution  $\psi$  was fundamentally different from the ordinary wave function in terms of its physical meaning:  $\psi(x, y, z, t)$  is not determined exclusively by the value of  $\psi$  at the initial moment (such an unambiguous relationship is postulated in nonrelativistic quantum mechanics).

Additionally, the formula expressing the likelihood of a certain condition might take on both positive and negative values, which have no physical significance. As a result, the Klein-Gordon equation was first disregarded. However, W. Pauli and W. Weisskopf found an appropriate interpretation for the equation in the context of quantum field theory in 1934 [2]. They quantized the equation by considering it as a field equation similar to Maxwell's equations for an electromagnetic field, making an operator [3-6].

### 3.2. The semi-inverse variational method for Klein Gordon equation:

As a result, in the second Chapter, we attempt to obtain the Lagrange function for the Klein-Gordon equation using the same condition.

Writing a functional test

$$J(r) = \int_0^{+\infty} L(r; R_{n,l}; R_{n,l_r}) dr$$
 (3.2)

Where  $L(r; R; R_r) = \left(r \frac{dR_{n,l}}{dr}\right)^2 + F(R)$  and we use the stationary form:

$$\delta R : \frac{d}{dr} \left( r^2 \frac{dR_{n,l}}{dr} \right)^2 + \frac{\delta F}{\delta R} = \frac{d}{dr} \left( r^2 \frac{dR_{n,l}}{dr} \right)^2 + \frac{2}{(\hbar c)^2} \left( (M(r)c^2 + S(r))^2 - \left( E - V(r) \right)^2 \right) r^2 R_{n,l}$$

So 
$$\frac{\delta F}{\delta R_{n,l}} = \frac{2}{(\hbar c)^2} \Big( (M(r) + S(r))^2 - \Big( E - V(r) \Big)^2 \Big) r^2 R_{n,l}$$
 then we can find  $F$  with:

$$F = \frac{1}{(\hbar c)^2} \left( (M(r)c^2 + S(r))^2 - \left( E - V(r) \right)^2 \right) r^2 R_{n,l}^2 + F_0$$

 $F_0$  is a constant equal 0

now we get the Lagrangian as mentioned in:

$$L(r; R_{n,l}; R_{n,l_r}) = \left(r \frac{dR_{n,l}}{dr}\right)^2 + \frac{1}{(\hbar c)^2} \left( (M(r)c^2 + S(r))^2 - \left(E - V(r)\right)^2 \right) r^2 R_{n,l}^2$$

$$L(r; R_{n,l}; R'_{n,l_r}) = \left(r \frac{dR_{n,l}}{dr}\right)^2 + \frac{1}{(\hbar c)^2} \left( (M(r) + S(r))^2 - \left(E - V(r)\right)^2 \right) r^2 R_{n,l}^2$$
(3.3)

After simplifying with putting  $\hbar = c = 1$  we get:

$$L(r; R_{n,l}; R_{n,lr}) = \left[ \left( \frac{dR}{dr} \right)^2 + \left( (M(r) + S(r))^2 - \left( E - V(r) \right)^2 \right) R^2 \right] r^2$$
 (3.4)

We conclude.

$$J(r) = \int_0^{+\infty} \left[ \left( \frac{dR_{n,l}}{dr} \right)^2 + \left( (M(r)c^2 + S(r))^2 - \left( E - V(r) \right)^2 \right) R^2 \right] r^2 dr$$
 (3.5)

### 3.2.1. Colombian potential:

The shape of the Kratzer potential is as follows [7]:

 $S(r) = \frac{A_1}{x^2} - \frac{B_1}{x}$  and  $V(r) = \frac{A_2}{x^2} - \frac{B_2}{x}$  with the Colombian potential is a special case from the Kratzer one with putting  $A_1 = 0$  and  $A_2 = 0$ .

For m(r) as constant value m = 1, the expression of Lagrange becomes:

$$J(r) = \int_0^{+\infty} \left[ \left( \frac{dR_{n,l}}{dr} \right)^2 + \left( (1 + S(r))^2 - \left( E - V(r) \right)^2 \right) R^2 \right] r^2 dr$$
 (3.6)

For special cases we put

### $A_1 = A_2 = 0$

And as a result, we may use  $B_1 = 0$  and  $B_2 = 0.1$  as examples. For instance, the radial trial function is  $R(r) = ae^{-kr}$ , therefore we can replace R(r) in equation (3.6). For this reason, we may express Lagrange's overall functionality as follows:

$$J(a,k) = \frac{a^2(0.25 + 0.245k^2 - 0.05kt - 0.25t^2)}{k^3}$$
(3.7)

The stationary condition offered by the following phrases is used in this instance:

$$\frac{\partial J(a,k)}{\partial a} = \frac{2a(0.25 + 0.245k^2 - 0.05kt - 0.25t^2)}{k^3}$$
(3.8a)

$$\frac{\partial J(a,k)}{\partial k} = \frac{a^2(-0.75 - 0.245k^2 + 0.1kt + 0.75t^2)}{k^4}$$
(3.8b)

We use the Mathematica packaging to resolve the nonlinear system of equations  $\partial J$  for all the applications in this paper in order to find the k, E, and other variables. A constant can be found by using the normalization condition, and we note that the energy values, which are already used

in Mathematica,  $k \approx 0.1$ ,  $E \approx 0.994937$  and  $R = ae^{-0.1r}$  which represent the ground state energy n = 0.

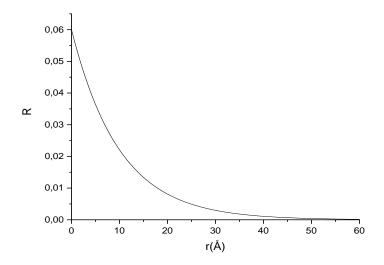


Fig.3.1. The Radial wave function R for  $B_2 = 0.1$  for the ground state n = 0

We'll proceed on to examine a further wave function with constants set to the same values of  $B_2$ ,  $R = (ar + b)e^{-kr}$ , which we'll insert in equation (2.6) to represent the generic Lagrange functional as follows:

$$J(a,b,k) = \frac{1}{k^5} (a^2(0.75 + 0.2475k^2 - 0.075kt - 0.75t^2) + abk(0.75 + 0.245k^2 - (3.9) - 0.75t^2) + b^2k^2(0.25 + 0.245k^2 - 0.05kt - 0.25t^2))$$

In this case we use the stationary condition provides by the following expressions:

$$\frac{\partial J(a,b,k)}{\partial a} = \frac{1}{k^5} (2a(0.75 + 0.2475k^2 - 0.075kt - 0.75t^2) + bk(0.75 + 0.245k - 0.1kt - 0.75t^2))$$

$$(3.10a)$$

$$\frac{\partial J(a,b,k)}{\partial b} = \frac{1}{k^5} \left( ak(0.75 + 0.245k^2 - 0.1kt - 0.75t^2) + 2bk^2(0.25 + 0.245k^2 - 0.05kt - 0.25t^2) \right)$$
(3.10b)

$$\frac{\partial J(a,b,k)}{\partial k} = \frac{2}{k^6} (b^2 k^2 (-0.375 - 0.1225k^2 + 0.05kt + 0.375t^2) + ack(-1.5) - 0.245k^2 + 0.15kt + 1.5t^2) + a^2 (-1.875 - 0.37125k^2 + 0.15kt + 1.875t^2))$$
(3.10c)

Always with Mathematica packaging to resolute the nonlinear system of equations  $\partial J$  for all the applications to find the k and t and other constants, a constant can be determined via the normalization condition and for this aims we get, $k \approx 0.05$ ,  $k \approx 0.998739$  and  $k = a(r-19.76)e^{-0.05r}$  which represent the first excited state energy k = 1.

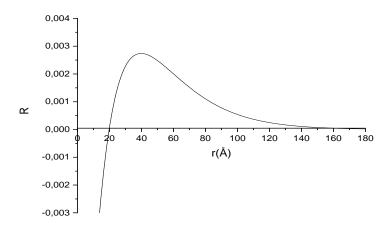


Fig. 3.2. The Radial wave function R for  $B_2 = 0.1$  for the first excited state n = 1

We'll proceed on to examine a further wave function with constants set to the same value of  $B_2$ ,  $R = (ar^2 + br + d)e^{-kr}$ , which we'll insert in equation (2.6) to represent the generic LaGrange functional as follows:

$$J(a,b,d,k) = \frac{1}{2k^7} (a^2(5.625 + 1.1175k^2 - 0.375kt - 5.625t^2) + ak(b(3.75 + 0.7425k^2 - 0.3kt - 3.75t^2) + dk(1.5 - 0.005k^2 - 0.15kt - 1.5t^2)) + k^2(bdk(0.75 + 0.245k^2 - 0.1kt - 0.75t^2) + b^2(0.75 + 0.2475k^2 - 0.075kt - 0.75t^2) + d^2k^2(0.25 + 0.245k^2 - 0.05kt - 0.25t^2)))$$

$$(3.11)$$

In this case we use the stationary condition provides by the following expressions:

$$\frac{\partial J(a,b,d,k)}{\partial a} = \frac{1}{k^7} (2a(5.625 + 1.1175k^2 - 0.375kt - 5.625t^2) + k(b(3.75 + 0.7425k^2 - 0.3kt - 3.75t^2) + dk(1.5 - 0.005k^2 - 0.15kt - 1.5t^2)))$$
(3.12a)

$$\frac{\partial J(a,b,d,k)}{\partial b} = \frac{1}{k^7} (ak(3.75 + 0.7425k^2 - 0.3kt - 3.75t^2) + k^2 (dk(0.75 + 0.245k^2 - 0.1kt - 0.75t^2) + 2b(0.75 + 0.2475k^2 - 0.075kt + 0.245k^2) - 0.075t^2)))$$

$$\frac{\partial J(a,b,d,k)}{\partial d} = \frac{1}{k^7} (ak^2(1.5 - 0.005k^2 - 0.15kt - 1.5t^2) + k^2 (bk(0.75 + 0.245 + 0.01kt - 0.75t^2) + 2dk^2 (0.25 + 0.245k^2 - 0.05kt - 0.25t^2)))$$

$$\frac{\partial J(a,b,d,k)}{\partial k} = \frac{2}{k^8} (a^2(-19.6875 - 2.79375k^2 + 1.125kt + 19.6875t^2) + k^2 (d^2k^2(-0.375 - 0.1225k^2 + 0.05kt + 0.375t^2) + bdk(-1.5 - 0.245k^2 + 0.15kt + 1.5t^2) + b^2 (-1.875 - 0.37125k^2 + 0.15kt + 1.875t^2)) + ak(dk(-3.75 + 0.0075k^2 + 0.3kt + 3.76t^2) + b(-11.25 - 1.485k^2 + 0.75kt + 11.25t^2)))$$

For all applications to obtain the constants k, t, and others, the nonlinear system of equations  $\partial J$  must always be solved using the Mathematica package. The constants can be found by using the normalization condition, and for this purpose, we obtain  $k \approx 0.03, b \approx -89.2239a$ ,  $d \approx 1324.68a$   $E \approx 0.999441$  and  $R = a(r - 89.2269r + 1324.68)e^{-0.03r}$  which represent the first second state energy n = 2.

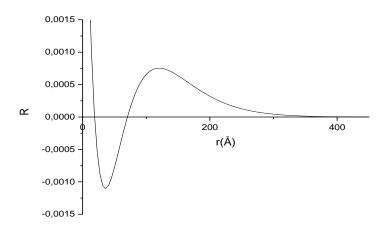


Fig.3.3. The Radial wave function R for  $B_2 = 0.1$  for the first excited state n = 2

The values of  $B_1$  are varied to increase the compatibility of the outcomes produced by this procedure, and the results are summarized in the table below.

Table 3.1. The eigenvalues of Coulomb potential for different values of  $B_2$  and  $B_1=0$ 

$B_2$	n	our results	<i>Ref</i> [8]
0.1		0.994937	0.99503
0.2	0	0.978945	0.98058
0.3		0.949662	0.9578
0.1	1	0.998739	0.998752
0.2		0.994833	0.995037
0.3		0.987872	0.988936
0.1		0.999441	0.999445
0.2	2	0.997725	0.997785
0.3		0.9947	0.995037

According to the drawn figures 3.1, 3.2 and 3.3 we observed:

n = 0: the curve has no node, so it corresponds to the ground state.

n = 1:The curve has a node, so it corresponds to the first excited state.

n = 2: the curve has two nodes, so it corresponds to the second excited state.

Table 3.1 displays the eigenvalues of Coulomb potential for different values of  $B_2$  and  $B_1 = 0$ . we noticed that :

- There is a correlation between rising quantum numbers (n) and increasing energy.
- When the value of B<sub>2</sub> grows, the energy drops.
- The results show good agreement with the findings in reference [8], with a maximum accuracy of 0.0003%.

# For $A_1 = A_2 = 0$ :

and as a result, we may use  $B_1 = 0.1$  and  $B_2 = 0$  as examples, where R(r) is the radial trial function and  $ae^{(-kr)}$  is the radial trial function. For this reason, we may express LaGrange's overall functionality as follows:

$$J(a,k) = \frac{1}{k^3} (a^2(0.25 - 0.05k + 0.255k^2 - 0.25t^2))$$
 (3.13)

In this case we use the stationary condition provides by the following expressions:

$$\frac{\partial J(a,k)}{\partial a} = \frac{2}{k^3} (a(0.25 - 0.05k + 0.255k^2 - 0.25t^2))$$
(3.14a)

$$\frac{\partial J(a,k)}{\partial k} = \frac{2}{k^3} (a^2(-0.375 + 0.05k - 0.1275k^2 + 0.375t^2))$$
(3.14b)

A constant can be found using the normalization condition, and for this purpose, we obtain  $k \approx 0.1$ ,  $E \approx 0.995086$  and  $R = ae^{-0.05r}$  which represent the first ground state energy n = 0. This is always done with Mathematica packaging to resolve the nonlinear system of equations  $\partial J$ .

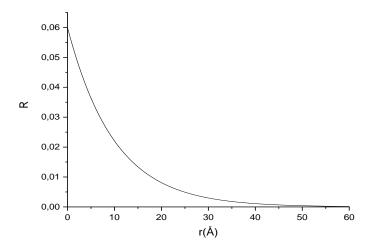


Fig.3.4. The Radial wave function R for  $B_1 = 0.1$  for the ground state n = 0

We'll proceed on to examine a further wave function with constants set to the same value of  $B_1$ ,  $R = (ar + b)e^{-kr}$ , which we'll insert in equation (3.6) to represent the generic LaGrange functional as follows:

$$J(a,b,k) = \frac{1}{k^5} (a^2(0.75 + (-0.075 + 0.2525k)k - 0.75t^2) + abk(0.75 + (-0.1 + 0.255k)k - 0.75t^2) + b^2k^2(0.25 + (-0.05 + 0.255k)k - 0.25t^2))$$
(3.15a)

In this case we use the stationary condition provides by the following expressions:

$$\frac{\partial J(a,b,k)}{\partial a} = \frac{1}{k^5} (2a(0.75 + (-0.075 + 0.2525k)k - 0.75t^2) + bk(0.75 + (-0.165k)k - 0.75t^2) + bk(0.75 + (-0.165k)k - 0.75t^2))$$
(3.15b)

$$\frac{\partial J(a,b,k)}{\partial b} = \frac{1}{k^5} (ak(0.75 + (-0.1 + 0.255k)k - 0.75t^2) + 2bk^2(0.25 + (-0.05 + 0.255k)k - 0.25t^2))$$
(3.15c)

$$\frac{\partial J(a,b,k)}{\partial k} = \frac{2}{k^6} (b^2 k^2 (-0.375 + 0.05k - 0.1275k^2 + 0.375t^2) + abk(-1.5) + 0.15k - 0.255k^2 + 1.5t^2) + a^2 (-1.875 + 0.15k - 0.37875k^2 + 1.875t^2))$$

$$(3.15c)$$

A constant can be found using the normalization condition, and for this purpose, we obtain  $k \approx 0.05, b \approx -20.267 \ E \approx 0.998762$  and  $R = a(r - 20.276)e^{-0.05r}$  which represent the first ground state energy n = 1. This is always done with Mathematica packaging to resolve the nonlinear system of equations  $\partial I$ .

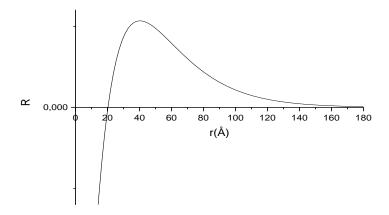


Fig.3.5. The Radial wave function R for  $B_1 = 0.1$  for the first excited state n = 1

We'll proceed on to examine a further wave function with constants set to the same value of  $B_2$ ,  $R = (ar^2 + br + d)e^{-kr}$ , which we'll insert in equation (3.6) to represent the generic LaGrange functional as follows:

$$J(a,b,d,k) = \frac{1}{k^7} (a^2(5.625 + k(-0.375 + 1.1325k) - 5.625t^2) + ak(b(3.75 + (-0.3 + 0.7575k)k - 3.75t^2) + dk(1.5 + (-0.15 + 0.005k)k - 1.5t^2)) + k^2(b^2(0.75 + (-0.075 + 0.2525k)k - 0.75t^2) + bdk(0.75 + (-0.1 + 0.255k)k - 0.75t^2) + d^2k^2(0.25 + (-0.05 + 0.255k)k - 0.25t^2)))$$

$$(3.16)$$

In this case we use the stationary condition provides by the following expressions:

$$\frac{\partial J(a,b,d,k)}{\partial a} = \frac{1}{k^7} (2a(5.625 + k(-0.375 + 1.1325k) - 5.625t^2) + k(b(3.75 + (-0.3 + 0.7575k)k - 3.75t^2) + dk(1.5 + (-0.15 + 0.005k)k - 1.5t^2)))$$
(3.17a)

$$\frac{\partial J(a,b,d,k)}{\partial b} = \frac{1}{k^7} (ak(3.75 + (-0.3 + 0.7575k)k - 3.75t^2) + k^2(2b(0.75 + (-0.075 + 0.2525k)k - 0.75t^2) + dk(0.75 + (-0.1 + 0.255k)k - 0.75t^2)))$$

$$\frac{\partial J(a,b,d,k)}{\partial d} = \frac{1}{k^7} (ak^2(1.5 + (-0.15 + 0.005k)k - 1.5t^2) + k^2(bk(0.75 + (-0 + 0.255k)k - 0.75t^2) + 2dk^2(0.25 + (-0.05 + 0.255k)k - 0.25t^2)))$$

$$\frac{\partial J(a,b,d,k)}{\partial k} = \frac{1}{k^8} (a^2(-19.6875 + 1.125k - 2.83125k^2 + 19.6875t^2) + k^2(d^2k^2(-0.375 + 0.05k - 0.1275k^2 + 0.375t^2) + bdk(-1.5 + 0.15k - 0.255k^2 + 1.5t^2) + b^2(-1.875 + 0.15k - 0.37875k^2 + 1.875t^2)) + ak(dk(-3.75 + 0.3k - 0.0075k^2 + 3.75t^2) + b(-11.25 + 0.75k - 1.515k^2 + 11.25t^2)))$$

Always with Mathematica packaging to resolute the nonlinear system of equations  $\partial J$  for all the applications to find the k and t and other constants, a constant can be determined via the normalization condition and for this aims we get, $k \approx 0.03$ ,  $k \approx -90.827a$ ,  $k \approx 1377.2a$   $k \approx 0.999448$  and  $k = a(r - 90.827r + 1377.2)e^{-0.03r}$  which represent the first second state energy k = 2.

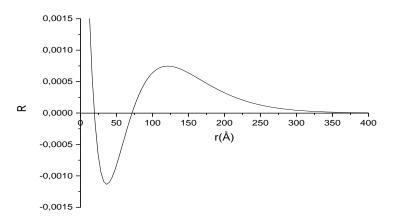


Fig. 3.6. The Radial wave function R for  $B_1 = 0.1$  for the first excited state n = 2

In order to further increase the compatibility of the outcomes produced by this approach, we varied the values of  $B_1$  as shown in the table below.

Table 3.2. The eigenvalues of Coulomb potential for different values of  $B_1$  and  $B_2$ =0

$B_1$	n	our results	<i>Ref</i> [8]
0.1		0.995086	0.994987
0.2	0	0.981307	0.979796
0.3		0.961108	0.953939
0.1	1	0.998762	0.998749
0.2		0.995181	0.994987
0.3		0.989631	0.988686
0.1		0.999448	0.999444
0.2	2	0.997834	0.997775
0.3		0.995278	0.994987

According to the drawn figures 3.4, 3.5 and 3.6 we observed:

n =0: the curve has no node, so it corresponds to the ground state.

n = 1:The curve has a node, so it corresponds to the first excited state.

n = 2: the curve has two nodes, so it corresponds to the second excited state.

Table 3.2 represent the eigenvalues of Coulomb potential for different values of  $B_1$  and  $B_2 = 0$ . we noticed that :

- There is a correlation between rising quantum numbers (n) and increasing energy.
- When the value of  $B_2$  grows, the energy drops.
- The results show good agreement with the findings in reference [8], with a maximum accuracy of 0.0002%.

## for $A_1 = A_2 = 0$ and $B_1 = B_2$ :

As a result, we may choose  $B_1 = B_2 = 0.1$ , where  $R(r) = ae^{-kr}$  is the radial trial function. R(r) is substituted in equation (3.6). For this reason, we may express LaGrange's overall functionality as follows:

$$J(a,k) = \frac{1}{k^3} (0.25a^2(1+k^2+k(-0.2-0.2t)-t^2))$$
(3.18)

In this case we use the stationary condition provides by the following expressions:

$$\frac{\partial J(a,k)}{\partial a} = \frac{1}{k^3} (0.5a(1+k^2+k(-0.2-0.2t)-t^2))$$
(3.19a)

$$\frac{\partial J(a,k)}{\partial k} = \frac{2}{k^4} (a^2(-0.375 - 0.125k^2 + k(0.05 + 0.05t) + 0.375t^2))$$
(3.19b)

The first ground state energy, n=0, is represented by  $\approx 0.2$ ,  $E\approx 0.9980198$ , and  $R=ae^{-0.2r}$  which are obtained when solving the nonlinear system of equations  $\partial J$  in Mathematica for all applications.

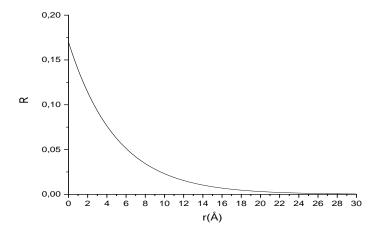


Fig.3.7. The Radial wave function R for  $B_1 = B_2 = 0.1$  for the first excited state n = 0

We'll continue with the same value of constants  $B_2$  but with another wave function  $R = (ar + b)e^{-kr}$  which we substitute it in the equation (3.6) and with Mathematica packaging we get, $k \approx 0.1, b \approx -10.025a$ ,  $E \approx 0.995012$  and  $R = a(r - 10.025)e^{-0.1r}$  which represent the first second state energy n = 1.

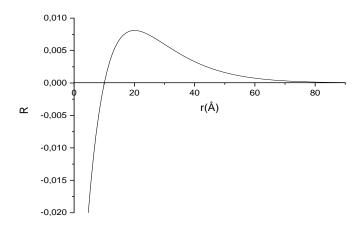


Fig.3.8. The Radial wave function R for  $B_1 = B_2 = 0.1$  for the first excited state n = 1

With the identical value of the constants  $B_2$  and a different wave function  $R = (ar^2 + br + d)e^{-kr}$  that we substitute into equation (3.6), we can describe the generic LaGrange function as follows:

$$J(a,b,d,k) = \frac{1}{k^7} (a^2(5.625 + 1.125k^2 + k(-0.375 - 0.375t) - 5.625t^2)$$

$$+ ak(b(3.75 - 0.3k + 0.75k^2 - 0.3kt - 3.75t^2) + dk(1.5 - 0.15k$$

$$- 0.15kt - 1.5t^2)) + k^2(bdk(0.75 - 0.1k + 0.25k^2 - 0.1kt$$

$$- 0.75t^2) + b^2(0.75 - 0.075k + 0.25k^2 - 0.075kt - 0.75t^2)$$

$$+ d^2k^2(0.25 - 0.05k + 0.25k^2 - 0.05kt - 0.25t^2)))$$

$$(3.20)$$

The stationary condition offered by the following phrases is used in this instance:

$$\frac{\partial J(a,b,d,k)}{\partial a} = \frac{1}{k^7} (2a(5.625 + 1.125k^2 + k(-0.375 - 0.375t) - 5.625t^2) 
+ k(b(3.75 - 0.3k + 0.75k^2 - 0.3kt - 3.75t^2) + dk(1.5 - 0.15k 
- 0.15kt - 1.5t^2)))$$
(3.21a)

$$\frac{\partial J(a,b,d,k)}{\partial b} = \frac{1}{k^7} (ak(3.75 - 0.3k + 0.75k^2 - 0.3kt - 3.75t^2) + k^2 (dk(0.75 - 0.1k + 0.25k^2 - 0.1kt - 0.75t^2) + 2b(0.75 - 0.075k + 0.25k^2 - 0.075kt - 0.75t^2)))$$

$$\frac{\partial J(a,b,d,k)}{\partial d} = \frac{1}{k^7} (ak^2 (1.5 - 0.15k - 0.15kt - 1.5t^2) + k^2 (bk(0.75 - 0.1k + 0.2 - 0.1kt - 0.75t^2) + 2dk^2 (0.25 - 0.05k + 0.25k^2 - 0.05kt - 0.25t^2)$$

$$\frac{\partial J(a,b,d,k)}{\partial k} = \frac{2}{k^8} (a^2 (-19.6875 - 2.8125k^2 + 19.6875t^2 + k(1.125 + 1.125t)) + k^2 (d^2k^2 (-0.375 + 0.05k - 0.125k^2 + 0.05kt + 0.375t^2) + bdk(-1.5 + 0.15k - 0.25k^2 + 0.15kt + 1.5t^2)$$

$$+ b^2 (-1.875 + 0.15k - 0.375k^2 + 0.15kt + 1.875t^2))$$

$$+ ak(dk(-3.75 + 0.3k + 0.3kt + 3.75t^2) + b(-11.25 + 0.75k - 1.5k^2 + 0.75kt + 11.25t^2)))$$

$$(3.21d)$$

Always with Mathematica packaging to resolute the nonlinear system of equations  $\partial J$  for all the applications to find the k and t and other constants, a constant can be determined via the normalization condition and for this aims we get, $k \approx 0.067$ ,  $b \approx -45.05a$ ,

 $d \approx 338.25 a \ E \approx 0.99778$  and  $R = a(r - 45.05r + 338.25)e^{-0.03r}$  which represent the first second state energy n = 2.

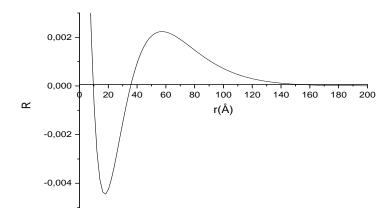


Fig.3.9. The Radial wave function R for  $B_1 = B_2 = 0.1$  for the first excited state n = 2

In order to further increase the compatibility of the outcomes produced by this approach, we varied the values of  $B_1$  as shown in the table below.

Table 3.3: The eigenvalues of Colombian potential for different values of  $B_1$  ( $B_1 = B_2$ )

$B_1$	n	our results	<i>Ref</i> [8]
0.1		0.980198	0.980099
0.2	0	0.923077	0.921538
0.3		0.834862	0.827431
0.1	1	0.995012	0.995006
0.2		0.990198	0.990099
0.3		0.95599	0.955495
0.1		0.99778	0.99778
0.2	2	0.99115	0.99115
0.3		0.980198	0.980198

According to the drawn figures 3.7, 3.8 and 3.9 we observed:

n =0: the curve has no node, so it corresponds to the ground state.

n = 1:The curve has a node, so it corresponds to the first excited state.

n = 2: the curve has two nodes, so it corresponds to the second excited state.

Table 3.3 represent the eigenvalues of Coulomb potential for different values of  $(B_2 = B_1)$ , we noticed that.

- There is a correlation between rising quantum numbers (n) and increasing energy.
- When the value of  $B_1$  and  $B_2$  rise, the energy drops.
- The results show good agreement with the findings in reference [8], with a maximum accuracy of 0.0001%.

## Pour $A_1 = A_2 = 0$ and $B_1 \neq B_2$ :

and as a result, we may utilize values like  $B_1 = 0.2$  and  $B_2 = 0.1$ , as well as the radial trial function  $R(r) = ae^{-kr}$ , by replacing R(r) in equation (3.6). For this reason, we may express LaGrange's overall functionality as follows:

$$J(a,k) = \frac{2}{k^3} (0.5a^2(0.25 - 0.1k + 0.265k^2 - 0.05kt - 0.25t^2))$$
 (3.22)

The stationary condition provided by the following phrases is what we utilize in this situation:

$$\frac{\partial J(a,k)}{\partial a} = \frac{2}{k^3} (a(0.25 - 0.1k + 0.265k^2 - 0.05kt - 0.25t^2))$$
(3.23a)

$$\frac{\partial J(a,k)}{\partial k} = \frac{2}{k^4} (a^2(-0.375 - 0.1325k^2 + k(0.1 + 0.05t) + 0.375t^2))$$
(3.23b)

We obtain  $k \approx 0.28$ ,  $E \approx 0.957843$  and  $R = ae^{-0.28r}$ , which represent the first ground state energy n = 0, when solving the nonlinear system of equations in Mathematica for all applications.

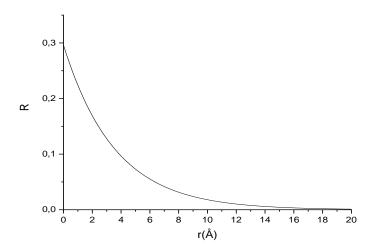


Fig.3.10. The Radial wave function R for  $B_1 = 0.2$  and  $B_2 = 0.1$  for the ground state n = 0

We'll proceed by keeping the variables  $B_1$  and  $B_2$  at their original values while substituting a different wave function,  $R = (ar + b)e^{-kr}$ , into equation (3.6). In this approach, we may define the generic LaGrange function as follows:

$$J(a,b,k) = \frac{1}{k^5} (abk(0.75 + 0.265k^2 + k(-0.2 - 0.1t) - 0.75t^2) + a^2(0.75 + 0.2575k^2 + k(-0.15 - 0.075t) - 0.75t^2) + b^2k^2(0.25 + 0.265k^2 + k(-0.1 - 0.05t) - 0.25t^2))$$
(3.24)

Here, we employ the stationary condition made possible by the following expressions:

$$\frac{\partial J(a,b,k)}{\partial a} = \frac{1}{k^5} (bk(0.75 + 0.265k^2 + k(-0.2 - 0.1t) - 0.75t^2) + 2a(0.75 + 0.2575k^2 + k(-0.15 - 0.075t) - 0.75t^2))$$
(3.24a)

$$\frac{\partial J(a,b,k)}{\partial b} = \frac{1}{k^5} \left( ak(0.75 + 0.265k^2 + k(-0.2 - 0.1t) - 0.75t^2) + 2bk^2(0.25 + 0.265k^2 + k(-0.1 - 0.05t) - 0.25t^2) \right)$$
(3.24b)

$$\frac{\partial J(a,b,k)}{\partial k} = \frac{2}{k^6} (b^2 k^2 (-0.375 - 0.1325k^2 + k(-0.1 - 0.05t) + 0.375t^2) 
+ abk(-1.5 - 0.265k^2 + k(-0.3 - 0.15t) + 1.5t^2) 
+ a^2 (-1.875 - 0.38625k^2 + k(-0.3 - 0.15t) + 1.875t^2))$$
(3.24c)

Always with Mathematica packaging to resolute the nonlinear system of equations  $\partial J$  for all the applications to find the k and t and other constants, a constant can be determined via the normalization condition and for this aims we get, $k \approx 0.05$ ,  $k \approx 0.05$ ,  $k \approx 0.998783$  and  $k = a(r-20.778)e^{-0.05r}$  which represent the first excited state energy  $k \approx 0.998783$ .

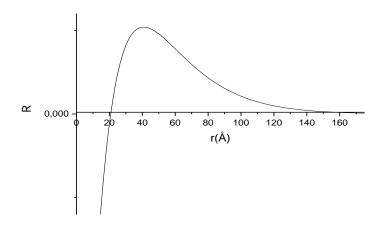


Fig.3.11. The Radial wave function R for  $B_1 = 0.2$  and  $B_2 = 0.1$  for the first excited state n = 1

We'll proceed with the same value of the constants  $B_2$  and another wave function  $R = (ar^2 + br + d)e^{-kr}$ , which we replace in equation (3.6), so that we can define the overall LaGrange function as follows:

$$J(a,b,d,k) = \frac{1}{k^7} (a^2(5.625 + 1.1475k^2 + k(-0.75 - 0.375t) - 5.625t^2)$$

$$+ ak(b(3.75 - 0.6k + 0.7725k^2 - 0.3kt - 3.75t^2) + dk(1.5 - 0.3k + 0.015k^2 - 0.15kt - 1.5t^2)) + k^2(bdk(0.75 - 0.2k + 0.265k^2 - 0.1kt - 0.75t^2) + b^2(0.75 - 0.15k + 0.2575k^2 - 0.075kt - 0.75t^2) + d^2k^2(0.25 - 0.1k + 0.265k^2 - 0.05kt - 0.25t^2)))$$

$$(3.25)$$

In this case we use the stationary condition provides by the following expressions:

$$\frac{\partial J(a,b,d,k)}{\partial a} = \frac{1}{k^7} (2a(5.625 + 1.1475k^2 + k(-0.75 - 0.375t) - 5.625t^2) + k(b(3.75 - 0.6k + 0.7725k^2 - 0.3kt - 3.75t^2) + dk(1.5 - 0.3k + 0.015k^2 - 0.15kt - 1.5t^2)))$$
(3.26a)

$$\frac{\partial J(a,b,d,k)}{\partial b} = \frac{1}{k^7} (ak(3.75 - 0.6k + 0.7725k^2 - 0.3kt - 3.75t^2) \\ + k^2 (dk(0.75 - 0.2k + 0.265k^2 - 0.1kt - 0.75t^2) + 2b(0.75 \\ - 0.15k + 0.2575k^2 - 0.075kt - 0.75t^2)))$$

$$\frac{\partial J(a,b,d,k)}{\partial d} = \frac{1}{k^7} (ak^2(1.5 - 0.3k + 0.015k^2 - 0.15kt - 1.5t^2) + k^2(bk(0.75 \\ - 0.2k + 0.265k^2 - 0.1kt - 0.75t^2) + 2dk^2(0.25 - 0.1k + 0.265k^2 \\ - 0.05kt - 0.25t^2)))$$

$$\frac{\partial J(a,b,d,k)}{\partial k} = \frac{2}{k^8} (a^2(-19.6875 - 2.86875k^2 + 19.6875t^2 + k(2.25 \\ + 1.125t)) + k^2(d^2k^2(-0.375 + 0.1k - 0.1325k^2 + 0.05kt \\ + 0.375t^2) + bdk(-1.5 + 0.3k - 0.265k^2 + 0.15kt + 1.5t^2) \\ + b^2(-1.875 + 0.3k - 0.38625k^2 + 0.15kt + 1.875t^2)) \\ + ak(dk(-3.75 + 0.6k - 0.0225k^2 + 0.3kt + 3.75t^2) \\ + b(-11.25 + 1.5k - 1.545k^2 + 0.75kt + 11.25t^2)))$$

The normalization condition can be used to determine a constant, and for this purpose, we obtain k = 0.044, b = -30.88, d = 159.72, E = 0.995103, and  $R = a(r - 30.88r + 159.72)e^{-0.044r}$ , which represent the first second state energy with n=2.

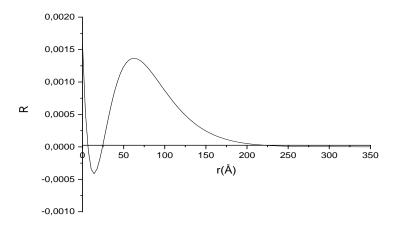


Fig.3.12. The Radial wave function R for  $B_1=0.2$  and  $B_2=0.1$  for the first excited state n=2

The results of this procedure are then resumed in the table below after we varied the values of  $B_1$  and  $B_2$  to further increase their compatibility.

Table 3.4: The eigenvalues of Colombian potential for different values of  $B_1$ .(  $B_1 \neq B_2$ )

$B_1$	$\boldsymbol{B}_2$	n	our results	<i>Ref</i> [8]
0.2	0.1		0.957843	0.955332
0.3	0.1	0	0.931013	0.919967
0.1	0.2		0.890096	0.879499
0.2	0.1	1	0.998783	0.988771
0.3	0.1		0.98149	0.979999
0.1	0.2		0.988514	0.988854
0.2	0.1		0.995103	0.995004
0.3	0.1	2	0.991569	0.991189
0.1	0.2		0.986618	0.986245

According to the drawn figures 3.10, 3.11 and 3.12 we observed:

n =0: the curve has no node, so it corresponds to the ground state.

n = 1:The curve has a node, so it corresponds to the first excited state.

n = 2: the curve has two nodes, so it corresponds to the second excited state.

Table 3.4 displays the eigenvalues of Colombian potential for different values of  $B_1$ .(  $B_1 \neq B_2$ ). We became aware of that.

- There exists an analogy between growing energy and growing quantum numbers (n).
- The energy decreases as  $B_1$  and  $B_2$  values increase. The results show good agreement with the findings in reference [8], with a maximum accuracy of 0.0001%.

#### 3.2.2. The Kratzer potential:

We start with special cases in Kratzer potential and variate the constants of  $A_1$ ,  $A_2$ ,  $B_1$ ,  $B_2$ . The first case is V(r) = 0 with  $A_2 = B_2 = 0$ 

So therefore, we can make use for example,  $A_1 = B_1 = 0.1$ , such as the radial trial function is  $R(r) = are^{-kr-\frac{A_1}{r}}$  we substitute R(r) in the equation (3.6) for this way we can expressed the general functional of LaGrange as below:

$$J(a,k) = \frac{1}{k^{5/2}} \left( a^2 (0.00632456 + (-0.004 - 0.04k)\sqrt{k} + (0.0765271 - 0.0126491 + 0.036k^{3/2} + 0.01897366k^2 - 0.00632456n^2) \right)$$
(3.28)

In this case we use the stationary condition provides by the following expressions:

$$\frac{\partial J(a,k)}{\partial a} = \frac{1}{k^{5/2}} \left( 2a(0.00632456 + (-0.004 - 0.04k)\sqrt{k} + (0.0765271 - 0.0126491k)k + 0.036k^{3/2} + 0.01897366k^2 - 0.00632456n^2) \right)$$
(3.29a)

$$\frac{\partial J(a,k)}{\partial k} = \frac{1}{k^{5/2}} \left( a^2 \left( -0.0158114 + 0.008\sqrt{k} - 0.11479065k + 0.004k^{3/2} - 0.00316228k^2 + 0.0158114n^2 \right) \right)$$
(3.29b)

The results  $k \approx 0.0007$ ,  $E \approx 0.995854$  and  $R = ae^{-0.0007r - 0.1/r}$ , which represent the first ground state energy n=0, are obtained when the nonlinear system of equations  $\partial J$  is solved using Mathematica's packaging for all applications to find the k and t and other constants.

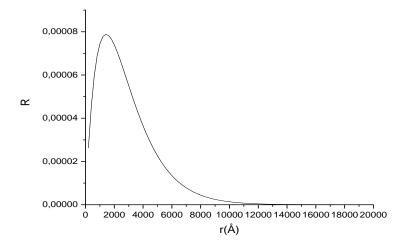


Fig.3.13. The Radial wave function R for  $A_1 = B_1 = 0.1$  and  $A_2 = B_2 = 0$  for the ground state n = 0

## The second case is S(r) = 0 with $A_1 = B_1 = 0$

Therefore, consequently, we may utilize values such as  $A_2 = 0.1$  and  $B_2 = 0.1$ , where  $R(r) = are^{-kr}$  is the radial trial function. R(r) is substituted in equation (3.6). For this reason, we may express LaGrange's overall functionality as follows:

$$J(a,k) = \frac{1}{k^5} (a^2(0.75 + 0.005k^3 - 0.005k^4 + k^2(0.2475 + 0.05t) - 0.075kt - 0.75t^2))$$
(3.30)

In this case we use the stationary condition provides by the following expressions:

$$\frac{\partial J(a,k)}{\partial a} = \frac{2}{k^5} (a(0.75 + 0.005k^3 - 0.005k^4 + k^2(0.2475 + 0.05t) - 0.075kt - 0.075k^2))$$
(3.31a)

$$\frac{\partial J(a,k)}{\partial k} = \frac{2}{k^6} (a^2(-1.875 - 0.005k^3 + 0.0025k^4 + k^2(-0.37125 - 0.075t) + 0.15kt + 1.875t^2))$$
(3.31b)

Always with Mathematica [34] packaging to resolute the nonlinear system of equations  $\partial J$  for all the applications to find the k and t and other constants, a constant can be determined via the normalization condition and for this aims we get, $k \approx 0.13$ ,  $E \approx 0.996868$  and  $R = are^{-0.28r}$  which represent the first ground state energy n = 0.

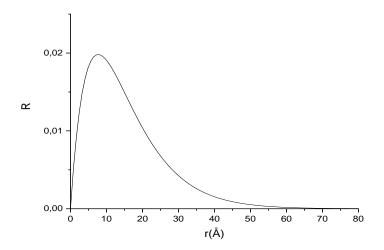


Fig.3.14. The Radial wave function R for  $A_2 = B_2 = 0.1$  for the ground state n = 0

We'll continue with the same value of constants  $A_2$  and  $B_2$  but with another wave function  $R = (ar + b)re^{-kr}$  which we substitute it in the equation (3.6) for this way we can expressed the general functional of LaGrange as below:

$$J(a,b,k) = \frac{1}{k^7} (a^2(5.625 + 0.0075k^3 - 0.0025k^4 + k^2(1.1175 + 0.15t) - 0.375kt - 5.625t^2) + abk(3.75 + 0.01k^3 - 0.005k^4 + k^2(0.7425 + 0.15t) - 0.3kt - 3.75t^2) + b^2k^2(0.75 + 0.005k^3 - 0.005k^4 + k^2(0.2475 + 0.05t) - 0.075kt - 0.75t^2))$$
(3.32)

In this case we use the stationary condition provides by the following expressions:

$$\frac{\partial J(a,b,k)}{\partial a} = \frac{1}{k^7} (2a(5.625 + 0.0075k^3 - 0.0025k^4 + k^2(1.1175 + 0.15t)) - 0.375kt - 5.625t^2) + bk(3.75 + 0.01k^3 - 0.005k^4 + k^2(0.7425 + 0.15t) - 0.3kt - 3.75t^2))$$

$$\frac{\partial J(a,b,k)}{\partial b} = \frac{1}{2k^7} (ak(3.75 + 0.01k^3 - 0.005k^4 + k^2(0.7425 + 0.15t) - 0.3kt - 3.75t^2) + 2bk^2(0.75 + 0.005k^3 - 0.005k^4 + k^2(0.2475 + 0.05t) - 0.075kt - 0.75t^2))$$
(3.32b)

$$\frac{\partial J(a,b,k)}{\partial k} = \frac{2}{k^8} (b^2 k^2 (-1.875 - 0.005k^3 + 0.0025k^4 + k^2 (-0.37125) - 0.075t) + 0.15kt + 1.875t^2) + abk (-11.252 - 0.015k^3 + 0.005k^4 + k^2 (-1.485 - 0.3t) + 0.75kt + 11.25t^2) + a^2 (-19.6875 - 0.015k^3 + 0.00375k^4 + k^2 (-2.79375) - 0.375t) + 1.125kt + 19.6875t^2))$$
(3.32c)

We obtain  $k \approx 0.07, b \approx -27.1$   $E \approx 0.998931$  and  $R = a(r - 27.1)re^{-0.07r}$ , which represent the first excited state energy n = 1, when solving the nonlinear system of equations  $\partial J$  in Mathematica for all applications.

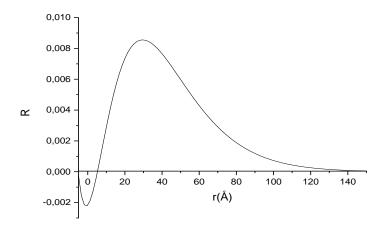


Fig.3.15. The Radial wave function R for  $A_2 = B_2 = 0.1$  for the first excited state n = 1

Then, we variate the values of  $B_1$  and  $B_2$  to improve more the compatibility of the results which obtained by this method and resume it in the table below.

$A_2$	$B_2$	n	our results	<i>Ref</i> [8]
0.1	0.1		0.996868	0.996528
0.2	0.2	0	0.989223	0.989796
0.2	0.1		0.997317	0.997449
0.1	0.2		0.9861111	0.987382
0.1	0.1	1	0.998931	0.998967
0.2	0.2		0.996558	0.996528
0.2	0.1		0.999143	0.999132
0.1	0.2		0.995682	0.995868

Table 3.5: The eigenvalues of Kratzer potential for different values of  $A_2$  and  $B_2$  with S(r) = 0.

According to the drawn figures 3.13, 3.14 and 3.15 we observed:

n =0: the curve has no node, so it corresponds to the ground state.

n = 0:The curve has no node, so it corresponds to the ground state.

n =1: the curve has a node, so it corresponds to the first excited state.

Table 3.5 shows the eigenvalues of Kratzer potential for different values of  $A_2$  and  $B_2$  with S(r) = 0. We became aware of that.

- There exists an analogy between growing energy and growing quantum numbers (n).
- The energy increases as  $A_2$  increase.
- As  $B_2$  grows, the energy decreases.
- The results show good agreement with the findings in reference [8], with a maximum accuracy of 0.0003%.

# The third case is V(r) = S(r) with $A_1 = B_1$ and $A_2 = B_2$ :

Consequently, we may employ equations like,  $A_1 = A_2 = 0.1$  and  $B_1 = B_2 = 0.1$ , such as the radial trial function, which is  $R(r) = are^{-kr}$ . R(r) is substituted in equation (3.6). For this reason, we may express LaGrange's overall functionality as follows:

$$J(a,k) = \frac{1}{k^5} (a^2(0.75 + k(-0.075 - 0.075t) + k^2(0.3 + 0.05t) - 0.75t^2))$$
(3.33)

In this case we use the stationary condition provides by the following expressions:

$$\frac{\partial J(a,k)}{\partial a} = \frac{1}{k^5} (2a(0.75 + k(-0.075 - 0.075t) + k^2(0.3 + 0.05t) - 0.75t^2))$$
(3.34a)

$$\frac{\partial J(a,k)}{\partial k} = \frac{1}{k^6} (2a^2(-1.875 + k^2(-0.45 - 0.075t) + k(0.15 + 0.15t) + 1.875t^2))$$
(3.34b)

Always with Mathematica packaging to resolute the nonlinear system of equations  $\partial J$  for all the applications to find the k and t and other constants, a constant can be determined via the normalization condition and for this aims we get, $k \approx 0.21$ ,  $E \approx 0.989327$  and  $R = are^{-0.21r}$  which represent the ground state energy n = 0.

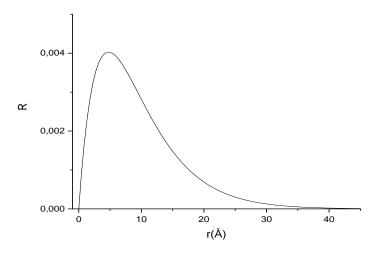


Fig.3.16. The Radial wave function R for V(r) = S(r) for the ground state n = 0

The variables  $A_1 = A_2 = 0.1$  and  $B_1 = B_2 = 0.1$  will remain the same, but we'll replace them in equation (3.6) with a different wave function,  $R = (ar + b)re^{-kr}$ . For this reason, we may express LaGrange's overall functionality as follows:

$$J(a,b,k) = \frac{1}{k^7} (a^2(5.625 + k(-0.375 - 0.375t) + k^2(1.275 + 0.15t) - 5.625t^2)$$

$$+ abk(3.75 + k(-0.3 - 0.3t) + k^2(0.9 + 0.15t) - 3.75t^2)$$

$$+ b^2k^2(0.75 + k(-0.075 - 0.075t) + k^2(0.3 + 0.05t) - 0.75t^2))$$

$$(3.35)$$

In this case we use the stationary condition provides by the following expressions:

$$\frac{\partial J(a,b,k)}{\partial a} = \frac{1}{k^7} (2a(5.625 + k(-0.375 - 0.375t) + k^2(1.275 + 0.15t) 
- 5.625t^2) + bk(3.75 + k(-0.3 - 0.3t) + k^2(0.9 + 0.15t) 
- 3.75t^2))$$
(3.36a)

$$\frac{\partial J(a,b,k)}{\partial b} = \frac{1}{k^7} (ak(3.75 + k(-0.3 - 0.3t) + k^2(0.9 + 0.15t) - 3.75t^2) + 2bk^2(0.75 + k(-0.075 - 0.075t) + k^2(0.3 + 0.05t) - 0.75t^2))$$
(3.36b)

$$\frac{\partial J(a,b,k)}{\partial k} = \frac{2}{k^8} (b^2 k^2 (-1.875 + k^2 (-0.45 - 0.075t) + k(0.15 + 0.15t)$$

$$+ 1.875t^2) + abk (-11.25 + k^2 (-1.8 - 0.3t) + k(0.75 + 0.75t)$$

$$+ 11.25t^2) + a^2 (-19.6875 + k^2 (-3.1875 - 0.375t)$$

$$+ 19.6875t^2 + k(1.125 + 1.125t)))$$
(3.36c)

k and E are constants can be found by using the normalization condition, and for this purpose, we get,  $k \approx 0.1, b \approx -17.87$   $E \approx 0.996581$  and  $R = a(r - 17.87)re^{-0.1r}$ , which represent the first excited state energy n = 1. Always using Mathematica packaging, we can solve the nonlinear system of equations  $\partial I$  to find the k and t and other constants.

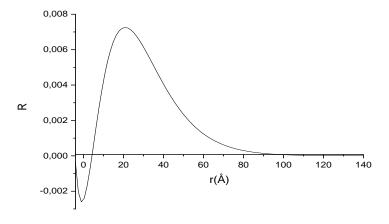


Fig.3.17. The Radial wave function 
$$R$$
 for  $A_2 = A_1 = B_1 = B_2 = 0.1$  for the first excited state  $n = 1$ 

The results of this procedure are then resumed in the table below after we varied the values of  $B_1$  and  $B_2$  to further increase their compatibility.

Table 3.6: The eigenvalues of Kratzer potential for S(r) = V(r).

$A_1 = A_2$	$B_1 = B_2$	n	our results	<i>Ref</i> [8]
0.1	0.1		0.989327	0.988278
0.2	0.2	0	0.966975	0.965587
0.2	0.1		0.991686	0.991397
0.1	0.2		0.957793	0.953113
0.1	0.1	1	0.996581	0.99624
0.2	0.2		0.9879726	0.987449
0.2	0.1		0.9969827	0.996862
0.1	0.2		0.9863851	0.984959

According to the drawn figures 3.16 and 3.17 we observed:

- n = 0: the curve has no node, so it corresponds to the ground state.
- n = 1: the curve has a node, so it corresponds to the first excited state.

Table 3.5 displays the eigenvalues of Kratzer potential for S(r) = V(r). We became aware of that.

- There exists an analogy between growing energy and growing quantum numbers (n).
- The energy increases as  $A_2$  increase.
- As  $B_2$  grows, the energy decreases.
- The results show good agreement with the findings in reference [8], with a maximum accuracy of 0.0003%.

The tables that are shown demonstrate that the semi-inverse variational technique yields eigenvalues for various potentials. The accuracy and effectiveness of this method in resolving

quantum mechanics issues involving diverse potentials are demonstrated by the results, which agree well with established references. Furthermore, the study investigates how the eigenvalues change as a function of various factors by setting the value and contrasting the results with fresh values. This research demonstrates the sensitivity of the quantum states to variations in the potential function and offers insightful information about how the system behaves when its potential parameters are varied. The tables support the semi-inverse variational method's validity and its ability to examine intricate quantum potentials overall. As a result of the method's ability to find precise eigenvalues for diverse potentials, it is a promising instrument for the study of quantum mechanics and provides useful details on how quantum systems behave under various circumstances.

### 3.2.3. Harmonic Oscillator:

for M=1

For m(r) as constant value m, S(r)=0, l=0 and  $\hbar=m=1$ , the expression of Lagrange becomes:

$$J(r; R_{n,l}; R_{n,l_r}) = \int_{0}^{+\infty} \frac{1}{2} \left[ \left( \frac{dR_{n,l}}{dr} \right)^2 + \left( M^2 - \left( E - V(r) \right)^2 \right) R_{n,l}^2 \right] r^2 dr$$
 (3.37)

consequently, we may use, for instance,  $\omega = \frac{1}{10}$  and  $V(r) = \frac{1}{2}M\omega^2r^2$  [9-10] radial trial function is  $R(r) = ae^{-kr^2}$  in these stages as Harmonic Oscillator potential. In the equation (3.37), R(r) is substituted, and we may formulate the generic LaGrange function as follows:

$$J(a,k) = \frac{a^2(-3 + 320k(3n + 400k(1 + 3k - n^2)))\sqrt{\frac{\pi}{2}}}{1024000k^{7/2}}$$
(3.38)

In this case we use the stationary condition provides by the following expressions:

$$\frac{\partial J(a,k)}{\partial a} = \frac{a(-3+320k(3n+400k(1+3k-n^2)))\sqrt{\frac{\pi}{2}}}{512000k^{7/2}}$$
(3.39a)

$$\frac{\partial J(a,k)}{\partial k} = -\frac{3a^2(-7 + 128000k^3 + 1600kn - 128000k^2(-1 + n^2))\sqrt{\frac{\pi}{2}}}{2048000k^{9/2}}$$
(3.39b)

We use Mathematica packaging to resolute the nonlinear system of equations  $\partial J$  for all the applications in this paper to find the k and t and other variables, a constant can be determined via the normalization condition and we note hat t represent the energy value, have been already used in Mathematica and for this aims we get,  $k \approx 0.05$ ,  $E \approx 1.14562$  and  $R_{00} = ae^{-0.05r^2}$ .

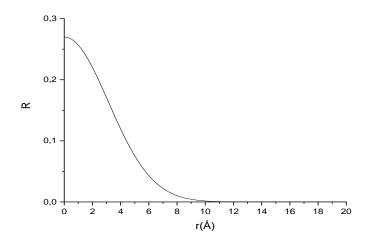


Fig.3.18. The wave function  $R_{00}$  for Harmonic oscillator potential (  $\omega = 0.1$ ).

We'll proceed on to another wave function,  $R = are^{-kr^2}$ , which we'll insert in equation (3.37), allowing us to describe the generic LaGrange functional as follows:

$$J(a,k) = \frac{a^2(-21 + 1600k(3n + 80k(3 + 7k - 3n^2)))\sqrt{\frac{\pi}{2}}}{4096000k^{9/2}}$$
(3.40)

The stationary condition provides the following expressions:

$$\frac{\partial J(a,k)}{\partial a} = \frac{a(-21 + 1600k(3n + 80k(3 + 7k - 3n^2)))\sqrt{\frac{\pi}{2}}}{2048000k^{9/2}}$$
(3.41a)

$$\frac{\partial J(a,k)}{\partial k} = -\frac{3a^2(-63 + 896000k^3 + 11200kn - 640000k^2(-1 + n^2))\sqrt{\frac{\pi}{2}}}{8192000k^{9/2}}$$
(3.41b)

Always with our packaging we get,  $k \approx 0.00073$ ,  $E \approx 0.075$  and  $R_{10} = are^{-0.075r^2}$ .

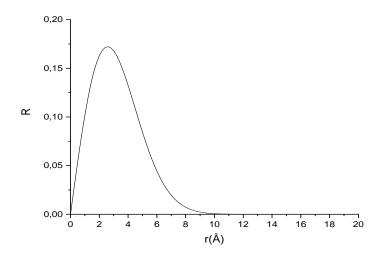


Fig. 3.19. The wave function  $R_{10}$  for Harmonic oscillator potential (  $\omega = 0.1$  ).

In order to describe the generic LaGrange functional as follows, let's move on to another wave function,  $R = (ar^2 + b)e^{-kr^2}$ , which we replace in equation (3.37).

$$J(a,b,k) = \frac{1}{16384000k^{11/2}} \left( (3a^2(-63 + 1600k(7n + 80k(5 + 11k - 5n^2))) + 24abk(-7 + 1600k(n + 80k(1 + k - n^2))) + 16b^2k^2(-3 + 320k(3n + 400k(1 + 3k - n^2)))) \sqrt{\frac{\pi}{2}} \right)$$
(3.42)

and for the stationary condition provides the following expressions:

$$\frac{\partial J(a,b,k)}{\partial a} = \frac{1}{16384000k^{11/2}} \left( (6a(-63 + 1600k(7n + 80k(5 + 11k - 5n^2))) + 24bk(-7 + 1600k(n + 80k(1 + k - n^2)))) \sqrt{\frac{\pi}{2}} \right)$$
(3.43a)

$$\frac{\partial J(a,b,k)}{\partial b} = \frac{1}{16384000k^{11/2}} \left( (24ak(-7 + 1600k(n + 80k(1 + k - n^2))) + 32bk^2(-3 + 320k(3n + 400k(1 + 3k - n^2)))) \sqrt{\frac{\pi}{2}} \right)$$
(3.44b)

$$\frac{\partial J(a,b,k)}{\partial k} = \frac{1}{32768000k^{13/2}} \left( 3(a^2(-693 + 7040000k^3 + 100800kn - 4480000k^2(-1 + n^2)) + 8abk(-63 + 384000k^3 + 11200kn - 640000k^2(-1 + n^2)) + 16b^2k^2(-7 + 128000k^3 + 1600kn - 128000k^2(-1 + n^2)) \right) \sqrt{\frac{\pi}{2}}$$
(3.44c)

For this we get  $b = -185.345k \approx 0.0078$ ,  $E \approx 1.24294$  and  $R_{20} = a(r^2 - 185.345)e^{-0.0078r^2}$ .

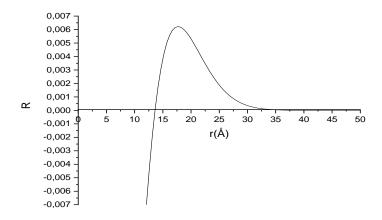


Fig. 3.20. The wave function  $R_{20}$  for Harmonic oscillator potential (  $\omega = 0.1$  ).

We'll proceed by using a different wave function,  $R = (ar^3 + br)e^{-kr^2}$ , and substituting it into equation (3.37). In this fashion, we may describe the generic LaGrange function as follows:

$$J(a,b,k) = \frac{1}{65536000k^{13/2}} \left( (3a^2(-693 + 1600k(63n + 400k(7 + 15k - 7n^2))) + 24abk(-63 + 1600k(7n + 80k(5 + 7k - 5n^2))) + 16b^2k^2(-21 + 1600k(3n + 80k(3 + 7k - 3n^2)))) \sqrt{\frac{\pi}{2}} \right)$$
(3.45)

It offers the following formulations for the stationary condition:

$$\frac{\partial J(a,b,k)}{\partial a} = \frac{1}{65536000k^{13/2}} \left( (6a(-693 + 1600k(63n + 400k(7 + 15k - 7n^2))) + 24bk(-63 + 1600k(7n + 80k(5 + 7k - 5n^2)))) \sqrt{\frac{\pi}{2}} \right)$$
(3.46a)

$$\frac{\partial J(a,b,k)}{\partial b} = \frac{1}{65536000k^{13/2}} \left( (24ak(-63 + 1600k(7n + 80k(5 + 7k - 5n^2))) + 32bk^2(-21 + 1600k(3n + 80k(3 + 7k - 3n^2)))) \sqrt{\frac{\pi}{2}} \right)$$
(3.46b)

$$\begin{split} \frac{\partial J(a,b,k)}{\partial k} &= -\frac{1}{131072000k^{15/2}} \bigg( 3(21a^2(-429 + 3200000k^3 + 52800kn \\ &- 1920000k^2(-1+n^2)) + 16b^2k^2(-63 + 896000k^3 + 11200kn \\ &- 640000k^2(-1+n^2)) + 56abk(-99 + 640000k^3 + 14400kn \\ &- 640000k^2(-1+n^2))) \sqrt{\frac{\pi}{2}} \bigg) \end{split} \tag{3.46c}$$

For this we get  $b = -17.482k \approx 0.067$ ,  $E \approx 1.3478$  and  $R_{30} = a(x^3 - 17.482r)e^{-0.067r^2}$ .

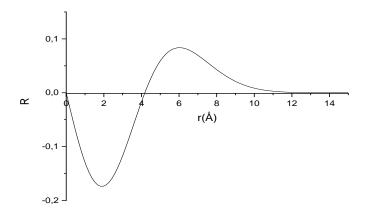


Fig. 3.21. The wave function  $R_{30}$  for Yukawa potential (  $\omega=0.1$  ). the remaining results of different values  $\omega$  are resumed in Table 3.7

Table 3.7: Energy eigenvalues of Klein Gordon oscillator for different values of ω

n	$\omega = 0.1$		$\omega = 0.001$		$\omega = 0.0001$	
	Our results	Ref [11]	Our results	Ref [11]	Our results	Ref [11]
0	1.1456228	1.09545	1.0014995	1.001	1.00014999	1.0001
1	1.1660254	1.18322	1.0017070	1.002	1.00017078	1.0002
2	1.2429356	1.26491	1.0034991	1.003	1.00034998	1.0003
3	1.3577966	1.34164	1.0037895	1.00399	1.00037931	1.0004

According to the plotted figures 3.18, 3.19, 3.20 and 3.21 we observed:

n =0: the curve has no node, so it corresponds to the ground state.

n = 1: the curve has a node, so it corresponds to the first excited state.

n = 2: the curve has a node, so it corresponds to the second excited state.

n = 3: the curve has more than two nodes, so it corresponds to the third excited state.

Table 3.7 shows the energy eigenvalues of Klein Gordon oscillator for different values of  $\omega$ . We became aware of that.

- There exists an analogy between growing energy and growing quantum numbers (n).
- There exists an analogy between growing energy and growing quantum numbers (n)
- The results show good agreement with the findings in reference [11], with a maximum accuracy of 0.0003%.

## 3.2.4. Perturbed Coulomb potential.

For m(r) as constant value M=1 and  $\hbar=c=1$ , the expression of Lagrange becomes:

$$J(r; R_{n,l}; R_{n,lr}) = \int_{0}^{+\infty} \left[ \left( \frac{dR_{n,l}}{dr} \right)^{2} + \left( (M - S(r))^{2} - \left( E - V(r) \right)^{2} \right) R_{n,l}^{2} \right] r^{2}$$
(3.47)

As an outcome, we can employ the perturbed coulomb potential with the form  $-\frac{A}{r} + Br$  [12], for instance,  $A = \frac{1}{5}$ ,  $B = \frac{1}{100}$ , with perturbed values  $V(r) = -\frac{A}{r} + Br$  and S(r) = 0. In these phases, the radial trial function, which has the Coulomb potential  $R(r) = ae^{-kr}$ , is used. To solve for r in the equation (3.47), we use R(r). For this reason, we may express LaGrange's overall functionality as follows:

$$J(a,k) = \frac{1}{k^5} (a^2(-0.000075 + 0.23k^4 + 0.0075kn - 0.1k^3n + k^2(0.001 + 0.25 - 0.25n^2)))$$
(3.48)

These expressions may be obtained from the stationary condition:

$$\frac{\partial J(a,k)}{\partial a} = \frac{1}{k^5} (2a(-0.000075 + 0.23k^4 + 0.0075kn - 0.1k^3n + k^2(0.001 + 0.25 - 0.25n^2)))$$
(3.49a)

$$\frac{\partial J(a,k)}{\partial k} = \frac{1}{k^6} (2a^2(0.0001875 - 0.115k^4 - 0.015kn + 0.1k^3n + k^2(-0.0015 - 0.375 + 0.375n^2)))$$
(3.49b)

Always with our packaging we get,  $k \approx 0.352$ ,  $E \approx 1.02878$  and  $R_{00} = ae^{-0.352r^2}$ .

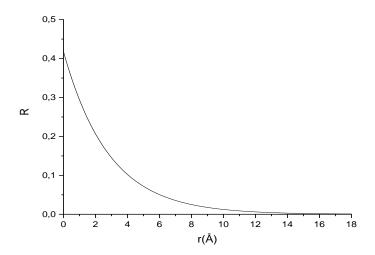


Fig. 3.22. The wave function  $R_{00}$  for perturbed coulomb potential ( A=0.2 , B=0.01) for  $V(r)=\frac{A}{r}+Br \text{ and } S(r)=0$ 

The ground state energies are displayed in table 3.8 with various values for A and B.

Table 3.8: The ground states energies of the perturbed coulomb potential for different values of A and B for  $V(r) = \frac{A}{r} + Br$  and S(r) = 0

A	В	our results	Ref [13]	Ref [12]
0.2	0	0.97894501037	0.97890631293	0.97890631293
	0.01	1.0287847048	1.027622(19)	1.027641
	0.05	1.15487890496	1.152(48)	1.1504
	0.1	1.2703186733	1.277(48)	1.2634
	0.2	1.4509308223	1.50(37)	1.4416
	0.3	1.59836405475	1.73(45)	1.5882
0.3	0	0.9492622940	0.9486832981	0.9486832981
	0.01	0.98502171845	0.9843795380(78)	0.9843836237
	0.05	1.08819164980	1.08612(08)	1.08611
	0.1	1.18677890797	1.18398(08)	1.18356
	0.2	1.34398199832	1.345(34)	1.3397
	0.3	1.47375379433	1.487(52)	1.4693
0.4	0	0.89973541084	0.894427191	0.894427191
	0.01	0.92438145539	0.9190495619	0.9190592557
	0.05	1.00378863065	0.99735023(19)	0.99732540
	0.1	1.083685815589	1.0579666(05)	1.07585618
	0.2	1.21437546978	1.20488(59)	1.20453
	0.3	1.32394120023	1.3138(20)	1.31261

According to the plotted figure 3.22,we observed n = 0: the curve has no node, so it corresponds to the ground state.

Table 3.8 shows the ground states energies of the perturbed coulomb potential for different values of A and B for V(r)=A/r+Br and S(r)=0. We became aware of that.

- The energy decreases when the value A increases.
- A rising of the value B is analogous to an increasing amount of energy.
- The results show good agreement with the findings in reference [8], with a maximum accuracy of 0.008%.

We may describe the generic LaGrange functional as follows by substituting the same wave function in equation (3.47) for another example where  $V(r) = \frac{A}{r}$  and S(r) = Br.

$$J(a,k) = \frac{a^2(0.000075 + 0.23k^4 + 0.0075k - 0.1k^3n + k^2(0.25 - 0.25n^2))}{k^5}$$
(3.50)

The stationary condition provides the following expressions:

$$\frac{\partial J(a,k)}{\partial a} = \frac{2a(0.000075 + 0.0075k + 0.23k^4 - 0.1k^3n + k^2(0.25 - 0.25n^2))}{k^5}$$
(3.51a)

$$\frac{\partial J(a,k)}{\partial k} = \frac{1}{k^6} (2a^2(-0.0001875 - 0.015k - 0.115k^4 + 0.1k^3n + k^2(-0.375 + 0.375n^2)))$$
(3.51b)

Always with our packaging we get,  $k \approx 0.358$ ,  $E \approx 1.028026$  and  $R_{00} = ae^{-0.352r^2}$ .

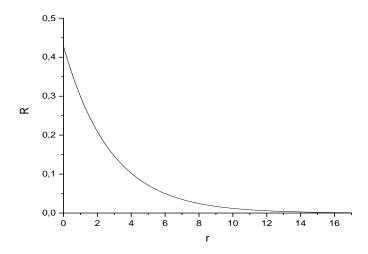


Fig.3.23. The wave function  $R_{00}$  for perturbed coulomb potential ( A=0.2 , B=0.01) for

$$V(r) = \frac{A}{r}$$
 and  $S(r) = Br$ 

The ground state energy with various values of A and B are displayed in table 3.10.

Table 3.9: The ground states energies of the perturbed coulomb potential for different values of A and B for  $V(r) = \frac{A}{r}$  and S(r) = Br

A	В	our results	<b>Ref</b> [13]	Ref [12]
0.2	0	0.97894501037	0.97890631293	0.97890631293
	0.01	1.02802586999	1.027622(19)	1.027641
	0.05	1.15007110053	1.152(48)	1.1504
	0.1	1.26006954745	1.277(48)	1.2634
	0.2	1.43009113672	1.50(37)	1.4416
	0.3	1.56774838360	1.73(45)	1.5882
0.3	0	0.949262293099	0.9486832981	0.9486832981
	0.01	0.98411217478	0.9843795380(78)	0.9843836237
	0.05	1.08288433761	1.08612(08)	1.08611
	0.1	1.17570115356	1.18398(08)	1.18356
	0.2	1.321725375996	1.345(34)	1.3397
	0.3	1.44111738667	1.487(52)	1.4693
0.4	0	0.89973541084	0.894427191	0.894427191
	0.01	0.923275641003	0.9190495619	0.9190592557
	0.05	0.99782183148	0.99735023(19)	0.99732540
	0.1	1.07151710634	1.0759666(05)	1.075856181.20453
	0.2	1.19026554022	1.20488(59)	1.20453
	0.3	1.27690759828	1.3138(20)	1.31261

According to the plotted figure 3.23, we observed n = 0: the curve has no node, so it corresponds to the ground state.

Table 3.9 displays the ground states energies of the perturbed coulomb potential for different values of A and B for V(r)=A/r and S(r)=Br.

- The energy decreases when the value A increases.
- A rising of the value B is analogous to an increasing amount of energy.
- The results show good agreement with the findings in references [12] and [13] , with a maximum accuracy of 0.03%.

The tables that are shown demonstrate that the semi-inverse variational technique yields eigenvalues for various potentials. The accuracy and effectiveness of this method in resolving quantum mechanics issues involving diverse potentials is demonstrated by the results, they agree

well with established references. Furthermore, the study investigates how the eigenvalues change as a function of various factors by setting the value of and contrasting the results with fresh values of. This research demonstrates the sensitivity of the quantum states to variations in the potential function and offers insightful information about how the system behaves when its potential parameters are varied. The tables support the semi-inverse variational method's validity and its ability to examine intricate quantum potentials overall. As a result of the method's ability in finding precise eigenvalues for diverse potentials, it is a promising instrument for the study of quantum mechanics and provides useful details on how quantum systems behave under various circumstances.

#### **Conclusion**

In this work, using the mentioned above technic, the Klein Gordon problem's energies solution was explored for case of the previous two potentials the harmonic and perturbed coulomb potentials [14]. We used the semi-inverse variation technique to obtain the results. The findings from implementing each state's wave functions' general form are given. The energy eigenvalue equations, along with related harmonic oscillator and perturbed coulomb potential eigenfunctions, have thus been obtained. It concludes the relativistic Klein Gordon have similar mathematical properties. If the relativity Klein Gordon problem, can be handled with a particular vector potential. The semi-inverse variational approach is used to determine the relativity Klein Gordon energies spectra and the accompanying wave equations for the Harmonic and Perturbed Coulomb potential. Using a variety of methodologies, it has been demonstrated that this method is effective and straightforward for realizing various arrangements of the Klein Gordon equation and other equations [15]. In this study, we propose a novel and enhanced approach to solve the Klein-Gordan equation by combining the previous potentials and the perturbed. For our calculation, we employ the semi-inverse variational technique. We determined the energy eigenvalues along with the radial wave function for both considered potentials. We noticed that the technic developed herein is extremely convenient to obtain satisfactory results approximation as for solving the Klein-Gordan equation furthermore, this approach can be used to enhance solid state computations in various areas of quantum physics or in conjunction with density functional theory [16-23].

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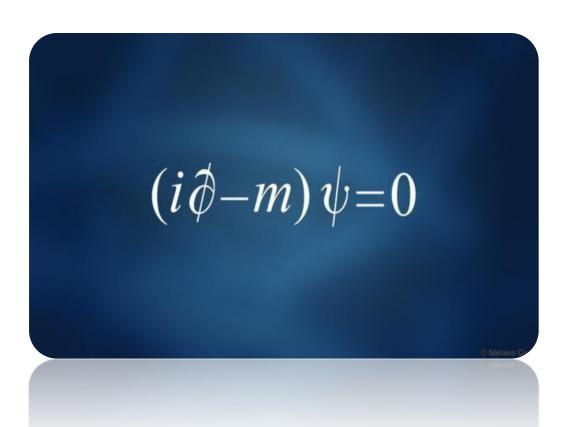
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## Chapter 04

### THE RESOLUTION OF DIRAC EQUATION WITH THE SEMI INVERSE VARIATIONAL METHOD



### **Chapter 4**

## THE RESOLUTION OF DIRAC EQUATION WITH THE SEMI INVERSE VARIATIONAL METHOD

### 4.1. The Dirac equation:

Dirac originally came up with the relativistic and quantum mechanical equation known as the Dirac equation to describe spin 1/2 free electrons. The creation of this astounding equation opened the door for the revolutionary discovery of anti-matter since Dirac described the equation's negative energy solutions as oppositely charged anti-electrons [1].

The Dirac equation with scalar and vector potential (S(r)) and V(r) is  $\hbar = c = 1$ 

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

where *E* is the relativistic energy of the system and  $p = -i\nabla$  is the three-dimensional momentum operator.  $\alpha$  and  $\beta$  are the usual  $4 \times 4$  Dirac matrices given as

$$\alpha = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \qquad \beta = \begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix}, \qquad i = 1,2,3,$$

$$(4.2)$$

where I is the 2  $\times$  2 unitary matrix and the three 2  $\times$  2 Pauli matrices  $\sigma_i$  are given as

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

The spin-orbit  $K = (\sigma \cdot L + 1)$  commutes with the Dirac Hamiltonian, and L is the spherical nucleons' orbital angular momentum. For the aligned spin j = l + (1/2) and the unaligned spin

j=l-(1/2), the eigenvalues of the spin-orbit coupling operator are  $\kappa=(j+(1/2))>0$  and  $\kappa=-(j+(1/2))<0$ , respectively. In the Pauli-Dirac representation, this means that

$$\psi_{nk}(r) = \begin{pmatrix} f_{nk}(r) \\ g_{nk}(r) \end{pmatrix} = \begin{pmatrix} \frac{F_{nk}(r)}{r} Y_{jm}^{l}(\theta, \varphi) \\ \frac{G_{nk}(r)}{r} Y_{jm}^{\tilde{l}}(\theta, \varphi) \end{pmatrix}$$
(4.4)

where  $f_{nk}(r)$  is the upper component and  $g_{nk}(r)$  is the lower component of the Dirac spinors  $Y_{jm}^l(\theta,\varphi)$  and  $Y_{jm}^{\tilde{l}}(\theta,\varphi)$  are spin and pseudospin spherical harmonics and m is the projection of the angular momentum on the z-axis. Substituting (3.4) into (3.1), one obtains two coupled differential equations for the upper and the lower radial wave functions as follows [2-6]:

$$\left(\frac{d}{dr} + \frac{\kappa}{r}\right) F_{nk}(r) = [M + E_{nk} - \Delta(r)] G_{nk}(r) 
\left(\frac{d}{dr} - \frac{\kappa}{r}\right) G_{nk}(r) = [M - E_{nk} + \sum(r)] F_{nk}(r)$$
(4.5)

with

$$\Delta(r) = V(r) - S(r)$$

$$\Sigma(r) = V(r) + S(r)$$
(4.6)

Solving (3.5) leads to a second-order Schrodinger-like differential equation for the upper and the lower components of the Dirac wavefunctions as follows:

$$\left[ \frac{d^2}{dr^2} - \frac{\kappa(\kappa - 1)}{r^2} \right] G_{nk}(r)$$

$$+ \left[ -\left(M + E_{nk} - \Delta(r)\right) \left(M - E_{nk} + \sum(r)\right) - \frac{\left(\frac{d\Sigma(r)}{dr}\right) \left(\frac{d}{dr} - \frac{k}{r}\right)}{M - E_{nk} + \sum(r)} \right] G_{nk}(r) = 0$$
(4.7a)

$$\left[\frac{d^{2}}{dr^{2}} - \frac{\kappa(\kappa - 1)}{r^{2}}\right] F_{nk}(r) + \left[-(M + E_{nk} - \Delta(r))(M - E_{nk} + \Sigma(r)) + \frac{(d\Delta(r)/dr)(d/dr + k/r)}{M + E_{nk} - \Sigma(r)}\right] F_{nk}(r) = 0$$
(4.7b)

### 4.1.1. Spin symmetry limit case:

In the limit of spin symmetry,  $d\Delta(r)/dr = 0$  or  $\Delta(r) = C_s = const$  Ref [7,8] Additionally, And  $\kappa(\kappa - 1) = \tilde{l}(\tilde{l} + 1)$  and  $\kappa(\kappa + 1) = l(l + 1)$ . When the vector potential V(r) equals the scalar potential S(r), the equation (3.7b) obtains.

$$\left[\frac{d^2}{dr^2} - \frac{\kappa(\kappa + 1)}{r^2} - (E_{nk} + M)\Sigma(r)\right] F_{nk}(r) = \left[M^2 - E_{nk}^2\right] F_{nk}(r)$$

$$\left[\frac{d^2}{dr^2} - \frac{\kappa(\kappa + 1)}{r^2} - (E_{nk} + M - C_s)\Sigma(r) - (E_{nk} + M - C_s)(M - E_{nk})\right] F_{nk}(r) = 0$$
(4.8)

And with (3.8), we have

$$G_{nk}(r) = \frac{1}{M + E_{nk}} \left[ \frac{d}{dr} + \frac{k}{r} \right] F_{nk}(r)$$
 (4.9)

### 4.1.2. Pseudospin symmetry case:

Meng and al [7,8] show that the precise symmetry may be inferred from equation (4.7a). In the Dirac equation, it appears when  $\frac{d\Sigma(r)}{dr} = 0$  or  $\Sigma(r) = C_{ps} = const$ . Equation (4.7a) with this symmetry states that.

$$\left[\frac{d^2}{dr^2} - \frac{\kappa(\kappa - 1)}{r^2} + \left(M - E_{nk} + C_{ps}\right)\Delta(r) + \left(E_{nk} + M - C_{ps}\right)(M - E_{nk})\right]G_{nk}(r) = 0$$
(4.10)

### 4.2. The Semi inverse variation method for Dirac equation

*U* is shifted to *Y* in the equation (2.3) for the Spin symmetry limit special case  $C_s = 0$  and the Euler formula (2.6) and factor (2.7). Assuming [9–11], the consistency criteria is now met.  $g(r) = r^2$ 

$$Y(r; F; F'; F'') = r^{2}U(r; F; F'; F'')$$

$$= r^{2}\frac{d^{2}F_{nk}(r)}{dr^{2}} + \frac{dF_{nk}(r)}{dr}$$

$$+ \left(-\frac{k(k-1)}{r^{2}} - (E_{nk} + M)V(r) + E_{nk}^{2} - M^{2}\right)r^{2}F_{nk}(r) = 0$$
(4.11)

For the equation (2.9), we create a generic functional process in an alternate manner as:

$$J(r) = \int_0^{+\infty} L(r; F; F'; F'') dr$$
 (4.12)

Which L(r; F; F'; F'') is the function of lagrange (lagrangian) depends on and its derivatives, guise reads:

$$L = 2\alpha \left(r\frac{dF_{nk}}{dr}\right)^2 + b\left(-\frac{k(k+1)}{r^2} - (E_{nk} + M)\sum(r) + E_{nk}^2 - M^2\right)(rF_{nk})^2 + f$$
(4.13)

Using equation (2.11) and the Euler-Lagrange condition, we've established.

$$2\alpha r^{2} \frac{d^{2}F_{nk}}{dr^{2}} - 2\alpha \frac{dF_{nk}}{dr} + 2b\left(-\frac{k(k+1)}{r^{2}} - (E_{nk} + M)V(r) + E_{nk}^{2} - M^{2}\right)r^{2}F_{nk} + \frac{\delta f}{\delta F_{nk}} = 0$$

$$(4.14)$$

We refer to  $\frac{\delta f}{\delta F_{nk}}$  as the variation derivative of f with respect to  $F_{nk}$ , expressed by:

$$\frac{\delta f}{\delta F_{nk}} = \frac{\partial f}{\partial F_{nk}} - \frac{d}{dr} \left( \frac{\partial f}{\partial F_{nk}'} \right) + \frac{d}{dr} \left( \frac{\partial f}{\partial F_{nk}''} \right) - \cdots \tag{4.15}$$

In order for equation (4.14) to match the original equation, we seek for the values of f,  $\alpha$  and b, and  $\alpha$  and

So 
$$\frac{\delta f}{\delta F_{nk}} = 2\left(-\frac{k(k+1)}{r^2} - (E_{nk} + M)V(r) + E_{nk}^2 - M^2\right)r^2F_{nk}$$
 then we can find F with:

$$F = \left(-\frac{k(k+1)}{r^2} - (E_{nk} + M)V(r) + E_{nk}^2 - M^2\right)r^2 F_{n,k}^2 + f_0$$

 $f_0$  is a constant

$$L = \left[ \left( \frac{dF_{nk}}{dr} \right)^2 + \left( -\frac{k(k+1)}{r^2} - (E_{nk} + M)\sum(r) + E_{nk}^2 - M^2 \right) F_{nk}^2 \right] r^2 dr \tag{4.16}$$

As a result, the problem's Lgrange may be expressed as:

$$J(r) = \int_0^{+\infty} \left[ \left( \frac{dF_{nk}}{dr} \right)^2 + \left( -\frac{k(k+1)}{r^2} - (E_{nk} + M) \sum (r) + E_{nk}^2 - M^2 \right) F_{nk}^2 \right] r^2 dr$$
 (4.17)

With the same method for the case of Pseudospin symmetry case and special one for  $C_{ps}$  we have applied the same conditions of Euler and the method of variation semi-inverse we got:

$$J(r) = \int_0^{+\infty} \left[ \left( \frac{dG_{nk}}{dr} \right)^2 + \left( -\frac{k(k+1)}{r^2} - (E_{nk} - M)\Delta(r) - E_{nk}^2 + M^2 \right) G_{nk}^2 \right] r^2 dr \qquad (4.18)$$

### 4.3. Dirac equation with harmonic oscillator:

### 4.3.1. Spin symmetry limit case for Dirac equation with harmonic oscillator potential:

In considering (4.8), we obtain

$$\left[\frac{d^2}{dr^2} - \frac{k(k+1)}{r^2} - (E_{nk} + M)\sum(r) + E_{nk}^2 - M^2\right] F_{nk}(r) = 0$$
(4.19)

The harmonic oscillator potential is given on the form.

$$\sum(r) = \frac{1}{2}m\omega^2 r^2 \tag{4.20}$$

where  $\omega$  is the pulsation.

So, for m = 1 the LaGrange in equation (2.16) becomes:

$$J(r) = \int_0^{+\infty} \left[ \left( \frac{dF_{nk}}{dr} \right)^2 + \left( -\frac{k(k+1)}{r^2} - \frac{1}{2} (E_{nk} + M) \omega^2 r^2 + E_{nk}^2 - M^2 \right) F_{nk}^2 \right] r^2 dr \qquad (4.21)$$

### 4.3.1.1 Some application on the harmonic oscillator for spin symmetry limit:

The approach is examined in this section using three examples. This application considers the harmonic oscillator potential. It is preferable to make educated guesses about the answers by formulating the trial radial wave functions as follows since the wave function disappears at the origin and at  $r \to \infty$ .

$$F_{nk} = h(r)e^{-kr^2} (4.22)$$

Where h(r) is polynomial function and k are constant quantities to be determined and are considered as variational parameters. These parameters are deduced from the condition of stationarity (minimization).

Fist example: The solution we are looking for is expressed as:

$$F = ae^{-kr^2} (4.23)$$

When we apply the stationary condition to equation (4.21) and substitute the wave function expression (4.23), we obtain.

$$J(a,k) = \frac{a^2 \sqrt{\frac{\pi}{2}} (3(1+t) + 8k(1+3k-t^2))}{128k^{5/2}}$$
(4.24a)

The following expressions are provided by the stationary condition.

$$\frac{\partial J(a,k)}{\partial a} = \frac{a\sqrt{\frac{\pi}{2}}(3(1+t) + 8k(1+3k-t^2))}{64k^{5/2}}$$
(4.24b)

$$\frac{\partial J(a,k)}{\partial k} = -\frac{3a^2\sqrt{\frac{\pi}{2}}(5 + 8k + 8k^2 + 5t - 8kt^2)}{256k^{7/2}}$$
(4.24c)

The normalizing condition may be used to calculate the values of k and the constant a given the resolution of the algebraic system.  $\int_0^\infty |R|^2 r^2 dr$ 

Each time that we use Mathematica, we obtain:  $k \approx 0.63$  And  $E \approx 2.18807$ 

We conclude that this outcome is consistent with the arrangement.: n = 1, l = 0 (state 1s)

The wave function becomes  $F_{00} = ae^{-0.63r^2}$ 

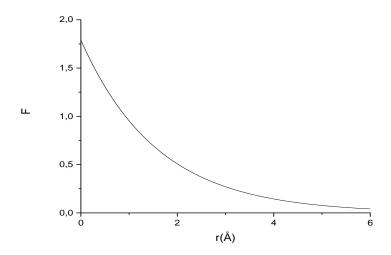


Fig.4.1. The wave function  $F_{10}$  for  $\omega = 1$ 

### second example:

$$F = (ar^2 + b)e^{-kr^2} (4.25)$$

Equation (4.21) may be changed to reflect the wave function expression (4.27) by applying the stationary condition.

$$J(a,g,k) = \frac{1}{2048k^{9/2}} \left( \sqrt{\frac{\pi}{2}} \left( 3a^2 (35(1+t) + 8k(5+11k-5t^2)) + 24abk(5(1+t) + 8k(1+k-t^2)) + 16c^2k^2 (3(1+t) + 8k(1+3k-t^2)) \right) \right)$$
(4.26a)

The stationary condition provides the following expressions.

$$\frac{\partial J(a,b,k)}{\partial a} = \frac{1}{2048k^{9/2}} \left( \sqrt{\frac{\pi}{2}} \left( 6a(35(1+t) + 8k(5+11k-5t^2)) + 24bk(5(1+t) + 8k(1+k-t^2)) \right) \right)$$
(4.26b)

$$\frac{\partial J(a,g,k)}{\partial b} = \frac{1}{2048k^{9/2}} \left( \sqrt{\frac{\pi}{2}} (24ak(5(1+t) + 8k(1+k-t^2)) + 32bk^2(3(1+t) + 8k(1+3k-t^2))) \right)$$

$$\frac{\partial J(a,g,k)}{\partial k} = \frac{-1}{4096k^{9/2}} \left( 3\sqrt{\frac{\pi}{2}} (16b^2k^2(5+8k+8k^2+5t-8kt^2) + 5a^2(88k^2 + 63(1+t) - 56k(-1+t^2)) + 8ack(24k^2+35(1+t) - 40k(-1 + (4.26d) + t^2))) \right)$$

$$(4.26c)$$

The normalizing condition may be used to determine the values of the constants and the values of k provided by the resolution of the algebraic system.  $\int_0^\infty |R|^2 r^2 dr$ 

Always with Mathematica we obtain:  $k \approx 0.74 \, a$ ,  $b \approx -1.01 a$  And  $E \approx 3.36826$ 

We deduce that this result corresponds to the configuration: n = 2, l = 0 (state 2s)

The wave function becomes  $F_{10} = a(r^2 - 1.01)e^{-0.74r^2}$ 

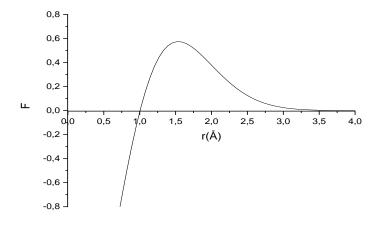


Fig.4.2. The wave function  $F_{20}$  for  $\omega = 1$ 

third example:

$$F = (ar^4 + br^2 + d)e^{-kr^2} (4.27)$$

Equation (4.21) is changed to include the expression for the wave function (4.32), and the stationary condition we derived is then applied.

$$J(a,b,d,k) = \frac{1}{32768k^{13/2}} \left( \sqrt{\frac{\pi}{2}} (105a^2(99(1+t) + 8k(9+19k-9t^2)) + 16k^2(3b^2(35(1+t) + 8k(5+11k-5t^2)) + 24bdk(5(1+t) + 8k(1+k-t^2)) + 16d^2k^2(3(1+t) + 8k(1+3k-t^2)) + 120ak(b(63(1+t) + 8k(7+11k-7t^2)) - 4dk(-7(1+t) + 8k(-1+k+t^2))) \right)$$

$$(4.28a)$$

The stationary condition provides the following expressions.

$$\frac{\partial J(a,b,d,k)}{\partial a} = \frac{1}{32768k^{13/2}} \left( \sqrt{\frac{\pi}{2}} \left( 210a(99(1+t) + 8k(9+19k-9t^2)) + 120k(b(63(1+t) + 8k(7+11k-7t^2)) - 4dk(-7(1+t) + 8k(-1+k+t^2))) \right) \right)$$
(4.28b)

$$\frac{\partial J(a,b,d,k)}{\partial b} = \frac{1}{2048k^{9/2}} \left( \sqrt{\frac{\pi}{2}} (120ak(63(1+t) + 8k(7+11k-7t^2)) + 16k^2(6b(35(1+t) + 8k(5+11k-5t^2)) + 24dk(5(1+t) + 8k(1+k-t^2))) \right)$$
(4.28c)

$$\frac{\partial J(a,b,d,k)}{\partial d} = \frac{1}{32768k^{13/2}} \left( \sqrt{\frac{\pi}{2}} \left( -480ak^2 \left( -7(1+t) + 8k(-1+k+t^2) \right) + 16k^2 \left( 24bk(5(1+t) + 8k(1+k-t^2) \right) + 32dk^2 \left( 3(1+t) + 8k(1+k-t^2) \right) + 3k(1+k-t^2) \right) \right)$$
(4.28d)

$$\frac{\partial J(a,b,d,k)}{\partial k} = \frac{-1}{65536k^{15/2}} \left( 3\sqrt{\frac{\pi}{2}} \left( 315a^2 (152k^2 + 143(1+t) - 88k(-1+t^2) \right) + 16k^2 (16d^2k^2(5+8k+8k^2+5t-8kt^2) + 5b^2(88k^2+63(1+t) - 56k(-1+t^2)) + 8bdk(24k^2+35(1+t) - 40k(-1+t^2)) \right)$$

$$+ 40ak(7b(88k^2 + 99(1+t) - 72k(-1+t^2)) - 4dk(40k^2 - 63(1+t) + 56k(-1+t^2))) \right)$$

$$+ (4.28e)$$

The normalizing condition may be used to derive the values of k and the constant a from the resolution of the algebraic system.  $\int_0^\infty |R|^2 r^2 dr$ 

When we use Mathematica, we obtain:  $k \approx 0.82 a$ ,  $b \approx -3.05 a$ , d = 1.4 And  $E \approx 4.35974$ 

We conclude that this outcome is consistent with the arrangement.: n = 2, l = 0 (state 3s)

The wave function becomes  $F_{20} = a(r^4 - 3.05r^2 + 1.4)e^{-0.82r^2}$ 

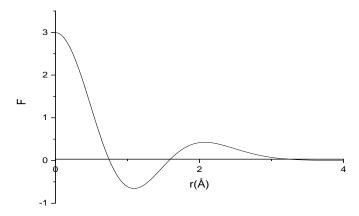


Fig.4.3. The wave function  $F_{30}$  for  $\omega = 1$ 

We continued displaying the findings in the table below for various values of  $\omega$ .

Table 4.1:The eigenvalues of Harmonic oscillator potential for different values of $\omega$ for Spin
symmetry limit case.

n	$\omega = 0.1$	<b>Ref</b> [12]	$\omega = 0.5$	<b>Ref</b> [12]	$\omega = 1$	<b>Ref</b> [12]
0	1.14485	1.14485	1.65139	1.65139	2.18807	2.18807
1	1.32464	1.32464	2.3518	2.3518	3.36826	3.36826
2	1.49266	1.49266	2.95546	2.95546	4.35974	4.35974

According to the drawn figures 4.1, 4.2 and 4.3 we observed:

- n = 1: the curve has no node, so it corresponds to the ground state.
- n =2:The curve has a node, so it corresponds to the first excited state.
- n = 3: the curve has two nodes, so it corresponds to the second excited state.

Table 4.1 the eigenvalues of Harmonic oscillator potential for different values of  $\omega$  for Spin symmetry limit case we noticed that :

- The energy increases as the values of  $\omega$  increase.
- An increase in energy is correlated with a rise in quantum number n.
- With inaccuracy of 0%, the results are in good agreement with the findings in reference [12].

### 4.3.2. Pseudospin symmetry case:

Using (4.10), we obtain

$$\left[\frac{d^2}{dr^2} - \frac{k(k-1)}{r^2} - (E_{nk} - M)\sum(r) + E_{nk}^2 - M^2\right]G_{nk}(r) = 0$$
(4.29)

On the form, the harmonic oscillator potential is provided.

$$\sum(r) = \frac{1}{2}m\omega^2 r^2 \tag{4.30}$$

where  $\omega$  is the pulsation.

So, for m = 1 the LaGrange in equation (2.16) becomes:

$$J(r) = \int_0^{+\infty} \frac{1}{2} \left[ \left( \frac{dG_{nk}}{dr} \right)^2 + \left( -\frac{k(k-1)}{r^2} - \frac{1}{2} (E_{nk} - M) \omega^2 r^2 + E_{nk}^2 - M^2 \right) G_{nk}^2 \right] r^2 dr \quad (4.31)$$

### 4.3.2.1. Some Application on the harmonic oscillator:

The approach is examined in this section using three examples. This application considers the harmonic oscillator potential. It is preferable to make educated guesses about the answers by

formulating the trial radial wave functions as follows since the wave function disappears at the origin and at  $r \to \infty$ .

$$G_{nk} = h(r)e^{-kr^2} (4.32)$$

Where k is a constant quantity that must be found and is regarded as a variational parameter, and h(r) is a polynomial function. These variables are derived from the stationarity (minimization) requirement.

<u>Fist example</u>: The solution we are looking for is expressed as:

$$G = ae^{-kr^2} (4.33)$$

When we apply the stationary condition to equation (4.40) and substitute the wave function expression (4.42), we obtain.

$$J(a,k) = \frac{a^2 \sqrt{\frac{\pi}{2}} (3(-1+t) + 8k(1+3k-t^2))}{128k^{5/2}}$$
(4.34a)

The stationary condition provides the following expressions.

$$\frac{\partial J(a,k)}{\partial a} = \frac{a\sqrt{\frac{\pi}{2}}(3(-1+t) + 8k(1+3k-t^2))}{64k^{5/2}}$$
(4.34b)

$$\frac{\partial J(a,k)}{\partial k} = -\frac{3a^2\sqrt{\frac{\pi}{2}}(-5 + 8k + 8k^2 + 5t - 8kt^2)}{256k^{7/2}}$$
(4.34c)

The normalizing condition may be used to calculate the values of k and the constant a given the resolution of the algebraic system.  $\int_0^\infty |R|^2 r^2 dr$ 

Mathematica consistently gives us:  $k \approx 0.28$  And  $E \approx 1.6438$ 

We conclude that this outcome is consistent with the arrangement.: n = 0, l = 0 (state 0s)

Wave function changes into  $G_{00} = ae^{0.28r^2}$ 

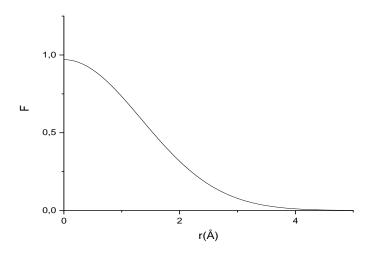


Fig.4.4. The wave function  $G_{00}$  for  $\omega = 1$ 

### second example:

$$G = (ar^2 + b)e^{-kr^2} (4.35)$$

Equation (4.40) is changed by substituting the formula for the wave function (4.46), and when the stationary condition is used, we obtain.

$$J(a,b,k) = \frac{1}{2048k^{9/2}} \left( \sqrt{\frac{\pi}{2}} \left( 3a^2 (35(-1+t) + 8k(5+11k-5t^2)) + 24abk(5(-1+t) + 8k(1+k-t^2)) + 16b^2k^2(3(-1+t) + 8k(1+3k-t^2)) \right) \right)$$
(4.36a)

The stationary condition provides the following expressions.

$$\frac{\partial J(a,b,k)}{\partial a} = \frac{1}{2048k^{9/2}} \left( \sqrt{\frac{\pi}{2}} \left( 6a(35(-1+t) + 8k(5+11k-5t^2)) + 24bk(5(-1+t) + 8k(1+k-t^2)) \right) + 24bk(5(-1+t) + 8k(1+k-t^2)) \right)$$
(4.36b)

$$\frac{\partial J(a,b,k)}{\partial b} = \frac{1}{2048k^{9/2}} \left( \sqrt{\frac{\pi}{2}} \left( 24ak(5(-1+t) + 8k(1+k-t^2)) + 32bk^2(3(-1+t) + 8k(1+3k-t^2)) \right) + 8k(1+3k-t^2) \right)$$
(4.36c)

$$\frac{\partial J(a,b,k)}{\partial k} = \frac{-1}{4096k^{11/2}} \left( 3\sqrt{\frac{\pi}{2}} \left( 16b^2k^2(-5 + 8k + 8k^2 + 5t - 8kt^2) + 5a^2(88k^2 + 63(-1+t) - 56k(-1+t^2)) + 8abk(24k^2 + 35(-1+t) - 40k(-1+t^2)) \right)$$
(4.36d)

The normalizing condition may be used to determine the values of the constant a and the values of k provided by the resolution of the algebraic system.  $\int_0^\infty |R|^2 r^2 dr$ 

Every time we use Mathematica, we:  $k \approx 0.47 \, a$ ,  $b \approx -1.61 a$  And  $E \approx 2.74597$ 

We conclude that this outcome is consistent with the arrangement.: n = 1, l = 0 (state 2s)

The wave function becomes  $G_{10} = a(r^2 - 1.61)e^{-0.47r^2}$ 

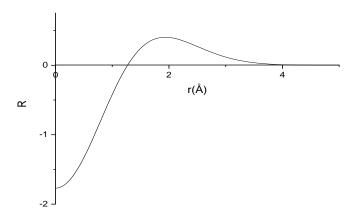


Fig.4.5. The wave function  $G_{10}$  for  $\omega = 1$ 

### third example:

$$G = (ar^4 + br^2 + d)e^{-kr^2} (4.37)$$

Equation (4.40) is changed by substituting the formula for the wave function (4.51), and when we use the stationary condition, we obtain.

$$J(a,b,d,k) = \frac{1}{32768k^{13/2}} \left( \sqrt{\frac{\pi}{2}} (105a^2(99(-1+t) + 8k(9+19k-9t^2)) + 16k^2(3b^2(35(-1+t) + 8k(5+11k-5t^2)) + 24bdk(5(-1+t) + 8k(1+k-t^2)) + 16d^2k^2(3(-1+t) + 8k(1+3k-t^2)) + 120ak(b(63(-1+t) + 8k(7+11k-7t^2)) - 4dk(7-7t + 8k(-1+k+t^2))) \right)$$

$$(4.38a)$$

These expressions are made possible by the stationary condition.

$$\frac{\partial J(a,b,d,k)}{\partial a} = \frac{1}{32768k^{13/2}} \left( \sqrt{\frac{\pi}{2}} \left( 210a(99(-1+t) + 8k(9+19k-9t^2)) + 120k(b(63(-1+t) + 8k(7+11k-7t^2)) - 4dk(7-7t + 8k(-1+k+t^2))) \right) \right)$$
(4.38b)

$$\frac{\partial J(a,b,d,k)}{\partial b} = \frac{1}{2048k^{9/2}} \left( \sqrt{\frac{\pi}{2}} (120ak(63(-1+t) + 8k(7+11k-7t^2)) + 16k^2(6b(35(-1+t) + 8k(5+11k-5t^2)) + 24dk(5(-1+t) + 8k(1+k-t^2))) \right)$$
(4.38c)

$$\frac{\partial J(a,b,d,k)}{\partial d} = \frac{1}{32768k^{13/2}} \left( \sqrt{\frac{\pi}{2}} \left( -480ak^2 \left( -7(1+t) + 8k(-1+k+t^2) \right) + 16k^2 (24bk(5(1+t) + 8k(1+k-t^2)) + 32dk^2 (3(1+t) + 8k(1+k-t^2)) + 3k(1+k-t^2) \right) \right)$$
(4.38d)

$$\frac{\partial J(a,b,d,k)}{\partial k} = \frac{-1}{65536k^{15/2}} \left( 3\sqrt{\frac{\pi}{2}} \left( 315a^2 (152k^2 + 143(-1+t) - 88k(-1+t^2) \right) \right) + 16k^2 (16d^2k^2(-5+8k+8k^2+5t-8kt^2) + 5b^2 (88k^2+63(-1+t) - 56k(-1+t^2)) + 8bdk(24k^2+35(-1+t) - 40k(-1+t^2)) + 40ak(7c(88k^2+99(-1+t) - 72k(-1+t^2)) + 4dk(40k^2 - 63(-1+t) + 56k(-1+t^2))) \right)$$

$$-4dk(40k^2 - 63(-1+t) + 56k(-1+t^2))))$$

The normalizing condition may be used to calculate the values of k and the constant a given the resolution of the algebraic system.  $\int_0^\infty |R|^2 r^2 dr$ 

Mathematica always gives us:  $k \approx 0.58$ ,  $b \approx -4.29a$ , d = 2.76a And  $E \approx 3.71797$ 

We determine that this outcome matches the setting.: n = 2, l = 0 (state 3s)

The wave function becomes  $G_{20} = a(r^2 - 4.29r + 2.76)e^{-0.58r^2}$ 

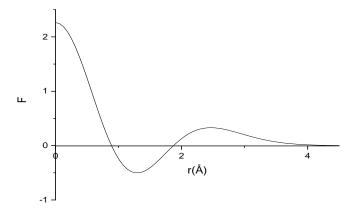


Fig.4.6. The wave function  $G_{20}$  for  $\omega = 1$ 

We continued displaying the findings in the table below for various values of  $\omega$ .

Table 4.2:The eigenvalues of Harmonic oscillator potential for different values of  $\omega$  for Pseudospin symmetry case.

n	$\omega = 0.1$	Ref [12]	$\omega = 0.5$	Ref [12]	$\omega = 1$	Ref [12]
0	1.01113	1.01113	1.22686	1.22686	1.6438	1.6438
1	1.05785	1.05785	1.78799	1.78799	2.74597	2.74597
2	1.13298	1.13298	2.34875	2.34875	3.71797	3.71797

According to the drawn figures 4.4, 4.5 and 4.6 we observed:

- n = 1: the curve has no node, so it corresponds to the ground state.
- n =2:The curve has a node, so it corresponds to the first excited state.
- n = 3: the curve has two nodes, so it corresponds to the second excited state.

Table 4.2 The eigenvalues of Harmonic oscillator potential for different values of  $\omega$  for Pseudospin symmetry case. we noticed that :

- The energy increases as the values of  $\omega$  increase.
- An increase in energy is correlated with a rise in quantum number n.
- With inaccuracy of 0%, the results are in good agreement with the findings in reference [12].

### 4.4. Dirac equation with Coulomb potential:

### **4.4.1.** Spin Symmetry Limit:

In considering (4.8), we obtain

$$\left[\frac{d^2}{dr^2} - \frac{\kappa(\kappa + 1)}{r^2} - (E_{nk} + M)\sum(r) + E_{nk}^2 - M^2\right] F_{nk}(r) = 0$$
(4.39)

On the form, the Coulomb potential is provided.

$$\sum(r) = \frac{A}{r} \tag{4.40}$$

where  $A = -\frac{e^2}{4\pi\varepsilon_0}$  and supposing  $e = 4\pi\varepsilon_0 = 1$ 

So, for m = 1 the LaGrange in equation (2.16) becomes:

$$J(r) = \int_0^{+\infty} \frac{1}{2} \left[ \left( \frac{dF_{nk}}{dr} \right)^2 + \left( \frac{k(k+1)}{r^2} + \frac{1}{r} (E_{nk} + M) + E_{nk}^2 - M^2 \right) F_{nk}^2 \right] r^2 dr \tag{4.41}$$

### 4.4.1.1. Some application on the coulomb potential in case of spin symmetry limit:

Three examples are used in this section to explore the methodology. We take the Coulombian potential into account in this application. It is preferable to make educated guesses about the answers by formulating the trial radial wave functions as follows since the wave function disappears at the origin and at  $r \to \infty$ ,.

$$F_{nk} = h(r)e^{-kr} (4.42)$$

We examine a few cases using various values of  $\kappa$  whether  $\kappa < 0$  or  $\kappa > 0$ 

First example: n = 0  $\kappa = 1$  l = 1

The solution we are looking for is expressed as:

$$F = are^{-kr} (4.43)$$

Equation (4.40) may be solved for r by substituting the wave function's expression (4.43) and the stationary condition.

$$J(a,k) = -\frac{a^4(-9 - 16k^2 + 9t^2 + 6k(1+t))}{1024k^5}$$
(4.44a)

The following expressions are provided by the stationary condition.

$$\frac{\partial J(a,k)}{\partial a} = -\frac{a^3(-9 - 16k^2 + 9t^2 + 6k(1+t))}{256k^5}$$
(4.44b)

$$\frac{\partial J(a,k)}{\partial k} = -\frac{3a^4(16k^2 - 8k(1+t) - 15(-1+t^2))}{1024k^6}$$
(4.44c)

The normalizing condition may be used to calculate the values of k and the constant a given the resolution of the algebraic system.  $\int_0^\infty |R|^2 r^2 dr$ 

Mathematica consistently gives us:  $k \approx 0.35$  and  $E \approx 0.882353$ 

We determine that this outcome matches the setting: n = 0, l = 1 (state 0p)

The wave function becomes  $F_{01} = are^{0.35r}$ 

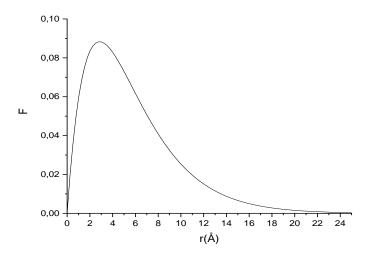


Fig.4.7. The wave function  $F_{01}$ 

### Second example: n = 1 $\kappa = 1$ l = 1

The conclusion that we seek is written as follows:

$$F = (ar + b)re^{-kr} (4.45)$$

When we apply the stationary condition to equation (4.40) and substitute the wave function expression (4.45), we obtain.

$$J(a,b,k) = \frac{1}{16k^7} (3(a^2(15+7k^2-15t^2-5k(1+t))+2abk(5+3k^2-5t^2-2k(1+t))+b^2k^2(2+2k^2-2t^2-k(1+t))))$$
(4.46a)

These phrases are made possible by the stationary condition.

$$\frac{\partial J(a,b,k)}{\partial a} = \frac{1}{16k^7} (3(2a(15+7k^2-15t^2-5k(1+t))+2bk(5+3k^2-5t^2-2k(1+t))))$$
(4.46b)

$$\frac{\partial J(a,b,k)}{\partial b} = \frac{1}{16k^7} (3(2ak(5+3k^2-5t^2-2k(1+t))+2bk^2(2+2k^2-2t^2-k(1+t))))$$
(4.46c)

$$\frac{\partial J(a,b,k)}{\partial k} = \frac{-1}{16k^8} \left( 3(2b^2k^2(5+3k^2-5t^2-2k(1+t)) + 5a^2(7k^2-6k(1+t)) - 21(-1+t^2) \right) + 4abk(6k^2-5k(1+t)-15(-1+t^2)) \right)$$
(4.46d)

The normalizing condition may be used to determine the values of the constant and the values of k provided by the resolution of the algebraic system.  $\int_0^\infty |R|^2 r^2 dr$ 

Mathematica consistently gives us:  $k \approx 0.32$ ,  $b \approx -6.17$  and  $E \approx 0.945946$ 

We conclude that this outcome is consistent with the arrangement.: n = 1, l = 1 (state 1p)

The wave function becomes  $F_{11} = (ar - 6.17)re^{0.32r}$ 

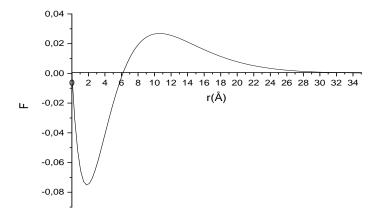


Fig.4.8. The wave function  $F_{11}$ 

### Third example: n = 0 $\kappa = -3$ l = 2

The clarification we seek is written as follows:

$$F = ar^2 e^{-kr} (4.47)$$

When we apply the stationary condition to equation (4.40) and substitute the wave function expression (4.47), we obtain.

$$J(a,k) = \frac{15a(3+3k^2-3t^2-k(1+t))}{8k^7}$$
 (4.48a)

The following expressions are provided by the stationary condition.

$$\frac{\partial J(a,k)}{\partial a} = \frac{15a(3+3k^2-3t^2-k(1+t))}{8k^7}$$
 (4.48b)

$$\frac{\partial J(a,k)}{\partial k} = -\frac{45a^2(7+5k^2-7t^2-2k(1+t))}{16k^8}$$
 (4.48c)

The normalizing condition may be used to calculate the values of k and the constant a given the resolution of the algebraic system.  $\int_0^\infty |R|^2 r^2 dr$ 

Mathematica always provides us with:  $k \approx 0.32$  and  $E \approx 0.945946$ 

We conclude that this outcome is consistent with the arrangement.: n = 0, l = 2 (state 0d)

The wave function becomes  $F_{02} = ar^2e^{0.32r}$ 

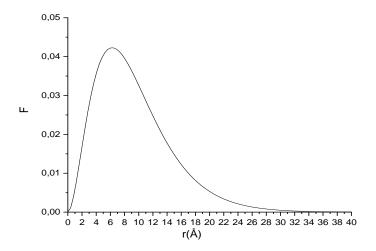


Fig.4.9. The wave function  $F_{02}$ 

### Fourth example: n = 1 $\kappa = -3$ l = 2

The reply that we seek is written as follows:

$$F = (ar + b)re^{-kr} (4.49)$$

Equation (4.40) may be solved for, and the stationary condition is applied by substituting the expression of the wave function (4.49) in it.

$$J(a,b,k) = \frac{1}{32k^9} (15(3a^2(28+16k^2-28t^2-7k(1+t))+6abk(7+5k^2-7t^2-2k(1+t))+2b^2k^2(3+3k^2-3t^2-k(1+t))))$$
(4.50a)

The stationary condition provides the following expressions.

$$\frac{\partial J(a,b,k)}{\partial a} = \frac{1}{32k^9} (15(6a(28+16k^2-28t^2-7k(1+t))+6bk(7+5k^2-7t^2-2k(1+t))))$$
(4.50b)

$$\frac{\partial J(a,b,k)}{\partial b} = \frac{1}{32k^9} (15(6ak(7+5k^2-7t^2-2k(1+t))+4bk^2(3+3k^2-3t^2-2k(1+t))) + 4bk^2(3+3k^2-3t^2-2k(1+t)))$$
(4.50c)

$$\frac{\partial J(a,b,k)}{\partial k} = \frac{-1}{16k^{10}} \left( 45(14a^2(9 + 4k^2 - 9t^2 - 2k(1+t)) + b^2k^2(7 + 5k^2 - 7t^2 - 2k(1+t)) + 2abk(15k^2 - 7k(1+t) - 28(-1+t^2)) \right)$$
(4.50d)

The normalizing condition may be used to calculate the values of k and the constant a given the resolution of the algebraic system.  $\int_0^{\infty} |R|^2 r^2 dr$ 

Each time we use Mathematica, we:  $k \approx 0.25$ ,  $b \approx -12.1875$  and  $E \approx 0.969231$ 

We conclude that this outcome is consistent with the arrangement.: n = 1, l = 2 (state 1d)

The wave function becomes  $F_{12} = a(r - 12.1875)re^{0.25r}$ 

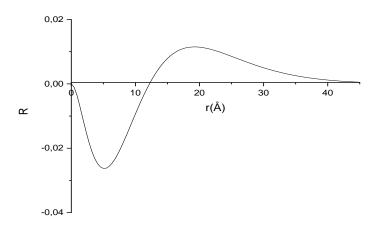


Fig.4.10. The wave function  $F_{12}$ 

In the table below, we repeated the results for various values of 1 and.

	7			D. C[12]			D (C[12]
n	l	К	semi inverse	Ref [13]	К	semi inverse	Ref [13]
0	1	1	0.882353	0.882353	-2	0.882353	0.882353
	2	2	0.945946	0.945946	-3	0.945946	0.945946
	3	3	0.969231	0.969231	-4	0.969231	0.969231
	4	4	0.980198	0.980198	-5	0.980198	0.980198
1	1	1	0.945946	0.945946	-2	0.945946	0.945946
	2	2	0.969231	0.969231	-3	0.969231	0.969231
	3	3	0.980198	0.980198	-4	0.980198	0.980198
	4	4	0.986207	0.986207	-5	0.986207	0.986207

Table 4.3: The eigenvalues of coulomb potential for different values of  $\kappa$  and l for spin symmetry case

According to the drawn figures 4.7, 4.8, 4.9 and 4.10 we observed:

- n = 0, l=1: the curve has no node, so it corresponds to the ground state.
- n = 1, l = 1: The curve has a node, so it corresponds to the first excited state.
- n = 0, l = 2: the curve has no node, so it corresponds to the ground state.
- n = 1, l=2: the curve has a node, so it corresponds to the first excited state.

Table 4.3 The eigenvalues of coulomb potential for different values of  $\kappa$  and 1 for spin symmetry case, we noticed that:

- An increase in energy is correlated with a rise in quantum numbers n,l and κ.
- With an inaccuracy of 0%, the results are in good agreement with the findings in reference [13].

Following the determination of the energy eigenvalues for various quantum numbers n and the variation of the pulsation constant  $\omega$  using equations (40) for the cases of spin symmetry limit and pseudo symmetry limit over the harmonic oscillator potential, it is obvious that the semi-inverse variation method was used. The results are shown in tables 4.1 and 4.2 When comparing it to earlier research in reference [13], we have identical findings with 0% incertitude, demonstrating the validity of this approach and demonstrating how accurate it is.

### **4.4.2.** Pseudospin Symmetry Limit:

Using (4.10), we obtain

$$\left[\frac{d^2}{dr^2} - \frac{\kappa(\kappa - 1)}{r^2} - (E_{nk} - M)\sum(r) + E_{nk}^2 - M^2\right] G_{nk}(r) = 0$$
(4.51)

Continuing with the same potential which is Coulomb potential.

So, for m = 1 the LaGrange in equation (2.16) becomes:

$$J(r) = \int_0^{+\infty} \frac{1}{2} \left[ \left( \frac{dG_{nk}}{dr} \right)^2 + \left( \frac{\kappa(\kappa - 1)}{r^2} - (E_{nk} - M) \frac{A}{r} - E_{nk}^2 + M^2 \right) G_{nk}^2 \right] r^2 dr \tag{4.52}$$

### 4.4.2.1. Some Application on the coulombmb potential in case of Spin Symmetry Limit:

The approach is examined in this section using three examples. We take the Coulombian potential into account in this application. It is preferable to make educated guesses about the answers by formulating the trial radial wave functions as follows since the wave function disappears at the origin and at  $r \to \infty$ .

$$G_{nk} = h(r)e^{-kr} (4.53)$$

We try to identify instances with various values of  $\kappa$  whether  $\kappa < 0$  or  $\kappa > 0$ 

First example: n = 0  $\kappa = 2$  l = 2

The clarification we desire is written as follows:

$$G = are^{-kr} (4.54)$$

Equation (4.53) may be changed to reflect the wave function expression (4.54), and when we apply the stationary condition, we obtain.

$$J(a,k) = \frac{3a^2(2+2k^2+k(-1+t)-2t^2)}{16k^5}$$
 (4.55a)

The stationary condition provides the following expressions.

$$\frac{\partial J(a,k)}{\partial a} = \frac{3a(2+2k^2+k(-1+t)-2t^2)}{8k^5}$$
 (4.55b)

$$\frac{\partial J(a,k)}{\partial k} = -\frac{3a^2(5+3k^2+2k(-1+t)-5t^2)}{8k^6}$$
 (4.55c)

The normalizing condition may be used to calculate the values of k and the constant a given the resolution of the algebraic system.  $\int_0^\infty |R|^2 r^2 dr$ 

Mathematica consistently gives us:  $k \approx 0.47$  and  $E \approx -0.882353$ 

We conclude that this outcome is consistent with the arrangement.: n = 0, l = 2 (state 0d)

The wave function becomes  $G_{02} = are^{0.47r}$ 

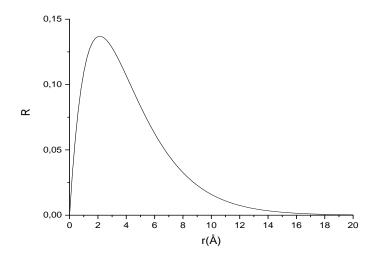


Fig.4.11. The wave function  $G_{02}$ 

### Second example: n = 1 $\kappa = 2$ l = 2

The conclusion that we need is written as follows:

$$G = (ar + b)re^{-kr} (4.56)$$

Substituting the expression of the wave function (4.56) in equation (4.53) and we apply the stationary condition we get.

$$J(a,b,k) = \frac{1}{16k^7} (3(a^2(15+7k^2+5k(-1+t)-15t^2)+2abk(5+3k^2+2k(-1+t)-5t^2)+b^2k^2(2+2k^2+k(-1+t)-2t^2)))$$
(4.57a)

The stationary condition provides the following expressions.

$$\frac{\partial J(a,b,k)}{\partial a} = \frac{1}{16k^7} (3(2a(15+7k^2+5k(-1+t)-15t^2)+2ck(5+3k^2+2k(-1+t)-5t^2)))$$
(4.57b)

$$\frac{\partial J(a,b,k)}{\partial b} = \frac{1}{16k^7} (3(2ak(5+3k^2+2k(-1+t)-5t^2)+2bk^2(2+2k^2+k(-1+t)-5t^2)+2bk^2(2+2k^2+k(-1+t)-5t^2)+2bk^2(2+2k^2+k(-1+t)-5t^2)+2bk^2(2+2k^2+k(-1+t)-5t^2)+2bk^2(2+2k^2+k(-1+t)-5t^2)+2bk^2(2+2k^2+k(-1+t)-5t^2)+2bk^2(2+2k^2+k(-1+t)-5t^2)+2bk^2(2+2k^2+k(-1+t)-5t^2)+2bk^2(2+2k^2+k(-1+t)-5t^2)+2bk^2(2+2k^2+k(-1+t)-5t^2)+2bk^2(2+2k^2+k(-1+t)-5t^2)+2bk^2(2+2k^2+k(-1+t)-5t^2)+2bk^2(2+2k^2+k(-1+t)-2t^2)+2bk^2(2+2k^$$

$$\frac{\partial J(a,b,k)}{\partial k} = \frac{-1}{16k^8} \left( 3(2b^2k^2(5+3k^2+2k(-1+t)-5t^2) + 5a^2(7k^2+6k(-1+t)-21(-1+t^2)) + 4abk(6k^2+5k(-1+t)-15(-1+t^2)) \right)$$
(4.57d)

The resolution of the algebraic system provides the values of k and the constant a can be determined via the normalization condition  $\int_0^{\infty} |R|^2 r^2 dr$ 

Always with Mathematica we get:  $k \approx 0.32$ ,  $c \approx -6.17$  and  $E \approx -0.945946$ 

We deduce that this result corresponds to the configuration: n = 1, l = 2 (state 1d)

The wave function becomes  $G_{12} = (ar - 6.17)re^{0.32r}$ 

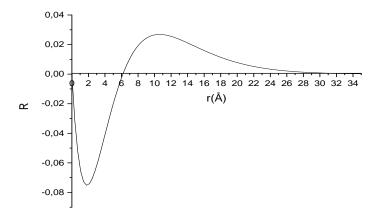


Fig.4.12. The wave function  $G_{12}$ 

third example: n = 1  $\kappa = -2$  l = 2

The answer we're seeking for is written as:

$$G = (ar + b)re^{-kr} (4.58)$$

Equation (4.53) may be changed to reflect the wave function expression (4.58), and when we apply the stationary condition, we obtain.

$$J(a,b,k) = \frac{1}{16k^7} (3(a^2(15+7k^2+5k(-1+t)-15t^2)+2abk(5+3k^2+2k(-1+t)-5t^2)+b^2k^2(2+2k^2+k(-1+t)-2t^2)))$$

$$(4.59)$$

The following expressions are provided by the stationary condition.

$$\frac{\partial J(a,b,k)}{\partial a} = \frac{1}{16k^7} (3(2a(15+7k^2+5k(-1+t)-15t^2)+2bk(5+3k^2+2k(-1+t)-5t^2)))$$
(4.60a)

$$\frac{\partial J(a,b,k)}{\partial b} = \frac{1}{16k^7} (3(2ak(5+3k^2+2k(-1+t)-5t^2)+2bk^2(2+2k^2+k(-1+t)-5t^2)+2bk^2(2+2k^2+k(-1+t)-2t^2)))$$
(4.60b)

$$\frac{\partial J(a,b,k)}{\partial k} = \frac{-1}{16k^8} \left( 3(2b^2k^2(5+3k^2+2k(-1+t)-5t^2) + 5a^2(7k^2+6k(-1+t)-2t^2) + 5a^2(7k^2+6k(-1+t)-2t^2) + 4abk(6k^2+5k(-1+t)-15(-1+t^2)) \right)$$
(4.60c)

The normalizing condition may be used to calculate the values of k and the constant a given the resolution of the algebraic system.  $\int_0^\infty |R|^2 r^2 dr$ 

Whenever we employ Mathematica, we:  $k \approx 0.32$ ,  $b \approx -6.17$  and  $E \approx -0.945946$ 

We determine that this outcome matches the setting: n = 1, l = 1 (state 1p)

The wave function becomes  $G_{11} = a(r - 6.17)re^{0.32r}$ 

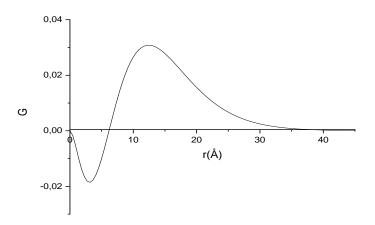


Fig.4.13. The wave function  $G_{11}$ 

### Fourth example: n = 2 $\kappa = -1$ l = 1

The answer we seek is written as follows:

$$G = (ar^2 + br + d)re^{-kr}$$

$$\tag{4.61}$$

Equation (4.53) may be changed by substituting the formula for the wave function (4.61), and when we apply the stationary condition, we obtain.

$$J(a,b,d,k) = \frac{1}{32k^9} (45a^2(28 + 8k^2 + 7k(-1+t) - 28t^2) + 30ak(b(21 + k(-6 + 7k) + 6kt - 21t^2) + 2dk(3 + (-1+k)k + kt - 3t^2))$$

$$+ 6k^2(b^2(15 + k(-5 + 7k) + 5kt - 15t^2) + 2bdk(5 + k(-2 + 3k) + 2kt - 5t^2) + d^2k^2(2 + k(-1 + 2k) + kt - 2t^2)))$$

$$(4.62a)$$

These expressions may be obtained from the stationary condition.

$$\frac{\partial J(a,b,d,k)}{\partial a} = \frac{1}{32k^9} (90a(28 + 8k^2 + 7k(-1+t) - 28t^2) + 30k(b(21 + k(-6 + 7k) + 6kt - 21t^2) + 2dk(3 + (-1+k)k + kt - 3t^2)))$$
(4.61b)

$$\frac{\partial J(a,b,d,k)}{\partial b} = \frac{1}{32k^9} (30ak(21 + k(-6 + 7k) + 6kt - 21t^2) + 6k^2(2b(15 + k(-5 + 7k) + 5kt - 15t^2) + 2dk(5 + k(-2 + 3k) + 2kt - 5t^2)))$$
(4.62c)

$$\frac{\partial J(a,b,d,k)}{\partial d} = \frac{-1}{16k^8} (60ak^2(3 + (-1+k)k + kt - 3t^2) + 6k^2(2bk(5 + k(-2 + 3k) + 2kt - 5t^2) + 2dk^2(2 + k(-1 + 2k) + kt - 2t^2)))$$
(4.62d)

$$\frac{\partial J(a,b,d,k)}{\partial k} = \frac{-1}{16k^8} (2k^2(2bdk(6+5k^2+3k(-1+t)-6t^2)+3b^2(5+3k^2+2k(-1+t)-5t^2)+d^2k^2(3+5k^2+2k(-1+t)-3t^2))$$

$$+2k(-1+t)-5t^2)+d^2k^2(3+5k^2+2k(-1+t)-3t^2))$$

$$+15a^2(7k^2+6k(-1+t)-21(-1+t^2))+12ak(dk(5+2k^2+2k(-1+t)-5t^2)+b(6k^2+5k(-1+t)-15(-1+t^2))))$$

$$(4.62e)$$

The normalizing condition may be used to calculate the values of k and the constant a given the resolution of the algebraic system.  $\int_0^{\infty} |R|^2 r^2 dr$ 

Each time we utilize Mathematica, we:  $k\approx 0.25$  ,  $b\approx -20.3125$  ,  $d\approx 82.5195$  and  $E\approx -0.969231$ 

We conclude that this outcome is consistent with the arrangement.: n = 2, l = 1 (state 2p)

The wave function becomes  $G_{21} = a(r^2 - 20.3125r + 82.5195)re^{0.25r}$ 

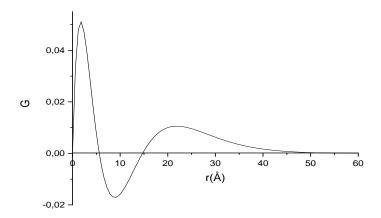


Fig.4.14. The wave function  $G_{21}$ 

In the table below, we tested the results for various values of l and  $\kappa$ .

Table 4.4: The eigenvalues of coulomb potential for different values of  $\kappa$  and l for pseudospin symmetry case

n	l	κ	semi inverse	Ref [13]	n	к	semi inverse	Ref [13]
0	1	2	-0.882353	-0.882353	1	-1	-0.945946	-0.945946
	2	3	-0.945946	-0.945946		-2	-0.969231	-0.969231
	3	4	-0.969231	-0.969231		-3	-0.980198	-0.980198
	4	5	-0.980198	-0.980198		-4	-0.986207	-0.986207
1	1	2	-0.945946	-0.945946	2	-1	-0.969231	-0.969231
	2	3	-0.969231	-0.969231		-2	-0.980198	-0.980198
	3	4	-0.980198	-0.980198		-3	-0.986207	-0.986207
	4	5	-0.986207	-0.986207		-4	-0.989848	-0.989848

According to the drawn figures 4.11, 4.12, 4.13 and 4.14 we observed:

- n = 0, l=1: the curve has no node, so it corresponds to the ground state.
- n = 1, l = 1: The curve has a node, so it corresponds to the first excited state.
- n = 0, l=2: the curve has no nodes, so it corresponds to the ground state.
- n = 1, l = 2: the curve has a node, so it corresponds to the first excited state.

Table 4.4 The eigenvalues of coulomb potential for different values of  $\kappa$  and 1 for pseudospin symmetry case. we noticed that :

- An increase in energy is correlated with a rise in quantum numbers n,l and  $\kappa$ .
- With an inaccuracy of 0%, the results are in good agreement with the findings in reference [13].

The Dirac equation was solved by Using the semi-inverse variation method, we investigated the energy eigenvalues for various quantum numbers (n, l, and  $\kappa$ ) according to the requirements of pseudospin symmetry and the spin symmetry limit over the coulomb potential. We observed the logic of the results, where the absolute value of energy at each level increases as the number of states (n, l) increases. After comparing the energy data in Tables 4.3 and 4.3 with those from past research in reference [13], we see that the results agree exactly and there are no margins of error, demonstrating the efficacy of the approach and how precise it is.

### **Conclusion**

In conclusion, we have investigated the spin symmetry and pseudospin symmetry requirements of the bound state solution of the Dirac equation with the harmonic oscillator and coulomb potentials. To get the results, we employed the semi-inverse variation approach. The outcomes obtained by applying the general form of each state's wave functions are described. Thus, we have obtained the energy eigenvalue equations and related harmonic oscillator and coulomb eigenfunctions in the case of spin symmetry and pseudospin symmetry, respectively. Particularly, it is discovered that the non-relativistic Schrödinger equation and the Dirac equation share mathematical similarities. If the solution of the non-relativistic Schrödinger equation with a specific vector potential can be obtained. The semi-inverse variational approach is used for determining the relativistic Dirac energy spectrum and the related wave functions for the Coulomb potential. It has been demonstrated that this method is an effective and straightforward technique for realizing various configurations of the Dirac equation.

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# General Conclusion

### **GENERAL CONCLUSION**

The semi-inverse approach of building generalized variational principles is provided here, demonstrating a novel theoretical foundation and new, diverse methods for constructing generalized variational principles of different fluid and elasticity issues. The semi-inverse approach will have a significant impact not only on fluid mechanics, but also on elasticity theorems.

In this thesis ,the time independent Schrödinger equation (radial portion) has been introduced in the first section. The current study's aim is to investigate the energy levels associated with the Schrödinger equation with different types of potentials employing the semi-inverse variation approach.

They used the semi-inverse variation approach to obtain the LaGrange expression of the Klein Gordon and Dirac equations. Then We figured out what the bound states were and the associate wave function.

We reviewed the semi-inverse technique findings by comparing them to the results obtained by using the related polynomials to solve the radial Schrödinger equation. The semi-inverse variational approach is a strong mathematical tool for developing a variational formulation for a wave type differential problem. So far, this method provides an effective and best strategy for establishing variational principles for a wide range of physical issues.

Particularly, the variational semi-inverse method is novel variational approach. Within the context of the introduction of the Schrödinger equation, we arrived at the proper findings given by a classical system and the quantum picture. The variational semi-inverse approach is used to solve the Schrödinger equation using the radial 3D potential. We examined certain state configurations, and the energies obtained are precise. A future effort is planned that will focus on the screened potential, which is challenging to address from a quantum standpoint.

The second section of the thesis begins with determining the significance of the semi-inverse variation approach and using knowledge of energy and related states. Its purpose is to ensure the method's effectiveness. Using this strategy, we were able to determine the limit states of

energy of the Klein Gordon equation with various potentials and gain certain results that proved to be conclusive enough to reach the equation's solutions.

In the previous thesis, we attempted to improve the efficacy of this method even further by calculating the Eigen energy by solving the Dirac equation with the harmonic oscillator potential and the Coulombian potential for the two cases considered, spin symmetry limit case and pseudo spin symmetry case. Exact results are obtained for the two cases considered.

### **Scientific Production**

### **Publications**

**Khalid Reggab**, Ahmed Gueddim, Abdelkrim Naas, (2023). Semi-inverse variational approach to solve the Klein-Gordon equation for harmonic- and perturbed Coulomb potentials. Studies In Engineering and Exact Sciences, Vol.4, No.1.

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### **International Communications**

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**Khalid Reggab**, Study Of Some Diatomic Molecules Properties Using The Pseudo-Harmonic Potential With The WKB Approximation, 1st International Conference on Materials Sciences and Applications (Hybrid) ICSMA'2023, 08th and 09th February 2023, Khenchela-Algeria.

**Khalid Reggab**, Resolution of differential equation (Schrodinger equation) via the numerical semi-inverse variation method, The first International Conference on Mathematical Sciences and Applications ICMSA'2023, May 2-3, 2023, Guelma-Algeria.

**Khalid Reggab**, Digital Transformation in Education and Educational Institutions and its Importance, The online international conference on: Modern Educational Technologies for Quality and Transformative Education: "Local Needs and Global Challenges", 4<sup>th</sup> May 2023.Batna-Algeria.

Aicha Aziza Ayad, Abdelkrim Naas, **Khalid Reggab**, Walid Serbout, Effect of annealing temperature on stability of methyl ammonium lead iodide CH<sub>3</sub>NH<sub>3</sub>PbI<sub>3</sub> structure, 1st International Conference on Renewable Solutions for Ecosystems: Towards a Sustainable Energy Transition ICRSEtoSET 2023, Djelfa on May 06-07, 2023, Algeria.

**Khalid Reggab,** The Numerical Investigation Of Eigenenergy's Of Schrodinger Equation For Nonlinear Potential, 11th International Summit Scientific Research Congress, December 15-17, 2023 / Gaziantep, Turkey.

**Khalid Reggab,** Energy spectrum of non-relativistic Schrodinger equation for nonlinear potential,1st International Future Engineering Conference,25-26,2023,Sirnak,Turkey

**Khalid Reggab**, The Analytical Analysis Of Energy Eigenvalues Of Some Selected Diatomic Molecules Via The WKB Approximation ,International Aegean Conferences Innovation Technologies & Engineering-IX, February 23-25, 2024,IZMIR, Turkey.

### **National Communications**

Meriem Kerara, Aicha Aziza Ayad, Ayoub Abdessabour, **Khalid Reggab**, Omar Meglali, Simulation of CIGS thin films solar cell with AMPS-1D, XIII<sup>émé</sup> Journées Maghrébines des Sciences des Matériaux JMSM'2020 tenues le 09-11 Mars 2020, Oran-Algeria

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**Khalid Reggab**, Resolution of Schrodinger Equation with Anharmonic Potential Via Nikiforov-Uvarov (NU) Method ,3rd National Conference on Applied Physics & Chemistry (3rdNCAPC23) held on March 12th &13th, 2023 in Laghouat-Algeria.

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