The discrete spectra of Dirac operators

Petr Zorin

A Thesis in

The Department of Mathematics

and Statistics

Presented in Partial Fulfillment of the Requirements for the Degree of Master of Science (Mathematics) at Concordia University

Montreal, Quebec, Canada

August 2011

CONCORDIA UNIVERSITY

School of Graduate Studies

This is to certify that the thesis prepared

By: Petr Zorin

Entitled: The discrete spectra of Dirac operators

and submitted in partial fulfillment of the requirements for the degree of

Master of Science (Mathematics)

complies with the regulations of the University and meets the accepted standards with respect to originality and quality.

Signed by the final Examining Committee:

Syed Twareque Ali

____ Chair

Alina Stancu

____ Examiner

Syed Twareque Ali

____ Examiner

Richard Hall

____ Supervisor

Approved by ________Jose Garrido____________________________

Chair of Department or Graduate Program Director

________Brian Lewis____________________________

Dean of Faculty

Date ________August 29, 2011____________________________

Abstract

The discrete spectra of Dirac operators.

Petr Zorin.

A single particle is bound by an attractive central potential and obeys the Dirac equation in d spatial dimensions. The Coulomb potential is one of the few examples for which exact analytical solutions are available. A geometrical approach called "the potential envelope method" is used to study the discrete spectra generated by potentials $V(r)$ that are smooth transformations $V(r) = g(-1/r)$ of the soluble Coulomb potential. When g has definite convexity, the method leads to energy bounds. This is possible because of the recent comparison theorems for the Dirac equation. The results are applied to study soft-core Coulomb potentials used as models for confined atoms. The spectral estimates are compared with accurate eigenvalues found by numerical methods.

Acknowledgements

I would like to express my gratitude first and foremost to my supervisor, Professor Richard L. Hall, without whom this work would not have been possible. His knowledge, support and tremendous patience have guided me througout this process. For the last two years his help and encouragement have taught me to believe and myself and not to give up.

I would also like to thank the staff of the Department of Mathematics and Statistics for the large role they played in the making of my thesis. Their resourcefulness and willingness to help have saved me a great deal of stress in difficult moments.

And last, but not least, I would like to say a special thank you to my mother Ludmila and brother Alexander who always believed in me, and to all of my friends who never doubted my abilities. Whithout each and every one of these people I would not be where I am today; they all played a part in my achievement.

To my mother and father,

Contents

List of Figures **vii**

List of Tables **x**

Introduction **1**

1 The Dirac equation in $d+1$ dimensions **4**

1.1 Schrödinger, Klein–Gordon, and Dirac equations 4

1.2 $\boldsymbol{\alpha}, \boldsymbol{\beta}$ algebra: general formulation 6

1.3 Central potentials $V(r)$ and $S(r)$ 11

1.4 Nonrelativistic limit 16

1.5 Some spectral generalities 18

2 The exact solution of the Coulomb problem **22**

2.1 The asymptotic iteration method 22

2.2 Solution of the Dirac Coulomb problem 26

3 Scaling laws **33**

3.1 Scaling for the Schrödinger equation 33

3.1.1 Scaling for the class of the power potentials $V(r) = v\,\mathrm{sgn}(q)r^q$ 35

3.1.2 Scaling for a class of soft–core Coulomb potentials 36

3.2 Scaling for the Dirac equation 37

4 Comparison Theorem **41**

4.1 Relativistic comparison Theorem for the Dirac equation 41

4.2 Some examples 44

5 Envelope theory **47**

5.1 The envelope method 47

5.2 An example 52

6 Numerical solutions **55**

6.1 The shooting method 55

6.2 Initial conditions for the Schrödinger equation 57

6.3 Initial conditions for the Dirac coupled equations 59

6.4 Maple code 61

7 Soft–Core Coulomb potentials - confined atoms **65**

7.1 Scaling 65

7.2 Monotonicity 67

7.3 Coulomb envelopes 69

Conclusion **71**

A Central Potentials **79**

A.1 Coulomb potential 79

A.2 Harmonic oscillator 80

A.3 Hulthén potential 81

A.4 Sech–squared potential 82

A.5 Soft–core Coulomb potential 83

A.6 Woods–Saxon potential 84

A.7 Yukawa potential 85

List of Figures

1.1 Graphs of the Schrödinger radial wave function $R(r)$ for the ground state and different v. 21

4.1 Laser–dressed (doted line) and cutoff (dashed line) Coulomb potentials with $l = 0.5$, $\lambda = 1$, $u = 0.73$, and $\beta = 1$. 45

4.2 Woods–Saxon (full line) and Laser–dressed Coulomb (doted line) potentials with $w = 1$, $R = 1$, $a = 1.3$, $l = 0.74$, and $\lambda = 1$. 46

5.1 The graph of $D''(u)$ for $n \geq k$. 50

5.2 The graph of $D''(u)$ for $n < k$. 50

5.3 Hulthén potential (full line) and the tangential potentials (dashed lines) at different touching points $t = 5,\ 10,\ 15,\ 20,\ 25$, with $\lambda = 0.2$ and $u = 100$. 54

6.1 Shooting method. 56

6.2 Dirac radial wave function $G(r)$. 64

7.1 The family of potentials $V(r) = -\dfrac{v}{(r^q + \beta^q)^{1/q}}$, with $\beta = 0.5$, $q = 10$, and $v = 0.1,\ 0.5,\ 1,\ 2,\ 5,\ 7,\ 10$. These potentials are monotonic in v: $\dfrac{\partial V}{\partial v}$. 68

7.2 The family of potentials $V(r) = -\dfrac{v}{(r^q + \beta^q)^{1/q}}$, with $v = 0.6$, $q = 15$, and $\beta = 0.1,\ 0.2,\ 0.5,\ 0.7,\ 1,\ 3,\ 7$. These potentials are monotonic in β: $\dfrac{\partial V}{\partial \beta}$. 69

7.3 The family of potentials $V(r) = -\dfrac{v}{(r^q + \beta^q)^{1/q}}$, with $v = 1$, $\beta = 1.5$, and $q = 1,\ 2,\ 3,\ 5,\ 10,\ 20,\ 100$. These potentials are monotonic in q: $\dfrac{\partial V}{\partial q}$. 70

7.4 Soft-Core Coulomb potential $V(r)$ (full line) and the tangentials potentials $V^{(t)}(r)$ (dashed lines) at different touching points $t = 0.01,\ 0.7,\ 1.5,\ 2,\ 3$, with $u = 58$, $\beta = 2$, and $q = 2$. Each tangential potential leads to a lower energy curve $E^{(t)}$. 72

List of Tables

4.1 Energy values of laser–dressed (E_L) and cutoff (E_C) Coulomb potentials 46

5.1 Comparison of the exact Hulthén energy eigenvalues E with its upper bounds E^U; $j = 1/2$ and $\tau = -1$. 53

7.1 Comparison the exact soft–sore Coulomb energy eigenvalues E with its lover bounds E^L. 71

Introduction

The first theory of quantum mechanics was the matrix theory. The development of the matrix formulation of quantum mechanics was done by the German physicists Werner Heisenberg[1] [1] and Max Born in 1925. But matrix theory was new to physics and was not very welcome. It was difficult for contemporaries to understand and apply, but it was reluctantly recognized and accepted as a theory of quantum mechanics. However, shortly after this theory was published, the Austrian physicist Erwin Schrödinger in 1926, fascinated by de Broglie's Ph.D thesis[2], constructed wave mechanics and the nonrelativistic Schrödinger equation as an approximation to the generalised case of de Broglie's theory [2, 3]. Soon after, Schrödinger [4] and von Neumann [5] showed that the matrix and wave theories of quantum mechanics were equivalent, the former treating operators in the Hilbert space l^2 and the latter in L^2. Schrödinger tried to make his quantum mechanics relativistic, but was not satisfied, because it was second order in time (the state at a later time is not predicted from the present). In 1928, the British physicist Paul Dirac introduced a satisfactory solution which required 4–spinor states and 4×4 matrix operators. Thus arose Dirac's relativistic quantum mechanical wave equation in three spatial dimensions.

With these two fundamental theories of quantum mechanics available, the field grew quickly. Quantum theory was applied to atoms, molecules, and solids, with

---

[1] Heisenberg was awarded the Nobel Prize in physics 1932 for this achievement.

[2] In 1924, the French physicist Louis de Broglie put forward his theory of matter waves by stating that particles can exhibit wave characteristics and vice versa. This theory was for a single particle and derived from the special relativity theory.

great success. The wave equation form of quantum mechanics is still generally used today. One of the main problems in relativistic quantum mechanics is to determine the solutions of the Dirac equation, in particular, to find the energy levels of a particle. But very few problems admit exact analytic solutions. Therefore methods that give approximate solutions are extremely important. In this thesis, we describe the envelope theory which allows us to approximate the energy eigenvalues by studying potentials $V(r)$ that are smooth transformations $V(r) = g(h(r))$ of soluble potentials $h(r)$.

We start the first Chapter with the derivation of three fundamental equations of Quantum Mechanics: the Schrödinger, Klein–Gordon and Dirac equations, guided by [6]. Then we consider the properties of certain Dirac matrices and state a theorem which gives the connection between the size of the Dirac matrices and the spatial dimension d. For central potentials, after the time dependence is determined, we derive a pair of Dirac coupled equations in d spatial dimensions [7]. We then obtain from these the radial Schrödinger equation in the nonrelativistic limit. At the end of this chapter we describe some spectral generalities concerning the Dirac energy eigenvalues.

In Chapter 2 we review the asymptotic iteration method [8, 9]. Then with its help we solve the pair of the Dirac coupled equations for a particle which is moving in a pure vector Coulomb field. As a result we get the formula for the Coulomb energies in d spatial dimensions.

In Chapter 3 we derive scaling laws for the Schrödinger and the Dirac radial equations for different central potentials.

We begin Chapter 4 with the relativistic Comparison Theorem for the Dirac equation, and the proof, following Hall [10, 13]. We then illustrate this theorem with some examples.

In Chapter 5 we review the envelope theory and demonstrate it by an example.

In Chapter 6 we briefly review the shooting method for finding numerical solutions to boundary–value problems. Then we consider initial conditions for the Schrödinger and Dirac equations with different potentials. Finally, we introduce a computer program, based on this theory, with which we can calculate the energy values for the Schrödinger and Dirac coupled equations with different potentials.

In Chapter 7 we consider a family of soft–core Coulomb potenials. In particular, we obtain the scaling law for this family with the Dirac Hamiltonian, establish monotonicity of the energy values, and give an approximate formula for the soft–core Coulomb energy eigenvalues.

In an appendix we include some general background information about specific potentials which we use in this thesis.

Throughout the thesis, the natural units $\hbar = c = 1$ are employed if it is not explicitly stated otherwise.

Chapter 1

The Dirac equation in $d+1$ dimensions

1.1 Schrödinger, Klein–Gordon, and Dirac equations

The classical nonrelativistic relation between the energy E and momentum $\mathbb{p}$ for a free particle of mass m reads

$$E = \frac{\mathbb{p}^2}{2m}. \tag{1.1}$$

We replace the energy E and the momentum $\mathbb{p}$ by their corresponding quantum mechanical operators

$$E \longrightarrow i\hbar\frac{\partial}{\partial t} \quad \text{and} \quad \mathbb{p} \longrightarrow \frac{\hbar}{i}\bigtriangledown,^{1} \tag{1.2}$$

and let them act on the wave function $\Psi(\boldsymbol{r}, t)$. Then the equation (1.1) becomes

$$i\hbar\frac{\partial\Psi}{\partial t} = -\frac{\hbar^2}{2m}\bigtriangledown^2\Psi, \tag{1.3}$$

---

[1] The nabla symbol $\bigtriangledown$ denotes the gradient and $\hbar = h/2\pi$ is the reduced Planck constant.

which is the well-known nonrelativistic time dependent Schrödinger equation for a free particle.

Let us now apply the same approach to the relativistic relation between energy and momentum, namely

$$E^2 = \mathbb{p}^2 c^2 + m^2 c^4, \tag{1.4}$$

where c is the speed of light. Using (1.2), we obtain the Klein–Gordon equation for a free particle of mass m:

$$-\hbar \frac{\partial^2 \Psi}{\partial t^2} = \left(-\hbar^2 c^2 \bigtriangledown^2 + m^2 c^4 \right) \Psi. \tag{1.5}$$

The Klein–Gordon equation presents some difficulties. For instance, it is a second order differential equation in the time t. This means that we can find the solution only if two boundary conditions are given, i.e. $\Psi(\boldsymbol{r},\ t)$ and $\partial \Psi(\boldsymbol{r},\ t)/\partial t$ for a given t. Also the Klein–Gordon equation admits negative energy solutions. Because of these problems, physicists searched for another equation which could combine quantum mechanics and special relativity. This equation must be a differential equation of first order in time so we will not run into the above mentioned problem of the Klein–Gordon equation, and also of first order with respect to derivatives of space coordinates so that the equation can be invariant under Lorentz transformations.

Dirac considered the square root

$$E = \sqrt{\mathbb{p}^2 c^2 + m^2 c^4},$$

and assumed that it cannot be extracted in some simple way. In the limit $\mathbb{p} \longrightarrow 0$, we find

$$\sqrt{\mathbb{p}^2 c^2 + m^2 c^4} \longrightarrow mc^2,$$

and for $m \longrightarrow 0$,

$$\sqrt{\mathbb{p}^2c^2 + m^2c^4} \longrightarrow \mathbb{p}c.$$

Then Dirac generalized the two last limits to

$$\sqrt{\mathbb{p}^2c^2 + m^2c^4} = \alpha\mathbb{p}c + \beta mc^2,$$

and, following a similar path as that to the Klein–Gordon equation, he obtained his famous equation.

$$i\hbar\frac{\partial\Psi}{\partial t} = \left(\alpha\mathbb{p}c + \beta mc^2\right)\Psi. \tag{1.6}$$

We shall determine the coefficients α and β in the next section.

1.2 $\boldsymbol{\alpha}, \boldsymbol{\beta}$ algebra: general formulation

Let us rewrite equation (1.6) in natural units $\hbar = c = 1$ in the following way

$$i\frac{\partial\Psi}{\partial t} = \left(\sum_{j=1}^{d}\alpha_j p_j + \beta m\right)\Psi, \qquad H = \sum_{j=1}^{d}\alpha_j p_j + \beta m, \tag{1.7}$$

where m is the mass of the particle and the operator p_j is defined by

$$p_j = -i\frac{\partial}{\partial x^j}, \quad 1 \leq j \leq d. \tag{1.8}$$

Equation (1.7) is the Dirac equation in $d+1$ dimensions for a free particle. The coefficients $\{\alpha_j\}$ and β cannot be simple numbers, otherwise (1.7) would not be form invariant with respect to simple spatial rotations, thus they are matrices, called Dirac matrices. Since $\{\alpha_j\}$ and β are matrices then Ψ has to be a column vector

$$\Psi = \begin{pmatrix} \psi_1(\boldsymbol{r}, t) \\ \psi_2(\boldsymbol{r}, t) \\ \dots \\ \psi_n(\boldsymbol{r}, t) \end{pmatrix},$$

therefore $\{\alpha_j\}$ and β have to be $n \times n$ square matrices. Following [14, 15] we consider their basic properties.

If we rewrite equation (1.7) for a free particle in the following form

$$\left(\sum_{j=1}^{d} \alpha_j p_j + \beta m - i \frac{\partial}{\partial t} \right) \Psi = 0,$$

and, multiply it on the left by the operator $\left(\sum_{j=1}^{d} \alpha_j p_j + \beta m + i \frac{\partial}{\partial t} \right)$, we obtain

$$\left(\sum_{i,j=1}^{d} \alpha_i \alpha_j p_i p_j + m \sum_{j=1}^{d} (\alpha_j \beta + \beta \alpha_j) p_j + m^2 \beta^2 + \frac{\partial^2}{\partial t^2} \right) \Psi = 0.$$

Since $\sum_{i,j=1}^{d} \alpha_i \alpha_j p_i p_j = \left(\sum_{i,j=1}^{d} \alpha_i \alpha_j p_i p_j + \sum_{i,j=1}^{d} \alpha_j \alpha_i p_j p_i \right)/2$, we finally obtain

$$-\frac{\partial^2 \Psi}{\partial t^2} = \left(\sum_{i,j=1}^{d} \frac{\alpha_i \alpha_j + \alpha_j \alpha_i}{2} p_i p_j + m \sum_{j=1}^{d} (\alpha_j \beta + \beta \alpha_j) p_j + m^2 \beta^2 \right) \Psi.$$

Each component $\psi_i(\boldsymbol{r}, t)$ of the spinor Ψ must satisfy the Klein–Gordon equation (1.5) (with $\hbar = c = 1$)

$$-\frac{\partial^2 \psi_i}{\partial t^2} = \left(\mathbb{p}^2 + m^2 \right) \psi_i.$$

The comparison of the last two equations gives us the following requirements for the matrices $\{\alpha_j\}$ and β:

$$\alpha_i \alpha_j + \alpha_j \alpha_i = 2\delta_{ij} \mathbb{1}, \tag{1.9}$$

$$\alpha_j \beta + \beta \alpha_j = 0, \tag{1.10}$$

$$\alpha_i^2 = \beta^2 = \mathbb{1}, \tag{1.11}$$

where

$$\delta_{ij} = \begin{cases} 1, & \text{if} \quad i = j, \\ 0, & \text{if} \quad i \neq j, \end{cases}$$

is the Kronecker delta symbol. The anticommutation relations (1.9), (1.10), and (1.11) define an algebra for the $\{\alpha_j\}$ and β matrices. The hamiltonian H in (1.7) has to be hermitian (self-adjoint), therefore Dirac matrices also have to be hermitian. This implies that the elements on the main diagonal are real, the matrices are symmetric with respect to the main diagonal, their eigenvalues are real, and

$$\alpha_j^\dagger = \alpha_j,^{2} \tag{1.12}$$

$$\beta^\dagger = \beta. \tag{1.13}$$

Since the $\{\alpha_j\}$ are hermitian, they are diagonalizable. Suppose that α_j in its eigen-representation has the form

$$\alpha_j = \begin{pmatrix} a_1 & 0 & 0 & \cdots & 0 \\ 0 & a_2 & 0 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \cdots & a_n \end{pmatrix}, \tag{1.14}$$

---

[2] The symbol "†" denotes the conjugate transpose of a matrix.

where $a_1, \ldots, a_n$ are eigenvalues of $\{\alpha_j\}$. Then (1.14) and (1.11) give us

$$\alpha_j^2 = \mathbb{1} = \begin{pmatrix} 1 & 0 & 0 & \cdots & 0 \\ 0 & 1 & 0 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \cdots & 1 \end{pmatrix} = \begin{pmatrix} a_1^2 & 0 & 0 & \cdots & 0 \\ 0 & a_2^2 & 0 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \cdots & a_n^2 \end{pmatrix},$$

from which we have $a_k = \pm 1, \; k = 1, \ldots, \; n$. The same argument applies to the matrix β. Thus the eigenvalues of $\{\alpha_j\}$ and β are equal to ± 1.

Multiply of (1.10) on the left by β yields (with $\beta^2 = \mathbb{1}$),

$$\beta \alpha_j \beta = -\alpha_j. \tag{1.15}$$

Using the identity [3] trAB =trBA from [16] with (1.11) and (1.15), we get

$$\text{tr } \alpha_j = \text{tr } \beta^2 \alpha_j = \text{tr } \beta \alpha_j \beta = -\text{tr } \alpha_j,$$

or tr $\alpha_j = -$tr α_j, this is possible only if

$$\text{tr } \alpha_j = 0. \tag{1.16}$$

Following the same reasoning we can obtain for the matrix β:

$$-\beta = \alpha_j \beta \alpha_j,$$

then

$$\text{tr } \beta = \text{tr } \alpha_j^2 \beta = \text{tr } \alpha_j \beta \alpha_j = -\text{tr } \beta.$$

---

[3] tr A, the trace of a square $n \times n$ matrix A, is defined to be the sum of the elements on the main diagonal.

Finally,

$$\text{tr}\ \beta = 0. \tag{1.17}$$

Now let us go back to the constraint (1.10), which we can rewrite in the following form

$$\alpha_j\beta = -\beta\alpha_j = (-\mathbb{1})\beta\alpha_j.$$

If we take the determinant of both sides of the above equation,

$$\det\alpha_j \det\beta = (-1)^n \det\beta \det\alpha_j$$

we find that n must be even.

Suppose that T is the $n \times n$ square matrix which transforms the matrix α_j into its diagonal form

$$T\alpha_j T^{-1} = \begin{pmatrix} a_1 & 0 & 0 & \cdots & 0 \\ 0 & a_2 & 0 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \cdots & a_n \end{pmatrix}. \tag{1.18}$$

Then (1.18) and identity trAB =trBA gives us

$$\text{tr} \begin{pmatrix} a_1 & 0 & 0 & \cdots & 0 \\ 0 & a_2 & 0 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \cdots & a_n \end{pmatrix} = \sum_{k=1}^{n} a_k = \text{tr}\ T\alpha_j T^{-1} = \text{tr}\ \alpha_j T T^{-1} = \text{tr}\ \alpha_j. \tag{1.19}$$

From (1.19) we can conclude that the trace of a matrix is the sum of its eigenvalues. But on the other hand, we know that the trace of the Dirac matrices is equal to zero and their eigenvalues are ±1. Thus the number of positive eigenvalues has to be the same as the number of negative eigenvalues.

According to the constraints (1.9), (1.10), and (1.11) the Dirac matrices should anticommute. Only three anticommuting 2×2 matrices exist [17]. They are the Pauli matrices $\sigma_m,\ m = 1,\ 2,\ 3$, given by

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

Therefore we can construct the Dirac matrices in terms of the Pauli matrices

$$\alpha_j = \begin{pmatrix} 0 & \sigma_m \\ \sigma_m & 0 \end{pmatrix} \quad \text{and} \quad \beta = \begin{pmatrix} \mathbb{1} & 0 \\ 0 & -\mathbb{1} \end{pmatrix}, \tag{1.20}$$

where $\mathbb{1}$ is the 2×2 unit matrix. The algebra of these matrices is a special case of a Clifford algebra [11, 12]. From (1.20) we can see that the Dirac matrices must be at least 4×4 dimensional. According to [18]–[21] we can state the following theorem:

Theorem 1.1. *Suppose that the size of the Dirac matrices is* $n \times n$. *If d+1 is even, then*

$$n = 2^{(d+1)/2}.$$

If d+1 is odd,

$$n = 2^{d/2}.$$

For example, if $d = 1$ or 2 then $n = 2$; if $d = 3$ or 4, $n = 4$.

1.3 Central potentials $V(r)$ and $S(r)$

The Dirac equation (1.7) in $d + 1$ dimensions for spherically symmetric vector and scalar potentials $V(r)$ and $S(r)$ respectively can be expressed in natural units $\hbar =$

$c = 1$ as [7, 22]

$$i\frac{\partial \Psi}{\partial t} = H\Psi, \qquad H = \sum_{j=1}^{d} \alpha_j p_j + \beta\left(m + S(r)\right) + \mathbb{1}V(r), \tag{1.21}$$

where m is the mass of the particle, $\mathbb{1}$ is the identity matrix, and the $(d+1)$ matrices $\{\alpha_j\}$ and β satisfy the anticommutation relations (1.9)–(1.11). Let us introduce the radial momentum and radial velocity operators respectively

$$p_r = r^{-1}\left(\sum_{j=1}^{d} x_j p_j - i\frac{d-1}{2}\right) \tag{1.22}$$

and

$$\alpha_r = r^{-1}\left(\sum_{j=1}^{d} \alpha_j x_j\right). \tag{1.23}$$

Let us now define a finite set of the orbital angular momentum operators L_{ij}, by the following algebraic relations [25]:

$$L_{ij} = x_i p_j - x_j p_i \overset{(1.8)}{=} -i\left(x_i\frac{\partial}{\partial x_j} - x_j\frac{\partial}{\partial x_i}\right), \tag{1.24}$$

$$L_{ij} = -L_{ji}, \tag{1.25}$$

$$L_{ij} = L_{ij}^{\dagger} \quad \text{(self-adjoint)}, \tag{1.26}$$

$$[L_{ij},\ L_{ik}] = iL_{jk}{}^{4}, \tag{1.27}$$

$$[L_{ij},\ L_{kl}] = 0, \quad \text{for} \quad i \neq j \neq k \neq l, \tag{1.28}$$

$$L_{ij}L_{kl} + L_{ki}L_{jl} + L_{jk}L_{il} = 0, \quad \text{for} \quad i \neq j \neq k \neq l, \tag{1.29}$$

where the indices $i,\ j,\ k,\ l$ can take the values $1,\ 2,\ \ldots,\ d$ (d is the dimension of

---

[4] The commutation relation $[a,\ b] = ab - ba$.

the space). Then the total orbital angular momentum has the form

$$L^2 = \sum_{i<j}^{d} L_{ij}^2. \tag{1.30}$$

We introduce now the generalized spin angular momentum σ_{ij}, and its basic properties [26]:

$$\sigma_{ij} = -\frac{i}{2}[\alpha_i,\ \alpha_j], \tag{1.31}$$

$$\sigma_{ij} = -\sigma_{ji}, \tag{1.32}$$

$$\sigma_{ij} = \sigma_{ij}^{\dagger}, \tag{1.33}$$

$$\sigma_{ij}^2 = 1 \quad \text{(the unit operator)}, \tag{1.34}$$

$$[\sigma_{ij},\ \sigma_{ik}] = i\sigma_{jk}, \quad \text{for} \quad i \neq j \neq k, \tag{1.35}$$

$$[\sigma_{ij},\ \sigma_{kl}] = 0, \quad \text{for} \quad i \neq j \neq k \neq l, \tag{1.36}$$

and again the indices $i,\ j,\ k,\ l$ can take the values $1,\ 2,\ \ldots,\ d$. It can be shown [27] that the total angular momentum and the operator $\hat{k}_d$ commute with the Hamiltonian H, where

$$\hat{k}_d = \beta\left(\sum_{i<j}^{d} \sigma_{ij} L_{ij} + \frac{d-1}{2}\right). \tag{1.37}$$

Using the information above and $\sum_{j=1}^{d}\left(x^j\right)^2 = r^2$ we can rewrite the Dirac Hamiltonian from (1.21) in terms of three operators: p_r, α_r, and $\hat{k}_d$, in the following way

$$H = \alpha_r p_r + \frac{i}{r}\alpha_r \beta \hat{k}_d + \beta(m + S(r)) + \mathbb{1}V(r). \tag{1.38}$$

If we find the eigenvalues of $\hat{k}_d$, then we can find the eigenvalues of H. For this purpose, we introduce the operator $\mathcal{L}$, such that

$$\mathcal{L} = \sum_{i<j}^{d} \sigma_{ij} L_{ij}, \tag{1.39}$$

and, according to (1.37), $\hat{k}_d$ becomes

$$\hat{k}_d = \beta \left(\mathcal{L} + \frac{d-1}{2} \right). \tag{1.40}$$

Since the potentials are spherically symmetric, the operators H, L^2, and $\mathcal{L}$ commute, i.e. $[H,\ \mathcal{L}] = 0$ and $[L^2,\ \mathcal{L}] = 0$. Thus, according to [17], these operators have common eigenfunctions, so we can find eigenvalues of $\mathcal{L}$ by establishing a relation between $\mathcal{L}$ and L^2. From (1.39) we have

$$\mathcal{L}^2 = \sum_{i<j}^{d} \sum_{k<l}^{d} \sigma_{ij} L_{ij} \sigma_{kl} L_{kl} = \mathcal{L}_1^2 + \mathcal{L}_2^2 + \mathcal{L}_3^2, \tag{1.41}$$

where $\mathcal{L}_1^2$ consists of terms with paired equal indices, i.e., $i = k$ and $j = l$; the second sum $\mathcal{L}_2^2$ includes terms with unequal indices, i.e., $i \neq j \neq k \neq l$; $\mathcal{L}_3^2$ – terms which can be contracted into $\sigma_{ij} L_{ij}$. So,

$$\mathcal{L}_1^2 = \sum_{i<j}^{d} \left(\sigma_{ij} L_{ij}\right)^2 \underset{(1.34)}{\overset{(1.30)}{=}} L^2. \tag{1.42}$$

Then the second partial sum has the form:

$$\mathcal{L}_2^2 = \sum_{i<j}^{d} \sum_{k<l}^{d} \sigma_{ij} L_{ij} \sigma_{kl} L_{kl}, \quad i \neq j \neq k \neq l, \tag{1.43}$$

and the third one is:

$$\mathcal{L}_3^2 = \sum_{i<j}^{d} \left(\sum_{k=1}^{d-1} \sigma_{ki} L_{ki} \sigma_{kj} L_{kj} + \sum_{k=j+1}^{d} \sigma_{ik} L_{ik} \sigma_{jk} L_{jk} \sum_{k=i+1}^{j-1} \sigma_{kj} L_{kj} \sigma_{ik} L_{ik} \right) \tag{1.44}$$

$$= -(d-2)L.$$

The terms in the sum (1.39) are symmetric, so all terms from (1.42) can be recovered by summing up only the following three terms (with the help of (1.27) and (1.34)):

$$\sigma_{ij}L_{ij}\sigma_{kl}L_{kl} + \sigma_{ik}L_{ik}\sigma_{jl}L_{jl} + \sigma_{jk}L_{jk}\sigma_{il}L_{il}$$

$$= \sigma_{ij}\sigma_{kl}(L_{ij}L_{kl} + L_{ik}L_{jl} + L_{jk}L_{il}) = 0, \quad i < j < k < l. \tag{1.45}$$

It can be shown that the numbers of terms involved in each partial sum are $N_1 = d(d-1)/2$ in $\mathcal{L}_1^2$, $N_2 = 6\sum_{i<j<k<l}^{d} 1 = d(d-1)(d-2)(d-3)/4$ in $\mathcal{L}_2^2$, and $N_3 = d(d-1)(d-2)$ in $\mathcal{L}_3^2$. Then the total number of terms is $N = N_1 + N_2 + N_3 = (d(d-1)/2)^2$. Using equations (1.42), (1.44), and (1.45) we find [5]

$$L^2 = \mathcal{L}(\mathcal{L} + d - 2). \tag{1.46}$$

Since the eigenfunctions of L^2 are doubly degenerate [23, 24], we may write

$$\mathcal{L}\psi_1 = l\psi_1, \tag{1.47}$$

$$\mathcal{L}\psi_2 = -(l + d - 2)\psi_2, \tag{1.48}$$

which lead to

$$L^2\psi_i = l(l + d - 2)\psi_i, \quad i = 1,\ 2. \tag{1.49}$$

Thus, the eigenvalues of $\hat{k}_d$ can be written as

$$k_d = \mp\left(j + \frac{d-2}{2}\right), \quad j = l \pm \frac{1}{2}. \tag{1.50}$$

---

[5] For an alternative way of getting this result see [25], Lemma 2.

Introducing $\tau = \pm 1$, we can rewrite k_d and j in the following way

$$k_d = \tau \left(j + \frac{d-2}{2} \right), \quad \text{with} \quad j = l - \frac{\tau}{2}. \tag{1.51}$$

By introducing the two–component wave function

$$\Psi = r^{-\frac{d-1}{2}} \begin{pmatrix} iG \\ -F \end{pmatrix}, \tag{1.52}$$

we obtain the radial Dirac equations in d dimensions (since time has been removed)

$$\frac{dG}{dr} = -\frac{k_d}{r} G + (E + m - V(r) + S(r))F, \tag{1.53}$$

$$\frac{dF}{dr} = \frac{k_d}{r} F - (E - m - V(r) - S(r))G. \tag{1.54}$$

Equations (1.53) and (1.54) can be reduced to three dimensions with $k_3 = \tau(j + 1/2)$ for $j = l - \tau/2$, which is in agreement with [14], and to two dimensions with $k_2 = \tau l - 1/2$.

1.4 Nonrelativistic limit

It is well known that, in nonrelativistic limit, the Dirac equation becomes the Schrödinger equation. In this section we derive the radial Schrödinger equation from the pair of the Dirac coupled equations.

Consider the relation between the Dirac and Schrödinger energies E and $\mathcal{E}$ respectively:

$$E = m + \mathcal{E}, \tag{1.55}$$

where m is the mass of the particle. Substitution of this relation and putting $S(r) = 0$

into the Dirac radial equations (1.53) and (1.54) gives us

$$\frac{dG}{dr} = (\mathcal{E} - V(r))F + 2mF - \frac{k_d}{r}G, \tag{1.56}$$

$$\frac{dF}{dr} = \frac{k_d}{r}F + (V(r) - \mathcal{E})G. \tag{1.57}$$

We assume that in nonrelativistic limit $|\mathcal{E}| \ll m$, therefore in equation (1.56) term $(\mathcal{E} - V(r))F$ is much less then the term $2mF$, so we can omit $(\mathcal{E} - V(r))F$ and (1.56) becomes

$$\frac{dG}{dr} = 2mF - \frac{k_d}{r}G. \tag{1.58}$$

Then we differentiate the last equation with respect to r:

$$\frac{d^2G}{dr^2} = 2m\frac{dF}{dr} + \frac{k_d}{r^2}G - \frac{k_d}{r}\frac{dG}{dr}.$$

Substituting (1.57) into the previous equation yields

$$\frac{d^2G}{dr^2} = 2m\frac{k_d}{r}F + 2m(V(r) - \mathcal{E})G + \frac{k_d}{r^2}G - \frac{k_d}{r}\frac{dG}{dr}. \tag{1.59}$$

Using (1.58), we can replace F in (1.59) and obtain

$$\frac{d^2G}{dr^2} = \frac{k_d^2 + k_d}{r^2}G + 2m(V(r) - \mathcal{E})G. \tag{1.60}$$

Replacing $G(r)$ by $R(r)$ in (1.60) gives us

$$\frac{1}{2m}\left[-\frac{d^2}{dr^2} + \frac{k_d(k_d+1)}{r^2}\right]R + V(r)R = \mathcal{E}R, \tag{1.61}$$

which is the radial Schödinger equation for a spherically symmetric potential $V(r)$ and a particle of mass m in d–dimensions. $R(r)$, like $G(r)$, satisfies $R(0) = 0$. We keep the function $G(r)$ instead of $F(r)$ because $m >> 1$ and from (1.58) $F = \frac{1}{2m}\frac{dG}{dr} + \frac{1}{2m}\frac{k_d}{r}G$.

Thus F approaches zero in the nonrelativistic limit. In quantum mechanics F is colled the small component and G is the big component of the wave function Ψ.

From the section above we have $k_d = \tau\left(j + \frac{d-2}{2}\right)$, where $j = l - \tau/2$ and $\tau = \pm 1$. According to [10] we can generalize the orbital–angular momentum quantum number l from the three–dimensional case to d-dimensions by introducing

$$l_d = l + \frac{d-3}{2}. \tag{1.62}$$

Thus the factor $k_d(k_d+1)$ in (1.61) for $\tau = \pm 1$ will take the form

$$k_d(k_d+1) = l_d(l_d+1). \tag{1.63}$$

Also we can derive (1.61) from $\left(-\frac{\triangle}{2m} + V(r)\right)\Psi = \mathcal{E}\Psi$ [6], by considering radial solutions of the form $\Psi(\boldsymbol{r}) = \psi(r)Y_l(\theta_0,\ \theta_1,\ \ldots,\ \theta_{d-1})$ and taking $\psi(r) = r^{-(d-1)/2}R(r)$ where $\psi(r)$ is spherically symmetric, Y_l is the generalized spherical harmonic [28], and $R(r)$ is the radial wavefunction. This deviation, for instance, can be found in [29] and [30].

1.5 Some spectral generalities

Let us consider equation (1.61) in three dimensions, thus, according to (1.62) and (1.63) it becomes

$$\frac{1}{2m}\left[-\frac{d^2}{dr^2} + \frac{l(l+1)}{r^2}\right]R + V(r)R = \mathcal{E}R, \tag{1.64}$$

which is the radial Schrödinger equation for a particle of mass m and a spherically symmetric potential $V(r)$ in three dimensions [17, 31] with $\hbar = c = 1$. With the

---

[6] $\triangle = \bigtriangledown^2$ is the Laplace operator or Laplacian.

sech–squared potential $V(r) = -v\,\mathrm{sech}^2\, r$ (A.8), and $l = 0$, equation (1.64) takes the form

$$-\frac{d^2}{dr^2}R - 2mv\,\mathrm{sech}^2(r)R = 2m\mathcal{E}R, \tag{1.65}$$

and the eigenvalues are given by, see (A.9),

$$\mathcal{E} = -\frac{1}{2m}\left[\left(2mv + \frac{1}{4}\right)^{1/2} - \left(n + \frac{1}{2}\right)\right]^2, \tag{1.66}$$

where $n = 1,\ 2,\ 3,\ \ldots$ labels the sequence of discrete eigenvalues. Therefore, according to (1.55), the Dirac energy E for the sech–squared potential is asymptotically

$$E = m - \frac{1}{2m}\left[\left(2mv + \frac{1}{4}\right)^{1/2} - \left(n + \frac{1}{2}\right)\right]^2. \tag{1.67}$$

In the nonrelativistic limit E approaches m, or, equivalently, $\mathcal{E}$ approaches zero. Therefore from the last two relations we conclude that these conditions will be satisfied if

$$v > v_L = \frac{n(n+1)}{2m}, \tag{1.68}$$

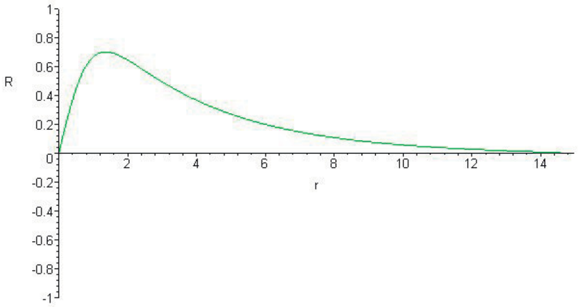
where v_L is the lower bound for the coupling v. In other words, this condition means that if $v \le v_L$, the discrete energy eigenvalue E does not exist and the pair of Dirac coupled equations cannot be solved.

We can verify the condition (1.68) using numerical methods for finding solutions of the Schrödinger and Dirac equations. We shall discuss these in Chapter 6. They allow us to find, for an arbitrary potential $V(r)$ and dimension d, the energy values, and also to plot the graph of the radial wave function.

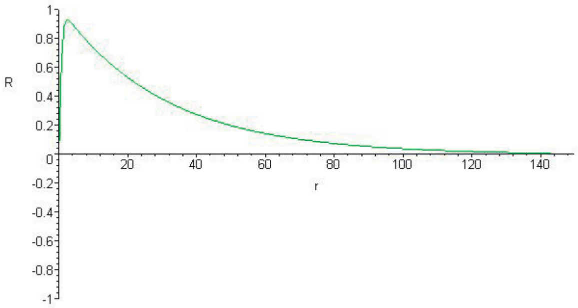
We start from the ground state $n = 1$ and take $m = 1/2$, thus condition (1.68) becomes $v > v_L = 2$. Then using numerical methods we solve equation (1.65) for different values of the coupling parameter.

As we can see from the Fig. 1.1, when the coupling satisfies condition (1.68), we get the energy values $\mathcal{E}_{NM}$ with the help of numerical methods, which are in agreement with the exact values of $\mathcal{E}$ from (1.66). We also obtain the graphs of the radial wave function $R(r)$ (Fig. 1.1 ***(a)*** and ***(b)***). On the other hand, when $v \leq v_L$ we can see from the Fig. 1.1 ***(c)*** and ***(d)*** that the graphs of $R(r)$ are "wrong"; thus the eigenvalues can not be calculated if v is too small.

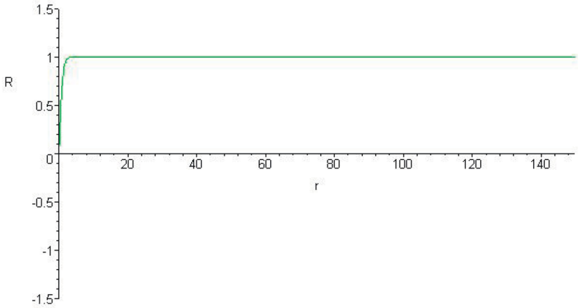
Hence, for short–range potentials, such as the sech–squared potential, there are no eigenvalues unless the coupling v is sufficiently large, $v > v_L$. As the coupling is increased beyond the critical value v_L, the eigenvalue E is reduced. Another boundary is reached when E approaches $-m$. In general, the eigenvalues lie in the interval $(-m,\ m)$, [14].



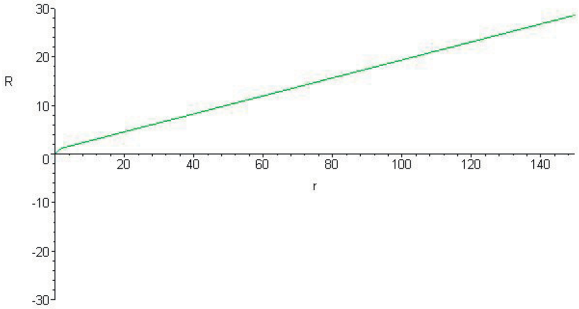
(a) $v = 3$, $\mathcal{E} = -0.09167$, and $\mathcal{E}_{NM} = -0.09167$.



(b) $v = 2.1$, $\mathcal{E} = -0.00109$, and $\mathcal{E}_{NM} = -0.00109$.



(c) $v = 2$, $\mathcal{E} = 0.00000$, and
$\mathcal{E}_{NM} = 0.00000$.



(d) $v = 1.5$, $\mathcal{E} = -0.03137$, and
$\mathcal{E}_{NM} = 0.00000$.

Figure 1.1: Graphs of the Schrödinger radial wave function $R(r)$ for the ground state and different v.

Chapter 2

The exact solution of the Coulomb problem

2.1 The asymptotic iteration method

In this section we consider the asymptotic iteration method (AIM) which was developed in [8] and [9]. Let us start from the first–order linear coupled differential equations:

$$\phi_1' = \lambda_0(x)\phi_1 + s_0(x)\phi_2, \tag{2.1}$$

$$\phi_2' = \omega_0(x)\phi_1 + p_0(x)\phi_2, \tag{2.2}$$

where $'$ denotes the operator d/dx, and $\lambda_0(x)$, $s_0(x)$, $\omega_0(x)$, and $p_0(x)$ are sufficiently differentiable in appropriate domains. If we take the derivative with respect to x from the equations (2.1) and (2.2) we obtain

$$\phi_1'' = \lambda_0'\phi_1 + \lambda_0\phi_1' + s_0'\phi_2 + s_0\phi_2',$$

$$\phi_2'' = \omega_0'\phi_1 + \omega_0\phi_1' + p_0'\phi_2 + p_0\phi_2',$$

and with (2.1) and (2.2) these equations become

$$\phi_1'' = \lambda_1(x)\phi_1 + s_1(x)\phi_2, \tag{2.3}$$

$$\phi_2'' = \omega_1(x)\phi_1 + p_1(x)\phi_2, \tag{2.4}$$

where

$$\lambda_1(x) = \lambda_0' + \lambda_0^2 + s_0\omega_0,$$

$$s_1(x) = s_0' + \lambda_0 s_0 + s_0 p_0,$$

$$\omega_1(x) = \omega_0' + \lambda_0\omega_0 + p_0\omega_0,$$

$$p_1(x) = p_0' + p_0^2 + s_0\omega_0.$$

If we continue to differentiate equations (2.3) and (2.4), after n steps, we will have

$$\phi_1^{(n+2)} = \lambda_{n+1}(x)\phi_1 + s_{n+1}(x)\phi_2, \tag{2.5}$$

$$\phi_2^{(n+2)} = \omega_{n+1}(x)\phi_1 + p_{n+1}(x)\phi_2, \tag{2.6}$$

with

$$\lambda_{n+1}(x) = \lambda_n' + \lambda_n\lambda_0 + s_n\omega_0, \tag{2.7}$$

$$s_{n+1}(x) = s_n' + \lambda_n s_0 + s_n p_0,$$

$$\omega_{n+1}(x) = \omega_n' + \omega_n\lambda_0 + p_n\omega_0,$$

$$p_{n+1}(x) = p_n' + p_n p_0 + \omega_n s_0.$$

Using (2.5), we can consider the ratio:

$$\frac{\phi_1^{(n+2)}}{\phi_1^{(n+1)}} = \frac{\lambda_{n+1}(\phi_1 + (s_{n+1}/\lambda_{n+1})\phi_2)}{\lambda_n(\phi_1 + (s_n/\lambda_n)\phi_2)}. \tag{2.8}$$

Meanwhile,

$$\frac{\phi_1^{(n+2)}}{\phi_1^{(n+1)}} = \frac{d}{dx}\left(\ln(\phi_1^{(n+1)}\right). \tag{2.9}$$

We now introduce the "asymptotic" aspect of the method. For sufficiently large $n = 1,\ 2,\ 3,\ \ldots$ we have

$$\frac{s_{n+1}}{\lambda_{n+1}} = \frac{s_n}{\lambda_n} := \alpha. \tag{2.10}$$

Joining equations (2.8), (2.9), and (2.10) we have

$$\frac{d}{dx}\ln\left(\phi_1^{(n+1)}\right) = \frac{\lambda_{n+1}}{\lambda_n},$$

then, with (2.7) and (2.10), the previous fraction becomes

$$\frac{\lambda_{n+1}}{\lambda_n} = \frac{d}{dx}(\ln(\lambda_n)) + \lambda_0 + \alpha\omega_0.$$

The last two equations give us

$$\ln\left(\phi_1^{(n+1)}\right) = \int^x \left(\frac{d}{dt}(\ln(\lambda_n(t))) + \lambda_0(t) + \alpha(t)\omega_0(t)\right) dt,$$

or

$$\phi_1^{(n+1)}(x) = C_1\lambda_n \exp\left(\int^x \lambda_0(t) + \alpha(t)\omega_0(t)\right) dt, \tag{2.11}$$

where C_1 is the constant of integration. From (2.5) we can write

$$\phi_1^{(n+1)} = \lambda_n(x)\phi_1 + s_n(x)\phi_2. \tag{2.12}$$

Substituting of (2.11) into (2.12), and using (2.10), we obtain

$$\lambda_n(x)\phi_1 + s_n(x)\phi_2 = C_1\lambda_n \exp\left(\int^x \lambda_0(t) + \alpha(t)\omega_0(t)\right) dt,$$

or

$$\phi_1(x) = C_1 \exp\left(\int^x \lambda_0(t) + \alpha(t)\omega_0(t)\right) dt - \alpha(x)\phi_2(x). \tag{2.13}$$

Also we can rewrite equation (2.2) in the following form

$$\phi_1(x) = (\phi_2'(x) - p_0(x)\phi_2(x))/\omega_0(x).$$

Combining the two last equations, we obtain

$$C_1\omega_0(x) \exp\left(\int^x [\lambda_0(t) + \alpha(t)\omega_0(t)]\right) dt - \alpha(x)\phi_2(x)\omega_0(x) = (\phi_2'(x) - p_0(x)\phi_2(x)),$$

or

$$\phi_2' + \xi(x)\phi_2 = \eta(x), \tag{2.14}$$

with

$$\xi(x) = \alpha(x)\omega_0(x) - p_0(x),$$

and

$$\eta(x) = C_1\omega_0(x) \exp\left(\int^x [\lambda_0(t) + \alpha(t)\omega_0(t)]\right) dt.$$

Equation (2.14) is a first–order linear differential equation and its solution is given by [33]

$$\phi_2 = \exp^{-1}\left[\int^x \xi(t)dt\right]\left[\int^x \eta(t)\exp\left[\int^x \xi(t)dt\right] dt + C_2\right]. \tag{2.15}$$

Substitution of the expressions for ξ and η into (2.15) yields the general solution of

$\phi_2(x)$:

$$\phi_2(x) = \exp\left(\int^x (p_0 - \alpha\omega_0)dt\right)\left[C_1\int^x \omega_0 \exp\left(\int^t (\lambda_0 - p_0 + 2\omega_0\alpha)d\tau\right)dt + C_2\right]. \tag{2.16}$$

We can use this solution and (2.13) to find $\phi_1(x)$:

$$\phi_1(x) = C_1 \exp\left(\int^x \lambda_0(t) + \alpha(t)\omega_0(t)\right)dt -$$

$$\alpha(x)\exp\left(\int^x (p_0 - \alpha\omega_0)dt\right)\left[C_1\int^x \omega_0 \exp\left(\int^t (\lambda_0 - p_0 + 2\omega_0\alpha)d\tau\right)dt + C_2\right]. \tag{2.17}$$

2.2 Solution of the Dirac Coulomb problem

Suppose we have a particle which is moving in a pure vector Coulomb field i.e. $S(r) = 0$ and

$$V(r) = -\frac{v}{r}, \tag{2.18}$$

where $v = \alpha Z$ is the coupling parameter, $\alpha = e^2/c\hbar \approx 1/137.037$ is the fine–structure constant, and Z is the atomic number. Thus equations (1.53) and (1.54) take the form

$$\frac{dG}{dr} = \left(E + m + \frac{v}{r}\right)F - \frac{k_d}{r}G, \tag{2.19}$$

$$\frac{dF}{dr} = \frac{k_d}{r}F - \left(E - m + \frac{v}{r}\right)G, \tag{2.20}$$

where $k_d = \tau\left(j + \frac{d-2}{2}\right)$ and $j = l - \tau/2$. Consider the behaviour of the functions $G(r)$ and $F(r)$ for small and large r. Near the origin ($r \longrightarrow 0$) the terms with r in the denominator become extremely large in comparison with the terms $E \pm m$, thus we can omit the small terms and equations (1.53) and (1.54) become

$$\frac{dG}{dr} = \frac{v}{r}F - \frac{k_d}{r}G, \tag{2.21}$$

$$\frac{dF}{dr} = \frac{k_d}{r}F - \frac{v}{r}G. \tag{2.22}$$

After taking the derivative with respect to r from the system above we get

$$\frac{d^2G}{dr^2} = \frac{v}{r}\frac{dF}{dr} - F\frac{v}{r^2} + G\frac{k_d}{r^2} - \frac{k_d}{r}\frac{dG}{dr},$$

$$\frac{d^2F}{dr^2} = \frac{k_d}{r}\frac{dF}{dr} - F\frac{k_d}{r^2} + G\frac{v}{r^2} - \frac{v}{r}\frac{dG}{dr}.$$

Then we substitute into the system above equations (2.21) – (2.22) and obtain

$$\frac{d^2G}{dr^2} = G\frac{k_d^2}{r^2} - G\frac{v^2}{r^2} - F\frac{v}{r^2} + G\frac{k_d}{r^2}, \tag{2.23}$$

$$\frac{d^2F}{dr^2} = F\frac{k_d^2}{r^2} - F\frac{v^2}{r^2} - F\frac{k_d}{r^2} + G\frac{v}{r^2}. \tag{2.24}$$

Using (2.21) and (2.22), we can replace the two last terms in (2.23) and (2.24) in the following way:

$$-F\frac{v}{r^2} + G\frac{k_d}{r^2} = \frac{1}{r}\frac{dG}{dr},$$

$$-F\frac{k_d}{r^2} + G\frac{v}{r^2} = \frac{1}{r}\frac{dF}{dr}.$$

Finally, for small r equations (2.19) and (2.20) have the form

$$\frac{d^2G}{dr^2} = G\frac{k_d^2 - v^2}{r^2} - \frac{1}{r}\frac{dG}{dr}, \tag{2.25}$$

$$\frac{d^2F}{dr^2} = F\frac{k_d^2 - v^2}{r^2} - \frac{1}{r}\frac{dF}{dr}. \tag{2.26}$$

These are the Cauchy–Euler equations with solution in the form [34]

$$H(r) = r^{\gamma}, \tag{2.27}$$

where $H(r)$ can be $G(r)$ or $F(r)$ as well, and

$$\gamma = \sqrt{k_d^2 - v^2}, \tag{2.28}$$

and $v^2 < k_d^2$ for the ground state, that is for $j = 1/2$; thus $v < 1$.

Now let us consider the case when r is large. When the terms with r in the denominator approach to zero and the system (2.19) – (2.20) becomes

$$\frac{dG}{dr} = (E + m)\,F, \tag{2.29}$$

$$\frac{dF}{dr} = (m - E)\,G, \tag{2.30}$$

and, after differentiation with respect to r,

$$\frac{d^2G}{dr^2} = (E + m)\,\frac{dF}{dr},$$

$$\frac{d^2F}{dr^2} = (m - E)\,\frac{dG}{dr}.$$

Using (2.29) and (2.30) in the last two equations we get the system of the Dirac coupled equations for $r \longrightarrow \infty$:

$$\frac{d^2G}{dr^2} = \left(m^2 - E^2\right) G,$$

$$\frac{d^2F}{dr^2} = \left(m^2 - E^2\right) F,$$

with the solution

$$T(r) = Ce^{-r\sqrt{m^2-E^2}}, \tag{2.31}$$

where $T(r)$ is either $G(r)$ or $F(r)$ and C is the constant of integration. Keeping in mind (2.27) and (2.31) we can introduce the radial functions $G(r)$ and $F(r)$ in the following form:

$$G(r) = \sqrt{m+E}\; r^\gamma e^{-r\sqrt{m^2-E^2}}(\phi_1 + \phi_2), \tag{2.32}$$

$$F(r) = \sqrt{m-E}\; r^\gamma e^{-r\sqrt{m^2-E^2}}(\phi_1 - \phi_2). \tag{2.33}$$

Now we make the substitution

$$r = r_1\rho \qquad \text{and} \qquad \frac{d}{dr} = \frac{1}{r_1}\frac{d}{d\rho} \tag{2.34}$$

with $r_1 = 1/\left(2\sqrt{m^2-E^2}\right)$ in (2.19) – (2.20) and (2.32) – (2.33), so

$$\frac{dG}{d\rho} = \left[r_1(m+E) + \frac{v}{\rho}\right] F(\rho) - \frac{k_d}{\rho}G(\rho), \tag{2.35}$$

$$\frac{dF}{d\rho} = \frac{k_d}{\rho}F(\rho) - \left[r_1(m-E) + \frac{v}{r}\right] G(\rho), \tag{2.36}$$

and

$$G(\rho) = \sqrt{m+E}\; r_1^\gamma \rho^\gamma e^{-\rho/2}(\phi_1(\rho) + \phi_2(\rho)), \tag{2.37}$$

$$F(\rho) = \sqrt{m-E}\ r_1^{\gamma}\rho^{\gamma}e^{-\rho/2}(\phi_1(\rho) - \phi_2(\rho)). \tag{2.38}$$

Substitution of (2.37) and (2.38) into (2.35) and (2.36) yields

$$\left(\frac{\gamma}{\rho} - \frac{1}{2}\right)(\phi_1 + \phi_2) + \frac{d\phi_1}{d\rho} + \frac{d\phi_2}{d\rho} =$$

$$-\frac{k_d}{\rho}(\phi_1 + \phi_2) + \left(r_1(m+E) + \frac{v}{\rho}\right)\sqrt{\frac{m-E}{m+E}}(\phi_1 - \phi_2),$$

$$\left(\frac{\gamma}{\rho} - \frac{1}{2}\right)(\phi_1 - \phi_2) + \frac{d\phi_1}{d\rho} - \frac{d\phi_2}{d\rho} =$$

$$\frac{k_d}{\rho}(\phi_1 - \phi_2) + \left(r_1(m-E) - \frac{v}{\rho}\right)\sqrt{\frac{m+E}{m-E}}(\phi_1 + \phi_2). \tag{2.39}$$

Adding the last two equations, and using $\sqrt{\frac{m-E}{m+E}} \overset{(2.34)}{=} 2r_1(m-E)$ and $\sqrt{\frac{m+E}{m-E}} \overset{(2.34)}{=} 2r_1(m+E)$, we obtain

$$\frac{2\gamma}{\rho}\phi_1 - \phi_1 + 2\frac{d\phi_1}{d\rho} = -2\frac{k_d}{\rho}\phi_2 +$$

$$\left[2r_1^2(m^2-E^2) + 2r_1(m-E)\frac{v}{\rho}\right](\phi_1 - \phi_2) + \left[2r_1^2(m^2-E^2) - 2r_1(m+E)\frac{v}{\rho}\right](\phi_1 + \phi_2).$$

According to (2.34) $2r_1^2(m^2-E^2) = 1/2$, thus

$$\frac{\gamma}{\rho}\phi_1 - \phi_1 + \frac{d\phi_1}{d\rho} = -\frac{k_d}{\rho}\phi_2 - \frac{2vr_1E}{\rho}\phi_1 - \frac{2vr_1m}{\rho}\phi_2.$$

Taking

$$a = 2vr_1E \quad \text{and} \quad b = 2vr_1m, \tag{2.40}$$

we finally obtain

$$\frac{d\phi_1}{d\rho} = \left(1 - \frac{a+\gamma}{\rho}\right)\phi_1 - \frac{b+k_d}{\rho}\phi_2. \tag{2.41}$$

Subtracting equations (2.39), and following the same reasoning, we get

$$\frac{d\phi_2}{d\rho} = \frac{b - k_d}{\rho}\phi_1 + \frac{a - \gamma}{\rho}\phi_2. \tag{2.42}$$

Following [9], we will use AIM to solve equations (2.41) and (2.42). Comparing equations (2.41) with (2.1), and (2.42) with (2.2), we find that

$$\lambda_0(\rho) = 1 - \frac{a + \gamma}{\rho}, \quad s_0(\rho) = -\frac{b + k_d}{\rho}, \quad \omega_0(\rho) = \frac{b - k_d}{\rho}, \quad p_0(\rho) = \frac{a - \gamma}{\rho}. \tag{2.43}$$

Then using the iteration formulas (2.7) and condition (2.10) we obtain

$$\text{if} \quad n = 0, \quad \text{then} \quad a = \gamma \quad \text{and} \quad b = -k_d,$$

$$\text{if} \quad n = 1, \quad \text{then} \quad a = 1 + \gamma \quad \text{and} \quad b = -k_d, \quad \pm\sqrt{1 + 2\gamma + k_d^2},$$

$$\text{if} \quad n = 2, \quad \text{then} \quad a = 2 + \gamma \quad \text{and} \quad b = -k_d, \quad \pm\sqrt{3 + 2\gamma + k_d^2}, \quad \pm\sqrt{4 + 4\gamma + k_d^2},$$

$$\text{if} \quad n = 3, \quad \text{then} \quad a = 3 + \gamma \quad \text{and}$$

$$b = -k_d, \quad \pm\sqrt{5 + 2\gamma + k_d^2}, \quad \pm\sqrt{8 + 4\gamma + k_d^2}, \quad \pm\sqrt{9 + 6\gamma + k_d^2}.$$

Finally, for arbitrary n, we have

$$a = n + \gamma \quad \text{and} \quad b = \pm\sqrt{s(2n - s) + 2s\gamma + k_d^2}, \tag{2.44}$$

where $s = 0,\ 1,\ 2, \ldots,\ n$. From (2.40) and (2.44) it follows that

$$n + \gamma = \frac{Ev}{\sqrt{m^2 - E^2}} \implies E = \pm\frac{m}{\sqrt{1 + \left(\dfrac{v}{n + \gamma}\right)^2}} \tag{2.45}$$

and

$$\pm\sqrt{s(2n-s)+2s\gamma+k_d^2}=\frac{mv}{\sqrt{m^2-E^2}} \implies E=\pm m\sqrt{1-\frac{v^2}{s(2n-s)+2s\gamma+k_d^2}}.$$

These two expressions for the energy must be equal, thus s must be either n or $n+2\gamma$. From (2.28) we see that γ is not an integer, but s and n should be integers, therefore we have only one possibility $s=n$. According to (2.44), b becomes $b=\pm\sqrt{n^2+2n\gamma+k_d^2}$ and, for $n=0$, b has to be equal to $-k_d$. Using (2.28), and introducing the "principal quantum number" defined as $n_r=n+|k_d|-\frac{d-3}{2}=1,\ 2,\ 3,\ \ldots$ in (2.45), we get the well–known formula for the Coulomb energy in d dimensions

$$E=m\left[1+\left(\frac{v}{n_r-|k_d|+(d-3)/2+\sqrt{k_d^2-v^2}}\right)^2\right]^{-1/2}. \tag{2.46}$$

According to [14], we exclude the negative sign in (2.46) because for positive coupling constant ($\alpha Z>0$), negative energies E do not fulfill the left hand side of the quantity (2.45) since $n+\gamma$ is positive.

Chapter 3

Scaling laws

3.1 Scaling for the Schrödinger equation

In three dimensions the Hamiltonian operator H from the Schrödinger equation (1.61) with $m = 1$, $l = 0$, can be written as

$$H = -\frac{1}{2}\frac{d^2}{dr^2} + V(r), \tag{3.1}$$

where $V(r) = vf(r)$ is the potential with $v > 0$, the coupling parameter, and $f(r)$ the shape of the potential. Suppose that H has the eigenvalues $E(v,\ 1)$ and we mark it in the following way

$$-\frac{1}{2}\frac{d^2}{dr^2} + vf(r) \longrightarrow E(v,\ 1) = F(v), \tag{3.2}$$

from which it immediately follows

$$-\frac{1}{2}\frac{d^2}{dr^2} + f(r) \longrightarrow F(1). \tag{3.3}$$

Assume that (3.2) is solved, i.e. we know the exact value of $F(v)$ for the potential $V(r) = vf(r)$, and we want to find the eigenvalues $E(v,\ a)$ for the potential $vf(r/a)$, where a is a positive real number, thus we can rewrite (3.2) in the following way

$$-\frac{1}{2}\frac{d^2}{dr^2} + vf\left(\frac{r}{a}\right) \longrightarrow E(v,\ a). \tag{3.4}$$

With the substitution $r = ax$, the operator d^2/dr^2 becomes

$$\frac{d^2}{dr^2} = \frac{d^2}{d(ax)^2} = \frac{1}{a^2}\frac{d^2}{dx^2},$$

and (3.4) takes the form

$$-\frac{1}{2}\frac{d^2}{dx^2} + a^2 vf(x) \longrightarrow a^2 E(v,\ a).$$

In accordance with (3.2) we also can write

$$-\frac{1}{2}\frac{d^2}{dx^2} + a^2 vf(x) \longrightarrow E(a^2 v,\ 1) = F(a^2 v).$$

Comparison of the last two expressions yields our first scaling law

$$E(v,\ a) = \frac{1}{a^2}E(a^2 v,\ 1) = \frac{1}{a^2}F(a^2 v). \tag{3.5}$$

As an example of (3.5), we consider (3.2) with the Hulthén potential (A.6) in the form

$$-\frac{1}{2}\frac{d^2}{dr^2} + v\left(\frac{-1}{e^r - 1}\right) \longrightarrow F(v) = -\frac{\left(2v - n^2\right)^2}{2}.$$

Using (3.5), we can easily find the eigenvalues $E(v,\ a)$ for the potential with the shape $f(r/a) = -1/(e^{r/a} - 1)$

$$E(v,\ a) = -\frac{\left(a^2 2v - n^2\right)^2}{2a^2}.$$

3.1.1 Scaling for the class of the power potentials $V(r) = v\,\mathrm{sgn}(q)r^q$

The Hamiltonian for the radial Schrödinger equation (1.61) in three dimensions, with $m = 1$, has the form

$$H = -\frac{1}{2}\frac{d^2}{dr^2} + \frac{l(l+1)}{2r^2} + V(r). \tag{3.6}$$

If we consider the family of power potentials $V(r) = v\,\mathrm{sgn}(q)r^q$, where $q > -2$ is the power parameter, and make the substitution $r = ax$ in (3.6). Similarly, from (3.2) we have

$$-\frac{1}{2}\frac{d^2}{dx^2} + \frac{l(l+1)}{2x^2} + va^{2+q}\,\mathrm{sgn}(q)x^q \longrightarrow a^2F(v). \tag{3.7}$$

We set $va^{2+q} = 1$, then $a = v^{-\frac{1}{2+q}}$, so the last expression becomes

$$-\frac{1}{2}\frac{d^2}{dx^2} + \frac{l(l+1)}{2x^2} + \mathrm{sgn}(q)x^q \longrightarrow v^{-\frac{2}{2+q}}F(v).$$

But, on the other side, using (3.3), we can write

$$-\frac{1}{2}\frac{d^2}{dx^2} + \frac{l(l+1)}{2x^2} + \mathrm{sgn}(q)x^q \longrightarrow F(1).$$

Comparing the last two expressions, we obtain the scaling law for the class of power potentials $V(r) = v\,\mathrm{sgn}(q)r^q$

$$F(v) = v^{\frac{2}{2+q}}F(1). \tag{3.8}$$

Now let us check the law (3.8). For this, we consider the Coulomb potential $V(r) = -v/r$, so $q = -1$ and the eigenvalues are given by (A.3)

$$F(v) = -\frac{2v^2}{(n+l)^2}.$$

It follows that

$$v^{\frac{2}{2+q}}F(1) = -v^2\frac{2}{(n+l)^2},$$

which confirms the law (3.8). We consider also the harmonic oscillator $V(r) = vr^2$ (A.4), so $q = 2$, and the energy values can be found using formula (A.5)

$$F(v) = (4n+2l-1)\sqrt{\frac{v}{2}} \quad \Longrightarrow \quad F(1) = (4n+2l-1)\sqrt{\frac{1}{2}},$$

thus

$$v^{\frac{2}{2+q}}F(1) = v^{1/2}(4n+2l-1)\sqrt{\frac{1}{2}},$$

which again confirms (3.8).

3.1.2 Scaling for a class of soft–core Coulomb potentials

Using the same notation as in the section above we derive the scaling law for the soft–core Coulomb potential (A.11)

$$V(r) = -\frac{v}{(r^q+\beta^q)^{1/q}}, \tag{3.9}$$

where $v > 0$ is the coupling parameter, $\beta > 0$ is the cutoff parameter, and $q \geq 1$ is the power parameter. It is clear that the soft–core Coulomb energy value depends on its parameters, i.e. $E = E(v,\ \beta,\ q)$. Using the Hamiltonian from the radial Schrödinger equation (1.61), with $m = 1$, we write

$$-\frac{1}{2}\frac{d^2}{dr^2} + \frac{l_d(l_d+1)}{2r^2} - \frac{v}{(r^q+\beta^q)^{1/q}} \longrightarrow E(v,\ \beta,\ q). \tag{3.10}$$

Substituting $r = ax$ into the last expression yields

$$-\frac{1}{2a^2}\frac{d^2}{dx^2} + \frac{l_d(l_d+1)}{2a^2x^2} - \frac{v}{(a^qx^q+\beta^q)^{1/q}} \longrightarrow E(v,\ \beta,\ q).$$

Factoring out β^q from the denominator, followed by multiplication by a^2 on both sides, yields

$$-\frac{1}{2}\frac{d^2}{dx^2}+\frac{l_d(l_d+1)}{2x^2}-\frac{av}{\left(x^q+\left(\frac{\beta}{a}\right)^q\right)^{1/q}}\longrightarrow a^2E(v,\ \beta,\ q).$$

In accordance with (3.10) we can also write

$$-\frac{1}{2}\frac{d^2}{dx^2}+\frac{l_d(l_d+1)}{2x^2}-\frac{av}{\left(x^q+\left(\frac{\beta}{a}\right)^q\right)^{1/q}}\longrightarrow E\left(av,\ \frac{\beta}{q},\ q\right).$$

Comparing the last two expressions, we arrive at the general scaling law for the class of soft–core Coulomb potentials

$$E(v,\ \beta,\ q)=\frac{1}{a^2}E\left(av,\ \frac{\beta}{q},\ q\right). \tag{3.11}$$

If we choose $a=1/v$ in (3.11), we obtain the special scaling law

$$E(v,\ \beta,\ q)=v^2E(1,\ v\beta,\ q), \tag{3.12}$$

and, with $a=\beta$, we get the second special scaling law

$$E(v,\ \beta,\ q)=\frac{1}{\beta^2}E(v\beta,\ 1,\ q). \tag{3.13}$$

3.2 Scaling for the Dirac equation

Let us rewrite the Dirac coupled equations (1.53)–(1.54) with $S(r)=0$ in the matrix form

$$H\Psi=E\Psi, \tag{3.14}$$

where

$$H = \begin{pmatrix} V(r) - m & \dfrac{d}{dr} + \dfrac{k_d}{r} \\ \dfrac{d}{dr} - \dfrac{k_d}{r} & V(r) + m \end{pmatrix} \quad \text{and} \quad \Psi = \begin{pmatrix} F(r) \\ G(r) \end{pmatrix}. \tag{3.15}$$

Consider the potential $V(r) = vf(r/a)$, where $v > 0$ and a is a positive real number, thus the eigenvalue E of H depens on three parameters: v, a, and m. In accordance with (3.1) and (3.2) we can write

$$\begin{pmatrix} vf(r/a) - m & \dfrac{d}{dr} + \dfrac{k_d}{r} \\ \dfrac{d}{dr} - \dfrac{k_d}{r} & vf(r/a) + m \end{pmatrix} \longrightarrow E(v,\ a,\ m). \tag{3.16}$$

Then we put $r = \delta x$, where δ is a positive real number, so

$$\frac{d}{dr} = \frac{1}{\delta}\frac{d}{dx},$$

therefore we can rewrite (3.16) as

$$\begin{pmatrix} \delta vf(\delta x/a) - \delta m & \dfrac{d}{dx} + \dfrac{k_d}{x} \\ \dfrac{d}{dx} - \dfrac{k_d}{x} & \delta vf(\delta x/a) + \delta m \end{pmatrix} \longrightarrow \delta E(v,\ a,\ m).$$

Using (3.16), we also can write

$$\begin{pmatrix} \delta vf(\delta x/a) - \delta m & \dfrac{d}{dx} + \dfrac{k_d}{x} \\ \dfrac{d}{dx} - \dfrac{k_d}{x} & \delta vf(\delta x/a) + \delta m \end{pmatrix} \longrightarrow E(\delta v,\ a/\delta,\ \delta m).$$

From the last two expressions, the first scaling law for the Dirac eigenvalues follows immedialtely

$$E(v,\ a,\ m) = \frac{1}{\delta} E\left(\delta v,\ \frac{a}{\delta},\ \delta m\right). \tag{3.17}$$

Now we consider the power potential $V(r) = vf(r) = v\,\mathrm{sgn}(q)r^q$ and rewrite (3.16) in simpler form

$$vf(r/a) = v\,\mathrm{sgn}(q)\left(\frac{r}{a}\right)^q \longrightarrow E(v,\ a,\ m), \tag{3.18}$$

or

$$vf(r/a) = \frac{v}{a^q}\,\mathrm{sgn}(q)r^q = \frac{v}{a^q} f(r) \longrightarrow E\left(\frac{v}{a^q},\ 1,\ m\right). \tag{3.19}$$

Since the left hand sides of (3.18) and (3.19) are equal, we can write the second scaling law

$$E(v,\ a,\ m) = E\left(\frac{v}{a^q},\ 1,\ m\right). \tag{3.20}$$

From (3.17) and (3.20), the general scaling law for the Dirac equation follows

$$E(v,\ a,\ m) = \frac{1}{\delta} E\left(\frac{v\delta^{q+1}}{a^q},\ 1,\ \delta m\right). \tag{3.21}$$

If we choose $\delta m = 1$, we obtain the special case of the law (3.21)

$$E(v,\ a,\ m) = mE\left(\frac{v}{a^q m^{q+1}},\ 1,\ 1\right). \tag{3.22}$$

Then, for the Hydrogen atom $q = -1$, the previous law becomes

$$E(v,\ a,\ m) = mE\left(va,\ 1,\ 1\right), \tag{3.23}$$

and, for the linear potential $q = 1$, we get the scaling law in the form

$$E(v,\ a,\ m) = mE\left(\frac{v}{am^2},\ 1,\ 1\right). \tag{3.24}$$

Now let us check the law (3.23) for the Coulomb potential. We know that in this case the energy eigenvalues are given by (2.46)

$$E(v,\ a,\ m) = m\left[1+\left(\frac{va}{n_r-|k_d|+(d-3)/2+\sqrt{k_d^2-(va)^2}}\right)^2\right]^{-1/2}.$$

The right hand side of (3.23) gives us

$$mE\left(va,\ 1,\ 1\right) = m\left[1+\left(\frac{va}{n_r-|k_d|+(d-3)/2+\sqrt{k_d^2-(va)^2}}\right)^2\right]^{-1/2},$$

which confirms the law (3.23).

Chapter 4

Comparison Theorem

4.1 Relativistic comparison Theorem for the Dirac equation

Let us rewrite equations (1.53) and (1.54) with $S(r) = 0$ in the following way

$$EG(r) = (V(r) + m)G(r) + \left(\frac{k_d}{r} - \frac{d}{dr}\right) F(r), \tag{4.1}$$

$$EF(r) = (V(r) - m)F(r) + \left(\frac{k_d}{r} + \frac{d}{dr}\right) G(r), \tag{4.2}$$

where the radial functions $G(r)$ and $F(r)$ are in $L^2\left([0,\ \infty),\ dr\right)$ and, for $d > 1$, satisfy the normalization condition[1]

$$(G(r),\ G(r)) + (F(r),\ F(r)) = \int_0^\infty \left(G^2(r) + F(r)^2\right) dr = 1. \tag{4.3}$$

The eigenvalue $E = E_{k_d \nu}$ corresponds to the state with $\nu = 0,\ 1,\ 2,\ \ldots$ nodes for the radial function $G(r)$, and k_d is defined by (1.51). In one dimension, the normalization

---

[1] $(f,\ g) = \int_a^b f(x)g(x)dx$ is an inner product of two square–integrable real–valued functions $f(x)$ and $g(x)$ on an interval $[a,\ b]$.

condition (4.3) becomes $\int_{-\infty}^{\infty}(G^2(x)+F(x)^2)\,dx=1$. With all these assumptions we can state, and then prove, the following theorem due to Hall [13]:

Theorem 4.1. *The real attractive central potential V(r, a) depends smoothly on the parameter a, and E(a)=* $E_{k_d\nu}(a)$ *is a corresponding discrete Dirac eigenvalue. Then*

$$\textit{if}\quad V'\geq 0,\quad \textit{then}\quad E'(a)\geq 0\quad \textit{and}\quad \textit{if}\quad V'\leq 0,\quad \textit{then}\quad E'(a)\leq 0, \tag{4.4}$$

where $'$ *is the operator* $\partial/\partial a$.

Proof: Differentiation of the equations (4.1)–(4.2) with respect to a gives

$$E'(a)G+E(a)G'=V'G+(V+m)G'+\left(\frac{k_d}{r}-\frac{d}{dr}\right)F', \tag{4.5}$$

$$E'(a)F+E(a)F'=V'F+(V-m)F'+\left(\frac{k_d}{r}+\frac{d}{dr}\right)G'. \tag{4.6}$$

Consider the quantity $\int_0^{\infty}((4.5)G+(4.6)F)dr$

$$E'(a)\underbrace{[(G,\ G)+(F,\ F)]}_{=1\text{ by }(4.3)}=(G,\ V'G)+(F,\ V'F)+W, \tag{4.7}$$

where

$$W=(G',\ (V+m)G)+\left(G,\ \left(\frac{k_d}{r}-\frac{d}{dr}\right)F'\right)-E(a)(G',\ G)+$$
$$(F',\ (V-m)F)+\left(F,\ \left(\frac{k_d}{r}+\frac{d}{dr}\right)G'\right)-E(a)(F',\ F). \tag{4.8}$$

Let us show that $W=0$. For this purpose, we prove the relation

$$(G,\ D_rF)=-(D_rG,\ F), \tag{4.9}$$

where the operator D_r is defined by $D_r=\partial/\partial r$. We know that $(G,\ D_rF)=\int_0^{\infty}GD_rFdr$, then using integration by parts $\int_0^{\infty}udv=[uv]_0^{\infty}-\int_0^{\infty}vdu$ with $u=$

$G \Longrightarrow du = dG$ and $dv = D_r F dr \Longrightarrow v = F$ we have

$$\int_0^{\infty} G D_r F dr = [GF]_0^{\infty} - \int_0^{\infty} D_r G F dr.$$

According to the boundary conditions $[GF]_0^{\infty} = 0$, thus (4.9) is proven. Similarly, it can be shown that $(F,\ D_r G) = -(D_r F,\ G)$. Relation (4.9) holds for $d > 1$. For the one–dimensional case, we can establish the corresponding result

$$(G(x),\ D_x F(x)) = [G(x)F(x)]_{-\infty}^{\infty} - \int_{-\infty}^{\infty} D_x G(x) F(x) dx = -(D_x G(x),\ F(x)),$$

with $D_x = \partial/\partial x$. Using (4.9) we can rewrite two terms of W in the following way

$$\left(G,\ \left(\frac{k_d}{r} - \frac{d}{dr}\right) F'\right) = \left(G',\ \left(\frac{k_d}{r} - \frac{d}{dr}\right) F\right)$$

and

$$\left(F,\ \left(\frac{k_d}{r} + \frac{d}{dr}\right) G'\right) = \left(F',\ \left(\frac{k_d}{r} + \frac{d}{dr}\right) G\right).$$

Therefore (4.8) becomes

$$W = \left(G',\ \underbrace{\left[(V+m)G + \left(\frac{k_d}{r} - \frac{d}{dr}\right) F - E(a)G\right]}_{=0 \text{ by } (4.1)}\right) +$$

$$\left(F',\ \underbrace{\left[(V-m)F + \left(\frac{k_d}{r} + \frac{d}{dr}\right) G - E(a)F\right]}_{=0 \text{ by } (4.2)}\right) = 0,$$

and (4.7) takes the form

$$E'(a) = (G,\ V'G) + (F,\ V'F). \tag{4.10}$$

From this relation it follows that if V' is non–negative, then $E'(a)$ is also non–negative. Similarly, if $V' \leq 0 \Longrightarrow E'(a) \leq 0$. These results complete the proof of the theorem.

$\square$

Now we can state the Comparison Theorem [10]:

Theorem 4.2 (Comparison Theorem)**.** *Suppose that* $E^{(1)}_{k_d\nu}$ *and* $E^{(2)}_{k_d\nu}$ *are the Dirac eigenvalues corresponding to two distinct attractive central potentials* $V^{(1)}(r)$ *and* $V^{(2)}(r)$*. Then*

$$\textit{if} \quad V^{(1)}(r) \leq V^{(2)}(r), \quad \textit{then} \quad E^{(1)}_{k_d\nu} \leq E^{(2)}_{k_d\nu}. \tag{4.11}$$

Proof: We assume that the potentials $V^{(1)}(r)$ and $V^{(2)}(r)$ are fixed. Then we define the one–parameter family of potentials $V(r,\ a)$ by

$$V(r,\ a) = V^{(1)}(r) + a\left(V^{(2)}(r) - V^{(1)}(r)\right), \tag{4.12}$$

where $a \in [0,\ 1]$. Suppose now that $E_{k_d\nu}(a) = E(a)$ is the eigenvalue which corresponds to $V(r,\ a)$, thus according to (4.12) $V(r,\ 0) = V^{(1)}(r)$ and $V(r,\ 1) = V^{(2)}(r)$, so $E^{(1)}_{k_d\nu} = E(0)$ and $E^{(2)}_{k_d\nu} = E(1)$. From (4.11), it follows that $V^{(2)}(r) - V^{(1)}(r) \geq 0$, so from (4.12) we have $\partial V(r,\ a)/\partial a = V^{(2)}(r) - V^{(1)}(r) \geq 0$. Since $\partial V(r,\ a)/\partial a \geq 0$, according to Theorem 4.1, $E'(a) \geq 0$ which implies that $E(a)$ is increasing and $E(0) \leq E(1)$; hence $E^{(1)}_{k_d\nu} \leq E^{(2)}_{k_d\nu}$.

$\square$

4.2 Some examples

Consider three potentials: the Woods–Saxon (A.14)

$$W(r) = -\frac{w}{1 + e^{\frac{r-R}{a}}}, \tag{4.13}$$

the laser–dressed Coulomb potential (A.13)

$$L(r) = -\frac{l}{(r^2 + \lambda^2)^{1/2}}, \tag{4.14}$$

and the cutoff Coulomb potential (A.12)

$$C(r) = -\frac{u}{r + \beta}, \tag{4.15}$$

where w, l, λ, u, and β are positive real parameters. First we compare the potentials $L(r)$ and $C(r)$. By choosing values for the parameters l, λ, u, and β, we make $L(r) > C(r)$ as is clear from Fig. 4.1. Then using numerical methods we solve the equations (4.1)–(4.2) with potentials (4.14), (4.15), and initial conditions (6.13) (to be disscussed in Chapter 6), and in three dimensions with $m = 1$. As the result, we get the energy values for the laser–dressed and the cutoff potentials, E_L and E_C respectively. They are given in the Table 4.1. According to Theorem 4.2, the potential ordering $L(r) > C(r)$ implies the spectral ordering $E_L > E_C$; this is confirmed numerically in Table 4.1 for various choices of the eigenvalue labels n, τ, and j.

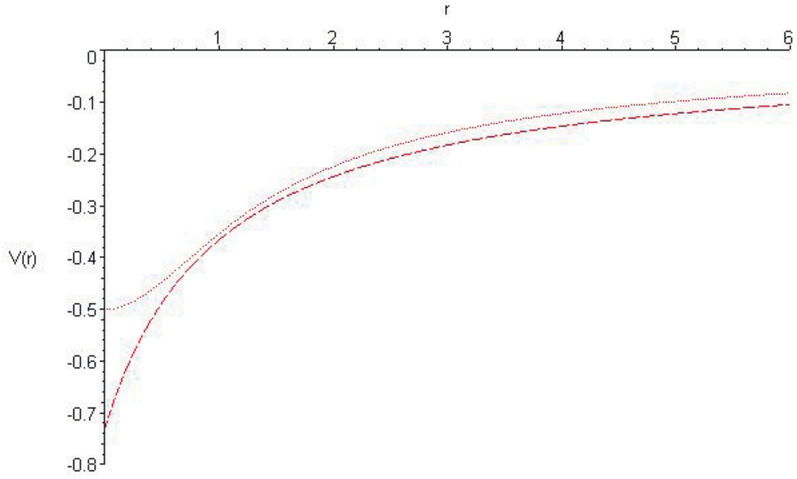


Figure 4.1: Laser–dressed (doted line) and cutoff (dashed line) Coulomb potentials with $l = 0.5$, $\lambda = 1$, $u = 0.73$, and $\beta = 1$.

Table 4.1: Energy values of laser–dressed (E_L) and cutoff (E_C) Coulomb potentials

n	τ	j	E_L	E_C
1	-1	1/2	0.909402	0.887474
	1		0.968006	0.949588
	-1	5/2	0.986091	0.974595
2		1/2	0.972553	0.957953
5			0.995206	0.991155
8			0.998095	0.996293

In Fig. 4.2 we compare potentials (4.13) and (4.14). We solve the pair of Dirac coupled equations with these potentials by using numerical methods with appropriate initial conditions in three dimensions. For the case $n = m = 1$, $\tau = -1$, and $j = -1/2$, equations (4.1)–(4.2) give us the energy value for the Woods–Saxon case $E_W = 0.872630$ and for laser–dressed potential $E_L = 0.825824$. According to Fig. 4.2, $W(r) > L(r)$, therefore Theorem 4.2 implies that $E_W > E_L$. This claim is confirmed by numerical methods since $E_W = 0.872630$ and $E_L = 0.825824$.

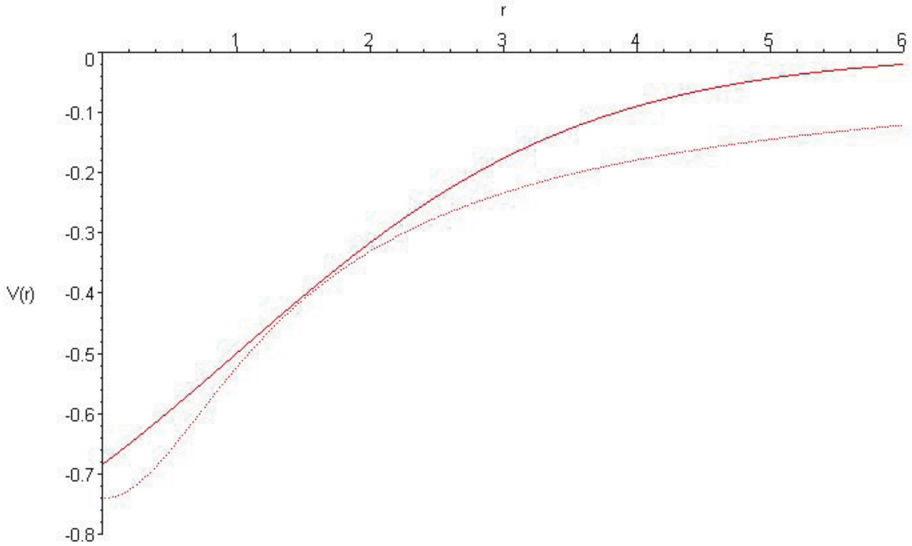


Figure 4.2: Woods–Saxon (full line) and Laser–dressed Coulomb (doted line) potentials with $w = 1$, $R = 1$, $a = 1.3$, $l = 0.74$, and $\lambda = 1$.

Chapter 5

Envelope theory

Here we introduce the envelope theory [35]–[37] and we give an example of its application. The Comparison Theorem 4.2 allows us to use the envelope method to approximate energy eigenvalues with the help of certain exact solutions, such as those for the Coulomb potential.

5.1 The envelope method

The central potential can be written as $V(r) = vf(r)$ where $v > 0$ is the coupling parameter and $f(r)$ is the shape of the potential. We assume that we can represent the shape $f(r)$ in the following way

$$f(r) = g(h(r)), \tag{5.1}$$

where $h(r)$ is the shape of a soluble potential and $g(h(r))$ is a smooth transformation function. We suppose that $g(h)$ is a monotone increasing function with definite convexity. We shall show that, if $g(h)$ is a convex ($g''(h) \geq 0$), envelope theory leads to a family of lower potentials which gives energy lower bounds. Conversely, in the case where $g(h)$ is a concave function ($g''(h) \leq 0$), we obtain an upper energy bounds.

According to (5.1), for a function $f(r)$, the family of functions $f^{(t)}(r)$ tangential at the point $r = t$ is given by[1]

$$f^{(t)}(r) = a(t) + b(t)h(r), \tag{5.2}$$

where

$$a(t) = g(h(t)) - g'(h(t))h(t), \quad \text{and} \quad b(t) = g'(h(t)). \tag{5.3}$$

Therefore we can write the shape $f(r)$ as

$$f(r) = \underset{t}{\text{envelope}} \left\{ f^{(t)}(r) \right\}. \tag{5.4}$$

If $g(h)$ is convex, its graph lies above its tangents and therefore $f(r) \geq f^{(t)}(r)$; meanwhile, if $g(h)$ is concave, we have $f(r) \leq f^{(t)}(r)$. With (5.2) and $v = 1$, the tangential potential becomes

$$V^{(t)}(r) = a(t) + b(t)h(r). \tag{5.5}$$

Now we suppose that $h(r)$ represents a Coulomb potential with unit coupling, i.e. $V(r) = h(r) = -1/r$. The radial equations (1.53)–(1.54) with potentials (5.5) and $S(r) = 0$ give us the tangential spectrum

$$E^{(t)} = a(t) + D(b(t)), \tag{5.6}$$

where $D(u)$ is the Dirac energy function for the Coulomb potential, which is given by (2.46) and, since $u < 1$, we require $b(t) < 1$.

---

[1] In many calculus books it can be found that for a given function $f(x)$ the equation of the tangent line at the point a is given by

$$y(x) = f(a) + f'(a)(x - a).$$

Suppose g is convex, then $f^{(t)}(r) \leq f(r)$. The Comparison Theorem 4.2 for the Dirac eigenvalues implies for each discrete eigenvalue

$$E^{(t)} \leq E. \tag{5.7}$$

According to (5.6) and (5.7), the best lower bound for E is the maximum of the right hand side of (5.6) over t, so

$$E \geq \max_{t} \left\{ E^{(t)} \right\} = \max_{t} \left\{ a(t) + D(b(t)) \right\}. \tag{5.8}$$

Similarly, in the concave case when $g''(h) \leq 0$, we obtain upper bounds for the energy values $E \leq \min\limits_{t} \left\{ E^{(t)} \right\}$. The Comparison Theorem 4.2 guarantees these bounds for each discrete eigenvalue. Using (5.4) we can write the family of lower bounds for E as

$$E^{L} = \operatorname*{envelope}_{t} \left\{ a(t) + D(b(t)) \right\}. \tag{5.9}$$

Now let us study the Dirac energy function $D(u)$ for the case $d = 3$. From (2.46) we have (with $m = 1$ and $d = 3$)

$$D(u) = \left[1 + \left(\frac{u}{n - k + \sqrt{k^2 - u^2}} \right)^2 \right]^{-1/2}, \tag{5.10}$$

where $n = 1,\ 2,\ 3,\ \ldots$ is the principal quantum number, $k = j + 1/2$ is the value of $|k_d|$ in three dimensions, and the Coulomb coupling u satisfies $u < 1$. Thus the first derivative of $D(u)$ has the form

$$\frac{dD(u)}{du} = - \left[\frac{2u}{\left(n - k + \sqrt{k^2 - u^2} \right)^2} + \frac{2u^3}{\sqrt{k^2 - u^2} \left(n - k + \sqrt{k^2 - u^2} \right)^3} \right] \times$$

$$2 \left[\frac{u^2}{\left(n - k + \sqrt{k^2 - u^2} \right)^2} + 1 \right]^{-3/2}, \tag{5.11}$$

and it is easy to see that $D'(u) < 0$ if $u \in (0,\ k)$. The expression of the second derivative of $D(u)$ is too complicated, so we will not introduce it here, instead we, using Maple, plot the family of the graphs of $D''(u)$ for two cases: $n \geq k$ and $n < k$, Fig. 5.1 and 5.2 respectively. From the graphs of the second derivative of the function $D(u)$ we see that $D''(u) < 0$. Finally, $D(u)$ is a positive, monotone decreasing and concave function of $u \in (0,\ k)$.

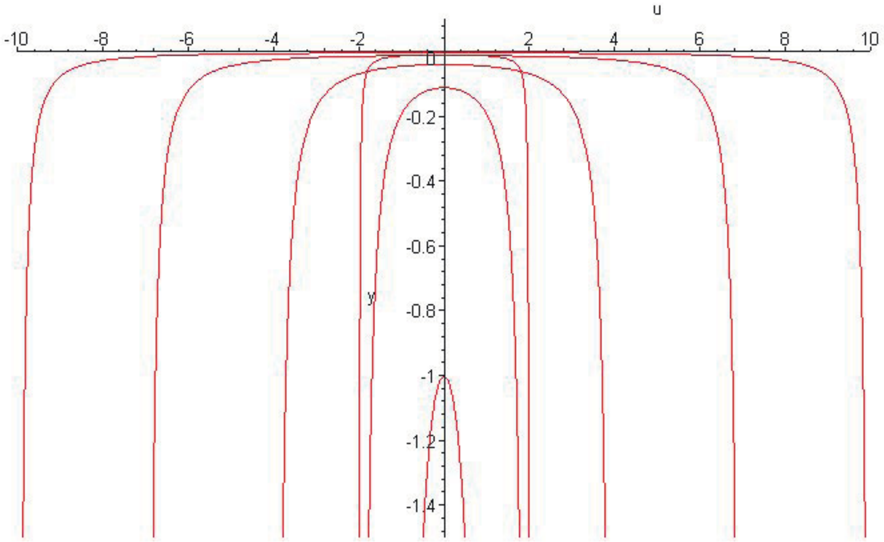


Figure 5.1: The graph of $D''(u)$ for $n \geq k$.

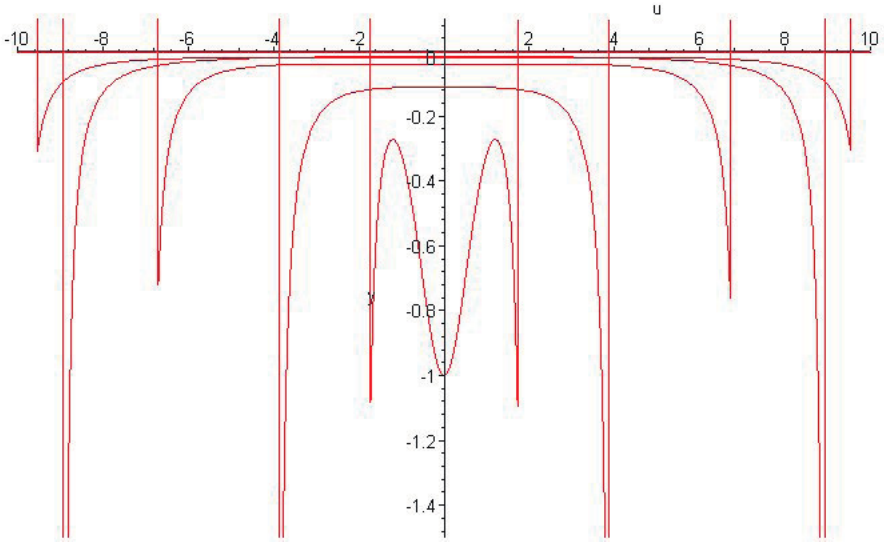


Figure 5.2: The graph of $D''(u)$ for $n < k$.

In order to find the envelope of the family E^L of tangential energy functions we, using (5.3), rewrite E^L in the following way

$$E^L = g(h) - g'(h)h + D(g'(h)). \tag{5.12}$$

Differentiation of the last equation with respect to h yields

$$-hg''(h) + D'(g'(h))g''(h) = 0.$$

After division by $g''(h)$ we find that the critical point is $h = D'(g'(h))$. Using the value for the critical point, and changing variables again to $u = g'(h)$ in (5.12), we obtain

$$E^L = E(u) = g(D'(u)) - uD'(u) + D(u). \tag{5.13}$$

Therefore the first and second derivatives of $E(u)$ with respect to u are

$$E' = D''\left(g(D') - u\right) \quad \text{and} \quad E'' = D''(g''D'' - 1) + D'''(g' - u). \tag{5.14}$$

From (5.3) and (5.8) we see that the energy function has the form

$$E^{(t)} = g(h) - hg'(h) + D(g'(h)). \tag{5.15}$$

From (5.13) and (5.14), it follows that $E(u)$ and $E^{(t)}$ have the same critical point and critical value. Finally, from (5.14), we find that if g is convex then the critical point is a minimum and if g is concave then the critical point is a minimum if $g''D'' < 1$ and a maximum if $g''D'' > 1$. Since we assumed that $g'' \geq 0$, we can write the following approximate formula

$$E \approx \min_u \left\{g(D'(u)) - uD'(u) + D(u)\right\}, \tag{5.16}$$

while for the case $g'' \leq 0$ we have

$$E \approx \begin{cases} \min\limits_{u} \left\{ g(D'(u)) - uD'(u) + D(u) \right\}, & \text{if} \quad g''D'' < 1, \\ \max\limits_{u} \left\{ g(D'(u)) - uD'(u) + D(u) \right\}, & \text{if} \quad g''D'' > 1. \end{cases} \tag{5.17}$$

5.2 An example

Consider the Hulthén potential (A.6)

$$H(r) = uf(r), \quad \text{and the shape} \quad f(r) = -\frac{1}{e^{r\lambda} - 1}, \tag{5.18}$$

where u and λ are real positive parameters. For a soluble potential, we take the Coulomb potential $V(r) = -v/r$ (A.2) with the shape $h(r) = -1/r$. According to (5.1), we can introduce $f(r)$ as

$$f(r) = g(h(r)) = -\frac{1}{e^{-\lambda/h(r)} - 1}. \tag{5.19}$$

Taking $x = -\frac{\lambda}{2h} > 0$, we can express $g(h)$ in terms of the hyperbolic cotangent as

$$g(x) = \frac{1 - \coth x}{2}. \tag{5.20}$$

So

$$\frac{dg}{dx} = \frac{1}{2\sinh^2 x} > 0, \tag{5.21}$$

and

$$\frac{d^2 g}{dx^2} = -\coth x \operatorname{csch}^2 x < 0. \tag{5.22}$$

Thus g is an increasing concave function and, according to the section above, we obtain optimized upper bounds for the Hulthén energy E

$$E \leq \min_t \left\{E^{(t)}(v)\right\} = \min_t \left\{ua(t) + D(ub(t))\right\}, \tag{5.23}$$

where $ub(t) < 1$. The coefficients $a(t)$ and $b(t)$ can be calculated using (5.3):

$$a(t) = \frac{1}{1 - e^{\lambda t}} + \frac{\lambda t}{4\sinh^2\left(\frac{\lambda t}{2}\right)}, \tag{5.24}$$

and

$$b(t) = \frac{\lambda t^2}{4\sinh^2\left(\frac{\lambda t}{2}\right)}. \tag{5.25}$$

With the help of mathematical softwhere (in our case Mathcad), we can calculate the values $E^U = \min_t \left\{E^{(t)}(v)\right\}$ and compare them with the values E of the energy for the potential (5.18) with different values of the parameters v, λ, τ. These are shown in Table 5.1.

Table 5.1: Comparison of the exact Hulthén energy eigenvalues E with its upper bounds E^U; $j = 1/2$ and $\tau = -1$.

n	v	λ	E	E^U
1	0.6	1	0.98946	1
	0.4	0.5	0.77699	0.78732
	1.8	2	0.99331	1
	0.29	0.3	0.39536	0.39911
	0.2	0.3	0.83607	0.83973
2	0.19	0.2	0.89402	0.90157
	0.67	0.7	0.99849	1
	0.088	0.09	0.81972	0.82126

Also, with (5.5), we obtain the set of the upper tangentials potentials

$$H(r) \leq V^{(t)}(r) = ua(t) + ub(t)h(r), \tag{5.26}$$

and the graphs of the Hulthén potential $H(r)$, which are given by (5.18), and the family of the tangential potentials $V^{(t)}(r)$ (given by (5.26)) shown in Fig. 5.3.

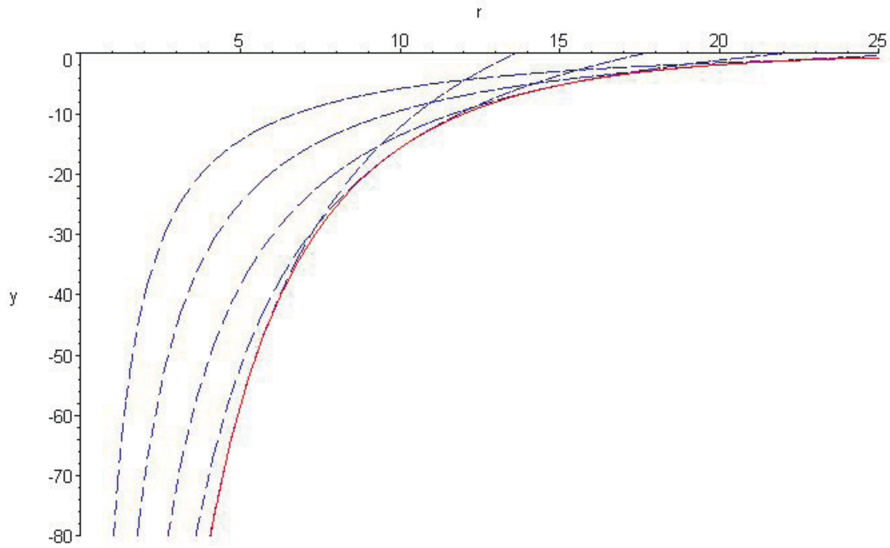


Figure 5.3: Hulthén potential (full line) and the tangential potentials (dashed lines) at different touching points $t = 5,\ 10,\ 15,\ 20,\ 25$, with $\lambda = 0.2$ and $u = 100$.

Chapter 6

Numerical solutions

6.1 The shooting method

The shooting method [38]–[41] is a method for solving a differential equation boundary value problem. This method reduces the boundary value problem to an initial value problem.

Suppose that we have a boundary value problem in the following form

$$\frac{d^2y}{dt^2} = f\left(t,\ y,\ \frac{dy}{dt}\right) \tag{6.1}$$

on $t \in [a,\ b]$ with the boundary conditions

$$\begin{cases} y(a) = \alpha, \\ y(b) = \beta. \end{cases} \tag{6.2}$$

Then we assume that $y'(a) = A$, so (6.2) reduces to

$$\begin{cases} y(a) = \alpha, \\ \dfrac{dy(a)}{dt} = A, \end{cases} \tag{6.3}$$

where the constant A must be chosen so that y satisfies the right–hand boundary condition $y(b) = \beta$. The shooting method gives an iterative procedure with which we can determine this constant A. Fig. 6.1 illustrates the solution of the boundary value problem given two distinct values of A. In one case, the value of $A = A_1$ gives a value for the initial slope which is too low to satisfy the boundary condition $y(b) = \beta$, whereas the value of $A = A_2$ is too large to satisfy this condition. However, A_1 and A_2 suggest the next guess: we have to adjust the value of A in (6.3) and find such an A which will lead to a solution which satisfies (6.2). The basic algorithm is as follows:

1. Solve the differential equation using any known method with the initial conditions $y(a) = \alpha$ and $y'(a) = A$.
2. Evaluate the solution $y(b)$ at $t = b$ and compare this value with the target value of $y(b) = \beta$.
3. Adjust the value of A (either bigger or smaller) untill a desired level of accuracy is achieved.

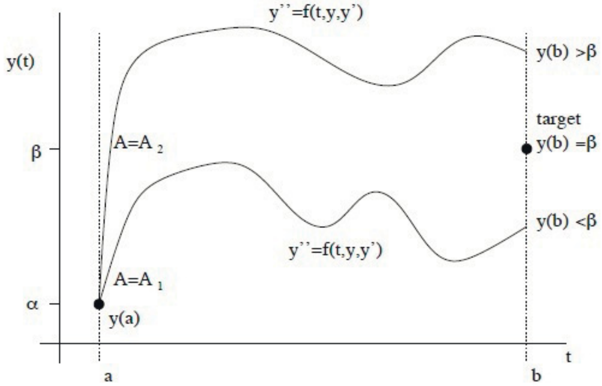


Figure 6.1: Shooting method.

Fig. 6.1 shows the solutions to the boundary value problem with $y(a) = \alpha$ and $y'(a) = A$. Here, two values of A are used to illustrate the solution's behavior and its lack of matching the correct boundary value $y(b) = \beta$.

In our applications, instead of the initial slope A, the adjustable parameter is the eigenvalue E given that the calculated wave function has the correct number of nodes for the eigenvalue sought.

6.2 Initial conditions for the Schrödinger equation

We start by finding suitable initial conditions near the origin ($r \longrightarrow 0$) for the Schrödinger equation in d dimensions. For this purpose, we consider equation (1.61) with (1.63)

$$-R''(r) + \left(\frac{l_d(l_d+1)}{r^2} + V(r)\right) R(r) = \mathcal{E} R(r), \tag{6.4}$$

where $'$ represents the derivative with respect to r, and $R(0) = 0$. We assume that $V(r) = vf(r)$ is not more singular than Coulomb so that $r^2V(r) \longrightarrow 0$ as $r \longrightarrow 0$, where $v > 0$ is the coupling parameter and $f(r)$ is the potential shape. For small r, we suppose $R(r)$ to be assymptotically of the form

$$\begin{cases} R(r) = br^q, \\ R'(r) = bqr^{q-1}, \end{cases} \tag{6.5}$$

where b and q are constants.

Firstly we consider the case $l_d = 0$, thus substitution of (6.5) into (6.4) and division by br^{q-2} yields

$$-(q-1)q + vr^2 f(r) = \mathcal{E} r^2.$$

After taking the limit from both sides of the previous equation as r approaches zero, we get

$$q(q-1) = 0, \quad \text{thus} \quad q = 0 \quad \text{or} \quad q = 1.$$

Since $R(0) = 0$, we keep $q = 1$ and set $b = 1$. Then the initial conditions (6.5) for small h have the form

$$\begin{cases} l_d = 0, \\ R(h) = h, \\ R'(h) = 1. \end{cases} \tag{6.6}$$

For the case $l_d > 0$, equation (6.4) with initial condition (6.5) takes the following form

$$-q(q-1) + l_d(l_d+1) + vr^2 f(r) = \mathcal{E} r^2,$$

and in the limit it becomes the quadratic equation

$$q^2 - q - l_d(l_d+1) = 0.$$

with the solutions

$$q_1 = l_d + 1 \quad \text{and} \quad q_2 = -l_d.$$

Again, since $R(0) = 0$, we keep the positive solution $q = l_d + 1$, so that the initial conditions (6.5) become

$$\begin{cases} l_d > 0, \\ R(h) = h^{l_d+1}, \\ R'(h) = (l_d+1)h^{l_d}, \end{cases} \tag{6.7}$$

with $b = 1$.

Examples of potentials satisfying these assumptions and conditions are the harmonic oscillator $V(r) = vr^2$, the Hydrogen–like atom $V(r) = -v/r$, and the sech–squared potential $V(r) = -v \operatorname{sech}^2 r$.

6.3 Initial conditions for the Dirac coupled equations

Let us now consider the Dirac coupled equations (1.53) and (1.54) with $S(r) = 0$, that is to say

$$G'(r) = -\frac{k_d}{r}G(r) + (E + m - V(r))\,F(r), \tag{6.8}$$

$$F'(r) = \frac{k_d}{r}F(r) - (E - m - V(r))\,G(r). \tag{6.9}$$

Suppose that the potential $V(r)$ satisfies $\lim_{r\to 0} rV(r) = -v \neq 0$. We again seek the initial conditions near the origin. Therefore, according to (2.27), we take the radial functions $G(r)$ and $F(r)$ to have the following forms

$$\begin{cases} G(r) = c_1 r^q, \\ F(r) = c_2 r^q, \end{cases} \tag{6.10}$$

where c_1, c_2, and q are constants greater then 0. After putting $c_2 = Bc_1$, where B is constant, in (6.10) and substituting it into (6.8) and (6.9), we obtain

$$EBr - vBV(r) + mBr = q + k_d,$$

$$Er - rV(r) - mr = -Bq + k_d B.$$

After taking the limit when $r \to 0$ from both sides of the last system of equations, we have

$$vB = q + k_d, \tag{6.11}$$

$$v = -Bq + k_d B. \tag{6.12}$$

The solution, q and B, of the last system is

$$q = \pm\sqrt{k_d^2 - v^2}, \quad B = \frac{k_d \pm \sqrt{k_d^2 - v^2}}{v}.$$

Since the wave functions have to be normalizable, we must choose the positive sign for q. Therefore the intial conditions for (6.8) and (6.9) with $c_1 = 1$ have the form (for small h)

$$\begin{cases} G(h) = h^{\sqrt{k_d^2 - v^2}}, \\ F(h) = \dfrac{k_d + \sqrt{k_d^2 - v^2}}{v} h^{\sqrt{k_d^2 - v^2}}. \end{cases} \tag{6.13}$$

This analysis is valid for example for the Coulomb potential $V(r) = -v/r$ and for a screened–Coulomb potential, such as the Yukawa potential (A.15)

$$V(r) = -\frac{a}{r} e^{-\lambda r}, \tag{6.14}$$

where a and λ are positive constants.

Now we consider the class of the potentials such that $\lim_{r \to 0} rV(r) = 0$, therefore the system (6.11)–(6.12) has two solutions

$$q = k_d \quad \text{and} \quad q = -k_d.$$

According to the boundary conditions, the radial wave functions G and F should vanish at the origin, therefore we keep $q = k_d$ and the initial conditions (6.10) with $B = 1$ become (for small h)

$$\begin{cases} G(h) = h^{k_d}, \\ F(h) = h^{k_d}. \end{cases} \tag{6.15}$$

6.4 Maple code

In the above section we described the shooting method in general. Here we adapt it for a program in Maple in the following way[1]: we start integrating numerically, if the eigenvalue is too large we get too many nodes, if not big enough we obtain fewer nodes than we need (this task is done by the block *nodes* in the Maple code). Then we solve for each trial eigenvalue the Dirac or Schrödinger equation with appropriate initial condition, and choose the eigenvalue which gives the best approximation. The wave function solutions have to vanish at infinity, but for our numerical analysis we have to choose an appropriate finite distance b at which the function must vanish. This choice can be a vexing issue: for Coulomb potentials $V(r) = -v/r$, an appropriate b may be as large as 50; for a short–range potential $V(r) = -ae^{\lambda r}$, b may turn out to be as small as 5. As an example, we introduce the Maple code for calculating energy eigenvalues for the Dirac coupled equations with the Coulomb potential.

```
> restart:  with(LinearAlgebra):  with(plots, listplot):
```

This part of the code creates the array of numbers on $[a,\ b]$, which we call a *mesh*.

```
> mesh:=proc(a, b, n) local h, i, m;
   m:=array(1..n+1);
   h:=(b-a)/n;
   for i from 0 by 1 to n do m[i+1]:=a+i*h; end do; m; end proc:
```

Here we create the potential. In this case, it is the Coulomb potential in the form (2.18).

```
> potential:=proc(v) local V;
   V:=-v/r; end proc:
```

In this block, we set up the system of the Dirac coupled equations (6.8) and (6.9) with initial conditions (6.13).

```
> dirsys:=proc(v, mass, energy, tau, j, d, h) local ds; global k_d;
```

---

[1] Adapted from a design of Professor R. L. Hall.

```
   k_d:=tau * (j + (d - 2)/2);
   ds:={diff(F(r), r)=(potential(v)+mass-energy)*G(r)+k_d*F(r)/r,
   diff(G(r), r)=(energy-potential(v)+mass)*F(r)-k_d*G(r)/r,
   G(h)=h^sqrt((k_d)^2-v^2), F(h)=(k_d + sqrt((k_d)^2-v^2))/v *
   h^(sqrt((k_d)^2-v^2))}; end proc:
```

Then we solve this system for the wave functions $G(r)$ and $F(r)$ by Fehlberg fourth–fifth order Runge–Kutta method with degree four interpolant - $rkf45$. Setting different values for r from array $mesh$, we form the matrix $(r,\ G(r))$.

```
>dirwaveG:=proc(v, mass, energy, tau, j, d, h, amesh, nmesh)
   local m, ds, mm;
   m:=mesh(h, amesh, nmesh);
   ds:=dsolve(dirsys(v, mass, energy, tau, j, d, h), {G(r), F(r)},
   numeric, method=rkf45, output=m);
   mm:=Matrix(ds[2,1]); SubMatrix(mm, [1..nmesh+1], [1, 3]);
   end proc:
```

This block counts the nodes and it is one of the key feaures of the shooting method described above.

```
>nodes:=proc(mat, n) local i, x1, x2, nc;
   nc:=0; x1:=mat[1,2];
   for i from 1 by 1 to n+1 do x2:=mat[i,2];
   if (x1*x2<0) then nc:=nc+1 end if;
   x1:=x2; end do; nc; end proc:
```

This is the heart of the code where we set up the node goal ng, which is the number of zeros of the function corresponding to the particular state studied. Also, we choose the lower $e1 = eL$ and the upper $e2 = eU$ limits for the possible energy values e. Afterwards, we let e be the average $e = (e1 + e2)/2$ which is our first trial eigenvalue. Then, using the numerical solution of the Dirac equation, we count its number of roots or nodes. If this number is less or equal than ng, then the eigenvalue e is too small, and we have to update the lower value $eL = e$. In the opposite situation, when the number of roots is greater a ng, then e is too big, and we have to change the upper limit $e = eU$. To check the solution e, we calculate the energy r_e using the formula (2.46).

```
>diregG:=proc(n, v, mass, tau, j, d, h, amesh, nmesh, eL, eU, m,
   nx, ymax) local e, e1, e2, ng, i, no, r_e;
   e1:=eL; e2:=eU; e:=(e1+e2)*0.5;
   ng:=n-1;
   for i from 1 by 1 to m do
   no:=nodes(eval(dirwaveG(v, mass, e, tau, j, d, h, amesh,
   nmesh)), nmesh);
   if (no<=ng) then e1:=e else e2:=e end if;
   e:=(e1+e2)*0.5; end do; e;
   r_e:=mass*(1+(v^2)/((n - abs(k_d) + (d-3)/2 +
   sqrt(k_d^2-v^2))^2))^(-1/2);
   printf("energy level=%d, energy=%3.7f, real_energy=%3.7f,
   v=%3.1f, mass=%d, tau=%d, j=%3.1f, dimension=%d, h=%3.5f,
   amesh=%d, nmesh=%d, eL=%d, eU=%d, m=%d, nx=%d, ymax=%d",
   n, e, r_e, v, mass, tau, j, d, h, amesh, nmesh, eL, eU, m,
   nx, ymax);
   listplot(dirwaveG(v, mass, e, tau, j, d, h, amesh, nx),
   view=[0..amesh, -ymax..ymax], color=green, axes=normal,
   labels=[r, G]); end proc:
```

Here we put the values of all the required variables and, as a result, we get the energy value *energy* and the graph of the radial function $G(r)$ (Fig. 6. 2).

```
>diregG(4, 0.5, 1.5, -1, 1/2, 3, 0.00001, 90, 50, -2, 5, 60,
```

```
   200, 1.2);
energy level=4, energy=1.4876102, real_energy=1.4876102, v=0.5, mass=1.5,
tau=-1, j=0.5, dimension=3, h=0.00001, amesh=90, nmesh=50, eL=-2, eU=5,
m=60, nx=200, ymax=1.2
```

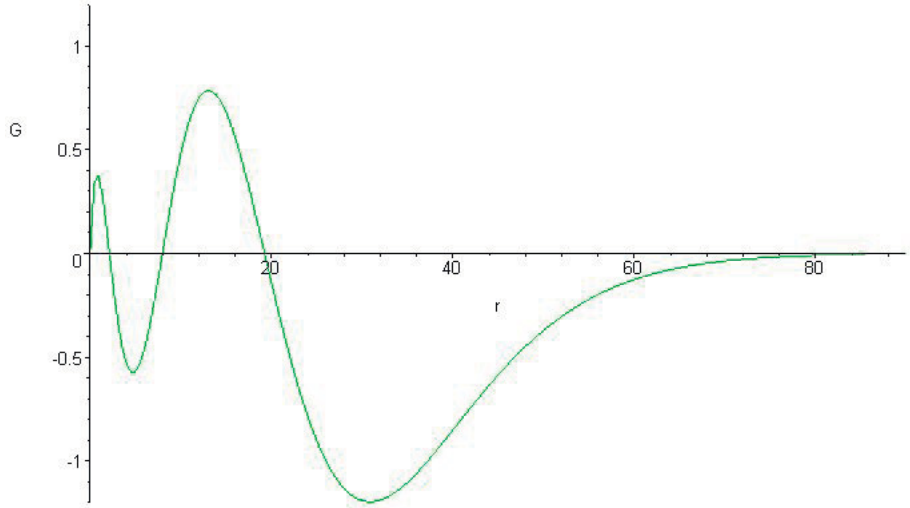


Figure 6.2: Dirac radial wave function $G(r)$.

The program calculates the energy value which satisfies (2.46). If we change the variables, such as the coupling parameter v, energy level n, dimension d, and so on, we will get the graph of the wave function $G(r)$ and the eigenvalues which still satisfy (2.46). Therefore we can conclude that our program works properly. Thus we can use this Maple code for other equations and other potentials (with suitable initial conditions) for which we do not know the exact answer. For this purpose, we simply have to change the Maple code, i.e. change the potential and initial conditions.

Chapter 7

Soft–Core Coulomb potentials - confined atoms

7.1 Scaling

In this section we derive the scaling law for a family of central soft–core Coulomb potentials for the Dirac coupled radial equations. For this purpose, we consider the Dirac Hamiltonian H in the form (3.15) with the potential (A.11). In this case, the energy eigenvalues depend on four parameters, i.e. $E = E(v,\ \beta,\ q,\ m)$, so

$$H = \begin{pmatrix} -\dfrac{v}{(r^q + \beta^q)^{1/q}} - m & \dfrac{d}{dr} + \dfrac{k_d}{r} \\ \dfrac{d}{dr} - \dfrac{k_d}{r} & -\dfrac{v}{(r^q + \beta^q)^{1/q}} + m \end{pmatrix} \longrightarrow E(v,\ \beta,\ q,\ m). \tag{7.1}$$

With the substitution $r = \delta x$, (7.1) becomes

$$H = \begin{pmatrix} -\dfrac{v\delta^2}{\left(x^q + \left(\frac{\beta}{\delta}\right)^q\right)^{1/q}} - \delta m & \dfrac{d}{dx} + \dfrac{k_d}{x} \\ \dfrac{d}{dx} - \dfrac{k_d}{x} & -\dfrac{v\delta^2}{\left(x^q + \left(\frac{\beta}{\delta}\right)^q\right)^{1/q}} + \delta m \end{pmatrix} \longrightarrow \delta E(v,\ \beta,\ q,\ m). \tag{7.2}$$

On the other hand, by using (7.1), we also can write

$$H = \begin{pmatrix} -\dfrac{v\delta^2}{\left(x^q + \left(\frac{\beta}{\delta}\right)^q\right)^{1/q}} - \delta m & \dfrac{d}{dx} + \dfrac{k_d}{x} \\ \dfrac{d}{dx} - \dfrac{k_d}{x} & -\dfrac{v\delta^2}{\left(x^q + \left(\frac{\beta}{\delta}\right)^q\right)^{1/q}} + \delta m \end{pmatrix} \longrightarrow E\left(v\delta^2,\ \frac{\beta}{\delta},\ q,\ \delta m\right). \tag{7.3}$$

Comparing (7.2) and (7.3), we obtain the scaling law for the family of the soft–core Coulomb potentials under the Dirac coupled equations, namely

$$E(v,\ \beta,\ q,\ m) = \frac{1}{\delta} E\left(v\delta^2,\ \frac{\beta}{\delta},\ q,\ \delta m\right). \tag{7.4}$$

Since δ can be any positive number, we set $\delta = \beta$ in (7.4) and obtain the first special scaling law

$$E(v,\ \beta,\ q,\ m) = \frac{1}{\beta} E\left(v\beta^2,\ 1,\ q,\ \beta m\right). \tag{7.5}$$

And, with $\delta = 1/m$, (7.4) becomes

$$E(v,\ \beta,\ q,\ m) = mE\left(\frac{v}{m^2},\ \beta m,\ q,\ 1\right). \tag{7.6}$$

7.2 Monotonicity

We now suppose that $m = 1$ and write $E(v,\ \beta,\ q,\ 1)$ as $E(v,\ \beta,\ q)$. We establish that the eigenvalues $E(v,\ \beta,\ q)$ are monotone in each of the three potential parameters: $v > 0$, $\beta > 0$, and $q \geq 1$. For this purpose, we consider the potential (A.11)

$$V(r) = -\frac{v}{\left(r^q + \beta^q\right)^{1/q}}. \tag{7.7}$$

From (7.7), it follows that

$$\frac{\partial V}{\partial v} = -\frac{1}{\left(r^q + \beta^q\right)^{1/q}},$$

and it is easy to see that $\left(r^q + \beta^q\right)^{1/q} > 0$, so $\partial V/\partial v < 0$. Then the derivative of V with respect to β is

$$\frac{\partial V}{\partial \beta} = \frac{v\beta^{q-1}}{\left(r^q + \beta^q\right)^{1/q+1}}.$$

It is also straightforward that, since $v\beta^{q-1} > 0$ and $\left(r^q + \beta^q\right)^{1/q+1} > 0$, then $\partial V/\partial \beta > 0$. Now we consider the derivative of V with respect to q

$$\frac{\partial V}{\partial q} = -v\left[\frac{\ln\left(r^q + \beta^q\right)}{q^2\left(r^q + \beta^q\right)^{1/q}} - \frac{\beta^q \ln \beta + r^q \ln r}{q\left(r^q + \beta^q\right)^{1/q+1}}\right].$$

After some algebra, we can rewrite it in the convenient form

$$\frac{\partial V}{\partial q} = \frac{v}{q^2}\frac{\beta^q\left[\ln \beta^q - \ln\left(r^q + \beta^q\right)\right] + r^q\left[\ln r^q - \ln\left(r^q + \beta^q\right)\right]}{\left(r^q + \beta^q\right)^{1/q+1}}.$$

We see that $v/q^2 > 0$, $\beta^q > 0$, $r^q > 0$, and $\left(r^q + \beta^q\right)^{1/q+1} > 0$. But $\ln \beta^q - \ln\left(r^q + \beta^q\right) = \ln\left[\beta^q/\left(r^q + \beta^q\right)\right] < 0$, since $\beta^q/\left(r^q + \beta^q\right) < 1$. Similarly, $\ln r^q - \ln\left(r^q + \beta^q\right) < 0$. Thus $\partial V/\partial q < 0$.

In summary, we have the following monotonic behaviour of the potential in the parameters $v,\ \beta$, and q :

$$\frac{\partial V}{\partial v} < 0, \quad \frac{\partial V}{\partial \beta} > 0, \quad \text{and} \quad \frac{\partial V}{\partial q} < 0. \tag{7.8}$$

These monotonicities are illustrated in Figures 7.1, 7.2, and 7.3. The special Comparison Theorem of R. L. Hall [13] (section 4.1 above), implies the following spectral monotonicities for each discrete eigenvalue:

$$\frac{\partial E}{\partial v} < 0, \quad \frac{\partial E}{\partial \beta} > 0, \quad \text{and} \quad \frac{\partial E}{\partial q} < 0. \tag{7.9}$$

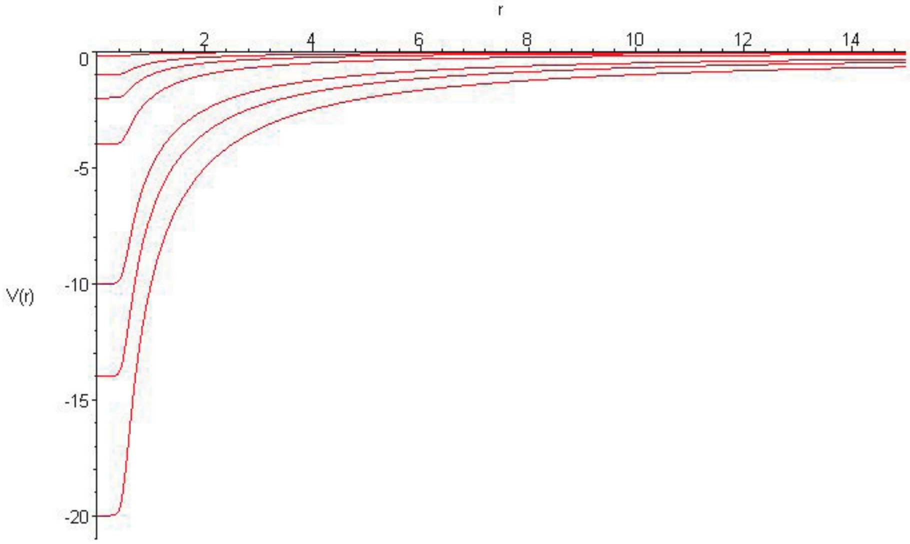


Figure 7.1: The family of potentials $V(r) = -\dfrac{v}{(r^q+\beta^q)^{1/q}}$, with $\beta = 0.5$, $q = 10$, and $v = 0.1,\ 0.5,\ 1,\ 2,\ 5,\ 7,\ 10$. These potentials are monotonic in v: $\dfrac{\partial V}{\partial v}$.

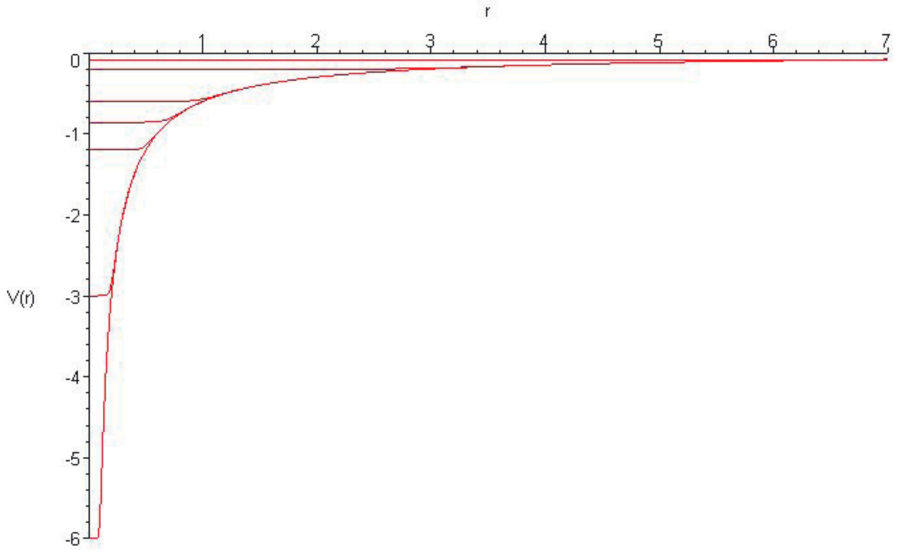


Figure 7.2: The family of potentials $V(r) = -\dfrac{v}{(r^q + \beta^q)^{1/q}}$, with $v = 0.6$, $q = 15$, and $\beta = 0.1,\ 0.2,\ 0.5,\ 0.7,\ 1,\ 3,\ 7$. These potentials are monotonic in β: $\dfrac{\partial V}{\partial \beta}$.

7.3 Coulomb envelopes

In this final section of our thesis, we apply the envelope theory which we described above in section 5.1. We rewrite the potential (7.7) in the following way

$$V(r) = uf(r), \quad \text{with the shape} \quad f(r) = -\frac{1}{(r^q + \beta^q)^{1/q}}, \tag{7.10}$$

where we replaced v by u to avoid confusion with the coupling parameter from the Colomb potential. As a potential with exact solutions, we take the Coulomb potential $V(r) = -v/r$, so its shape has the form $h(r) = -1/r$. Then, using (5.1), we introduce the shape $f(r)$ as

$$f(r) = g(h(r)) = -\frac{1}{\left[\left(-\frac{1}{h(r)}\right)^q + \beta^q\right]^{1/q}}. \tag{7.11}$$

Then

$$\frac{dg}{dh} = \frac{\left(-\frac{1}{h}\right)^{q-1}}{h^2\left[\left(-\frac{1}{h}\right)^q + \beta^q\right]^{1/q+1}}, \tag{7.12}$$

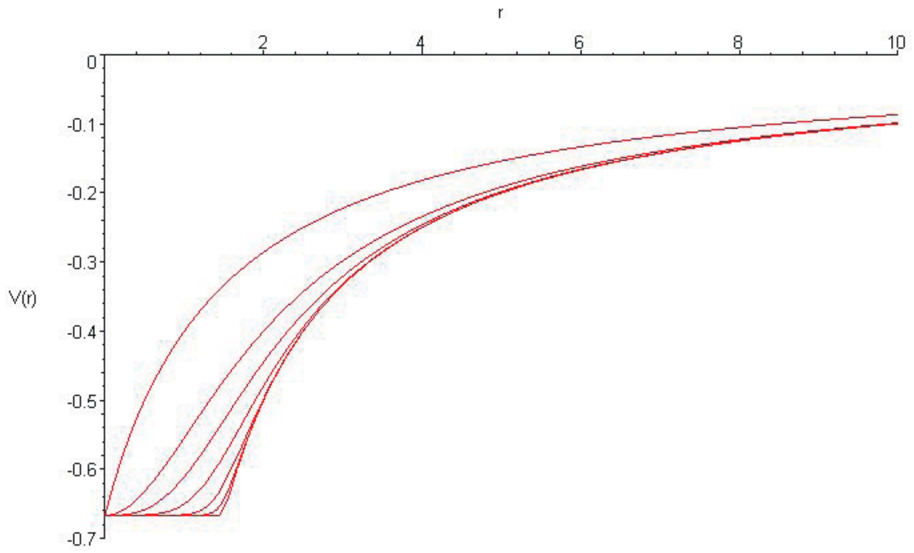


Figure 7.3: The family of potentials $V(r) = -\frac{v}{(r^q+\beta^q)^{1/q}}$, with $v = 1$, $\beta = 1.5$, and $q = 1,\ 2,\ 3,\ 5,\ 10,\ 20,\ 100$. These potentials are monotonic in q: $\frac{\partial V}{\partial q}$.

and

$$\frac{d^2g}{dh^2} = \frac{(q+1)\beta^q\left(-\frac{1}{h}\right)^q}{h^2\left[\left(-\frac{1}{h}\right)^q+\beta^q\right]^{1/q+2}}. \tag{7.13}$$

Since the quantity $-1/h > 0$, we conclude that $dg/dh > 0$ and $d^2g/dh^2 > 0$. Thus $g(h)$ is an increasing convex function and it leads to lower bounds for the soft–core Coulomb energy eigenvalues. Following the envelope theory, we find the coefficients $a(t)$ and $b(t)$, using (5.3),

$$a(t) = \frac{t^q}{(t^q+\beta^q)^{1/q+1}} - \frac{1}{(t^q+\beta^q)^{1/q}}, \tag{7.14}$$

and

$$b(t) = \frac{t^{q+1}}{(t^q+\beta^q)^{1/q+1}}. \tag{7.15}$$

Therefore we can calculate the lower bounds for the Dirac energy eigenvalues E for the class of soft–core Coulomb potentials, by using (5.8),

$$E \geq \max_{t} \left\{ va(t) + D(vb(t)) \right\}, \tag{7.16}$$

where $D(vb(t))$ is the Dirac energy function for the Coulomb potential, which is given by (5.10) provided $vb(t) < 1$.

With the help of the numerical methods described in Chapter 6, we calculate the "exact" energy values E (that is to say, accurate numerical estimates) and compare them with the lower bounds $E^L = \max\limits_{t} \{va(t) + D(vb(t))\}$. These are shown in the Table 7.1.

Table 7.1: Comparison the exact soft–sore Coulomb energy eigenvalues E with its lover bounds E^L.

n	u	β	q	j	τ	E	E^L
1	0.1	0.1	1	1/2	-1	0.99517	0.99509
	0.1	0.1	10			0.99499	0.99499
	0.9	10	10			0.92972	0.91850
	0.9	10	1			0.96198	0.95718
2	0.5	30	17	7/2	-1	0.99553	0.99497
	0.6	20	30	9/2	1	0.99631	0.99631
	0.2	0.1	3	3/2		0.99875	0.99875
3	0.2	4	7	5/2	-1	0.99920	0.99920
	0.3	40	70	1/2	1	0.99815	0.99713
5	0.9	0.8	4	1/2	-1	0.98358	0.98003
	0.4	54	40	3/2		0.99856	0.99776
9	0.8	74	3	1/2	1	0.99816	0.99697
11	0.2	0.1	19	1/2	-1	0.99983	0.99983

Also, from (5.5), we find the family of the lower tangential potentials

$$V(r) \geq V^{(t)}(r) = ua(t) + ub(t)h(r), \tag{7.17}$$

whose graphs are shown in Fig. 7.4.

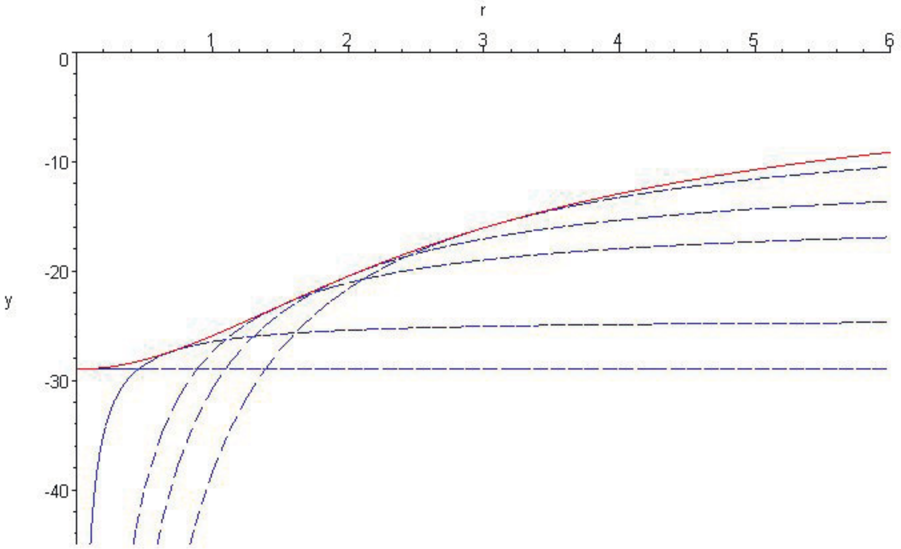


Figure 7.4: Soft-Core Coulomb potential $V(r)$ (full line) and the tangentials potentials $V^{(t)}(r)$ (dashed lines) at different touching points $t = 0.01,\ 0.7,\ 1.5,\ 2,\ 3$, with $u = 58$, $\beta = 2$, and $q = 2$. Each tangential potential leads to a lower energy curve $E^{(t)}$.

Conclusion

Analytic solutions to the Dirac equation are often very complicated, or not available. Therefore it is very useful to have an approximate analytic formula for the Dirac energy eigenvalues. The Comparison Theorem allows us to use a geometric approach to estimate the Dirac spectrum. In this thesis, we use the envelope method which allows us to obtain such spectral estimates. For instance, if the potential $V(r)$ is a convex transformation $V(r) = g(h)$ of the Coulomb potential $h(r) = -1/r$, then envelope theory allows us to obtain the optimized energy upper bound

$$E \leq \min_{u} \left\{ g(D'(u)) - uD'(u) + D(u) \right\},$$

where $D(u)$ is the hydrogenic energy function. Since this formula is essentially analytic, it can be used to determine approximately how the energy spectrum depends on all the parameters of the problem. As we can see from Table 7.1, this approximation gives very accurate results. Moreover, geometrical methods such as the envelope theory are very general and lead to the same formulae for the Schrödinger and Dirac problems in any d–dimensional space, and for each angular momentum sector.

Bibliography

[1] W. Heisenberg , Z. Physik **33**, 879–893 (1925).

[2] E. Schrödinger, Annalen der Physik **79**, 361–376 (1926).

[3] E. Schrödinger, *Collected Papers on Wave Mechanics*, (Chelsea Publishing Company, New York, 1982).

[4] E. Schrödinger, Annalen der Physik **79**, 734–756 (1926).

[5] J. von Neumann, *Mathematical foundations of quantum mechanics*, (Princeton University Press, Princeton, 1955).

[6] H. Haken, H. C. Wolf, *The Physics of Atoms and Quanta*, (Springer, Heidelberg, 1987).

[7] Y. Jiang, J. Phys. A. **38**, 1157 (2005).

[8] H. Ciftci, R. L. Hall, and N. Saad, J. Phys. A **36**, 11807 (2003).

[9] H. Ciftci, R. L. Hall, and N. Saad, Phys. Rev. A **72**, 022101 (2005).

[10] R. L. Hall, Phys. Rev. A **81**, 052101 (2010).

[11] E. Conte, EJTP **25**, 109126 (2011).

[12] J. S. R. Chisholm and A. K. Commons (Eds.), *Clifford Algebras and their Applications in Mathematical Physics*, (Reidel, Boston, 1986): *Clifford Algebra and the Interpretation of Quantum Mechanics* by D. Hestenes, 321–346.

[13] R. L. Hall, Phys. Rev. Lett. **101**, 090401 (2008).

[14] W. Greiner, *Relativistic Quantum Mechanics*, (Springer, Heidelberg, 1990).

[15] A. Messiah, *Quantum Mechanics*, (North Holland, Amsterdam, 1962).

[16] C. Chevalley, *Fundamental Concepts of Algebra*, (Academic Press Inc., New York, 1965).

[17] J. Griffiths, *Introduction to Quantum Mechancs*, (Pretice Hall, University of Michigan, 1995).

[18] D. J. Hurley, and M. A. Vandick, *Geometry, Spinors and Applications*, (Springer Praxis Publishing, Chichester, 2000).

[19] J. Polchinski, *String Theory*, Vol. 2, (Cambridge University Press, 1998).

[20] A. Proeyen, *Tools for supersymmetry*, arXiv: hep-th/9910030.

[21] P. C. West, *Supergravity, brane dynamics and string duality*, arXiv: hep-th/9811101.

[22] X–Y Gu, Z–Q Ma, and S–H Dong, Phys. Rev. A **67**, 062715 (2003).

[23] A. Wacker, *Quantum theory of angular momentum*, (Fysiska Institutionen, Lunds Universitet, 2008).

[24] J. Thompson, *Angular Momentum: An Illustrated Guide to Rotational Symmetries for Physical Systems*, (Wiley–VCH, Mörlenbach, 1994).

[25] A. Joseph, Rev. Mod. Phys. **39**, 829 (1967).

[26] R. Brauer and H. Weyl, Am. J. Math. **57**, 425 (1935).

[27] J. D. Bjorken and S. D. Drell, *Relativistic Quantum Mechanics*, (McGraw–Hill, New York, 1964).

[28] A. Sommerfeld, *Partial Differential Equations in Physics*, (New York: Academic, 1949). [The generalization of the ordinary spherical harmonics is considered on pp 227–232].

[29] R. L. Hall, Q. D. Katatbeh, and N. Saad, J. Phys. A: Math. Gen. **37**, 11629–11644 (2004).

[30] S–H Dong and Z–Q Ma, Phys. Rev. A **65**, 042717 (2002).

[31] W. Greiner, *Quantum Mechanics. An Introduction*, (Springer, Heidelberg, 2000).

[32] S. Flügge, *Practical Quantum Mechanics*, (Springer, New York, 1974).

[33] R. Larson, B. H. Edwards, *Calculus of a Single Variable: Early Transcendental Functions*, Fifth Edition, (Cengage Learning, Boston, 2010).

[34] A. Jeffrey, *Advanced engineering mathematics*, (Academic Press, Burlington 2002). [Cauchy-Euler equation is disscussed on page 309].

[35] R. L. Hall, J. Math. Phys. **25** (9), 2708–2715 (1984).

[36] R. L. Hall, J. Phys. A: Math. Gen. **19**, 2079–2086 (1986).

[37] R. L. Hall, J. Math. Phys. **34** (7), 2779–2788 (1993).

[38] A. L. Rodriguez, MSc Thesis: *Spectral Estimates for Schrödinger Operators*, (August 2008).

[39] G. Dahlquist, A. Bjorck, *Numerical Methods*, (Prentice-Hall, 1974).

[40] J. N. Kutz, *Notes for AMATH 301*, (2003). [The shooting method is discussed on pp 17–20].

[41] J. D. Pryce, *Numerical Solution of Sturm–Liouville Problems*, (Oxford Science Publications, New York, 1993).

[42] M. Hazewinkel, *Encyclopaedia of Mathematics: Supplement*, Vol. 3, (Netherlands, 1997).

[43] A. Inomata, H. Kuratsuji, and C. C. Gerry, *Path Integrals and Coherent States of SU(2) and SU(1, 1)*, (World Scientific Publishing Co. Pte. Ltd., Singapore, 1992).

[44] L. Hulthén and M. Sugawara, in S. Flügge (ed.): *Handbuch der Physik*, (Springer, 1957).

[45] C. S. Lam and Y. P. Varshni, Phys. Rev. A **4**, 1875 (1971).

[46] A. A. Berezin, Phys. Status. Solidi (b) **50**, 71 (1972).

[47] G. Pöschl, E. Teller, Z. Phys. **83**, 143 (1933).

[48] C. Eckart, Phys. Rev. **35**, 1303 (1930).

[49] B. Y. Tong, Solid State Commun. **104** (11), 679-682 (1997).

[50] F. Cooper, A. Kahare, and U. Sukhatme, Phys. Rept. **251**, 267 (1995).

[51] J. J. Weiss, J. Chem. Phys. **41**, 1120 (1964).

[52] A. Cimas, M. Aschi, C. Barrientos, V. M. Rayon, J. A. Sardo, and A. Largo, Chem. Phys. Lett. **374**, 594 (2003).

[53] N. Rosen and P. M. Morse, Phys. Rev. **42**, 210 (1932).

[54] R. L. Hall, N. Saad, K. D. Sen, and H. Ciftci, Phys. Rev. A. **80**, 032507 (2009).

[55] R. L. Hall, N. Saad, and K. D. Sen, J. Math. Phys. **51**, 022107 (2010).

[56] R. L. Hall and Q. D. Katatbeh, Phys. Lett. A. **294**, 163–167 (2002).

[57] C. H. Mehta and S. H. Patil, Phys. Rev. A **17**, 43 (1978).

[58] P. P. Ray and K. Mahata, J. Phys. A **22**, 3161 (1989).

[59] R. Dutt, U. Mukherji, and Y. P. Varshni, J. Phys. B: At. Mol. Phys. **18**, 3311-3318 (1985).

[60] J. P. Duarte and R. L. Hall, J. Phys. B: At. Mol. Opt. Phys. **27**, 1021–1025 (1994).

[61] C. A. S. Lima and L. C. M. Miranda, Phys. Rev. A **23**, 3335 (1981).

[62] V. K. Mittal, R. C. Verma, and S. C. Gupta, *Introduction to Nuclear and Particle Physics*, (Raj Press, New Delhi, 2009).

[63] P. Kennedy, R. L. Hall, and N. Dombey, Int. J. Mod. Phys. A **19**, 3557–3581 (2004).

[64] J. L. Basdevant, J. Rich, and M. Spiro, *Fundamentals in Nuclear Physics*, (Springer, 2005).

Appendix A

Central Potentials

The interactions between nucleons within a nucleus and between nucleons can be described using quantum mechanics. This type of interaction is very complicated and not precisely known. From the experiments, we know that it is of short range, attractive at distances comparable to the size of a nucleus, and is repulsive at very short distances. Because of the complexity of this interaction it is necessary to use approximations. The most widely used approximate potentials are called central potentials. They depend only on the distanee r of the particle from a center of force, and not on the direction of the vector $\boldsymbol{r}$ connecting that center with the particle, that is

$$\text{potential} = V(r), \quad r = ||\boldsymbol{r}||. \tag{A.1}$$

Therefore, the system of a particle in a central potential $V(r)$ is invariant under spatial rotations.

A.1 Coulomb potential

The Coulomb potential is an effective pair potential that describes the interaction between two point charges. It acts along the line connecting the two charges. Let r

be the distance between two particles of electric charge $Z_1 e$ and $Z_2 e$, respectively; so the electrostatic interaction potential of these two particles is given by [15]

$$V(r) = -\frac{Z_1 Z_2 e^2}{r}.$$

For the two identical particles $Z_1 = Z_2 = Z$, this potential becomes

$$V(r) = -\frac{v}{r}, \tag{A.2}$$

where the coupling constant $v = Ze^2$, in which $Z = 1$ for hydrogen, $Z = 2$ for singly ionized helium, and so on. The Coulomb potential admits continuum states (with $E > 0$), describing electron–proton scattering, as well as discrete bound states, representing the bound hydrogen atom.

Central potentials behaving like $1/r$ at the origin are often found in atomic and nuclear physics. With the exception of the Coulomb potential, none of these can be solved in terms of elementary functions for all orbital angular momentum. For example, the radial Schrödinger equation (1.61) in three dimensions with $m = 1$ gives the energy eigenvalues in a simple form [17]

$$E = -\frac{2v^2}{(n+l)^2}. \tag{A.3}$$

A.2 Harmonic oscillator

Whereas a breakthrough in atomic physics came with the quantum–mechanical solution of the central force problem with a Coulomb potential, a parallel breakthrough in nuclear physics resulted from the quantum–mechanical solution for nucleons in a spherical harmonic oscillator potential, which is given by [17]

$$V(r) = vr^2, \tag{A.4}$$

where the coupling $v = \frac{1}{2}\omega^2 > 0$, and ω represents the frequency of the oscillator. The quantum harmonic oscillator is the quantum–mechanical analog of the classical harmonic oscillator. Because an arbitrary potential can be approximated as a harmonic potential in the vicinity of a stable equilibrium point, it is one of the most important model systems in quantum mechanics. Furthermore, it is one of the few quantum–mechanical systems for which an exact solution is known. The Schrödinger equation with this potential yields the well–known energy eigenvalues in $d = 3$ and with $m = 1$ [17]

$$E = (4n + 2l - 1)\sqrt{\frac{v}{2}}. \tag{A.5}$$

A.3 Hulthén potential

The Hulthén potential [42, 43] is given by

$$V(r) = -\frac{u}{e^{\lambda r} - 1}, \tag{A.6}$$

where $u = Z\lambda$ and $\lambda = 1/a$, a is the screening parameter, Z is the atomic number.

The Hulthén potential is a short–range potential defined along a half line $0 < r < \infty$. This potential is a good approximation for the Yukawa potential or the screened Coulomb potential: for $r \ll a$, it is asymptotically like the Coulomb potential. Therefore it has been used in many branches of physics, such as nuclear physics [44], atomic physics [45], and solid state physics [46].

The Schrödinger equation (1.61) in three dimensions for this potential can be solved for s waves with $l = 0$ and $m = 1$ [32]

$$E = -\frac{\left(2v - n^2\right)^2}{2}. \tag{A.7}$$

If $l \neq 0$, the problem is not exactly soluble and must be solved numerically.

A.4 Sech–squared potential

The following potential interpolates between the square well and the harmonic oscillator

$$V(r) = -v\,\mathrm{sech}^2\,\alpha r, \tag{A.8}$$

where the coupling parameter $v > 0$ represents the potential depth and $\alpha > 0$ is the width of the potential. Potential (A.8) has been known under several different names since early days of quantum mechanics such as the Pöschl–Teller potential [47], the Eckart potential [48], and others. Therefore to avoid confusion, we shall name it by the function itself: sech–squared potential [49]. The sech–squared potential is one of the most important exponential–type potentials in the literature and it has been widely used in physics [50] and chemical physics [51, 52]. The Schrödinger equation for this potential can be solved in exact form and, for $\alpha = 1$, the energy values are given by [32]

$$E = -\frac{1}{2m}\left[\left(2mv + \frac{1}{4}\right)^{1/2} - \left(n + \frac{1}{2}\right)\right]^2, \tag{A.9}$$

where $n = 1,\ 2,\ 3,\ \ldots$ labels the sequence of discrete eigenvalues. Also the potential (A.8) is the special case (with $v_2 = 0$) of the Rosen–Morse potential [53]

$$V(r) = -v_1\,\mathrm{sech}^2\,\alpha r + v_2 \tanh \alpha r, \tag{A.10}$$

where v_1 and v_2 are the depth of the potential and α is the range of the potential. The Rosen–Morse potential plays a fundamental role in atomic, chemical and molecular physics, since it can be used to describe molecular vibrations and to obtain the energy spectra of linear and nonlinear systems. This potential is very useful for describing the interatomic interaction of linear molecules and is helpful for describing polyatomic vibration energies including the vibration states of the NH_3 molecule.

A.5 Soft–core Coulomb potential

Another family of potentials which is useful as model potentials in atomic and molecular physics is the family of the soft–core (truncated) Coulomb potentials [54, 55]

$$V(r) = -\frac{v}{(r^q + \beta^q)^{1/q}}, \tag{A.11}$$

where $v > 0$ is the coupling parameter, $\beta > 0$ is the cutoff parameter, and $q \geq 1$ is the power parameter. For $\beta > 0$, the potential is not singular as $r \longrightarrow 0$.

The specific potential corresponding to the power parameter $q = 1$ is called the cutoff Coulomb potential and given by [56]

$$C(r) = -\frac{u}{r + b}, \tag{A.12}$$

with the coupling $u > 0$ and cutoff parameter $b > 0$. $C(r)$ is an approximation to the potential due to a smeared charge distribution, rather than a point charge, and is appropriate for describing mesonic atoms [57]. The eigenvalues of the Schrödinger equation generated by the cutoff Coulomb potential has been studied by many authors who tried to estimate them. For instance, in [56] the simple formulas for upper and lower energy bounds for all the energy eigenvalues by the potential envelope method have been obtained. In [58] the method of the large–N expansion to approximate the bound state energies from $n = 1$ to $n = 4$ has been applied. And in [57] the authors analyzed in detail the S–wave bound–state eigenvalues of this potential as a function of b.

If $q = 2$, we obtain the laser–dressed Coulomb potential, which can be treated as an approximate stationary potential describing energy levels of the hydrogen atom in the electromagnetic wave field. However, the approximation has no bearing on the laser field strength and consequently the laser–dressed Coulomb potential potential is suitable for the description of an atom under either an intense or a weak laser field. This potential is given by [59, 60]

$$L(r) = -\frac{l}{(r^2 + \lambda^2)^{1/2}}, \tag{A.13}$$

where the coupling l is positive, and $\lambda > 0$ is the truncation parameter which is related to the strength of the irradiating laser field and has the range $\lambda = 20 - 40$ covering the experimental laser field strengths [61]. The parameter λ is related to the laser frequency $\omega(\mathrm{s}^{-1})$ and intensity $I(\mathrm{W\ cm}^{-2})$ by $\lambda = 6.5 \times 10^{24}\omega^{-2}I^{1/2}$ [59].

A.6 Woods–Saxon potential

The potential, which is a compromise between square well and harmonic oscillator potential, is

$$V(r) = -\frac{w}{1 + e^{\frac{r-R}{a}}}. \tag{A.14}$$

This potential is known as Woods–Saxon potential [62, 63]. In (A.14), w represents the potential well depth, a is a length representing the "surface thickness" of the nucleus, and $R = r_0 A^{1/3}$ is the nuclear radius where $r_0 = 1.25$ fm and A is the mass number.

The Woods-Saxon potential is a mean field potential for the nucleons (protons and neutrons) inside the atomic nucleus, which is used to describe approximately the forces applied on each nucleon, in the shell model for the structure of the nucleus. Typical values for the parameters are: $w \approx 50$ MeV, $a \approx 0.5$ fm. For large mass number A, this potential is similar to a potential well, because it is approximately flat in the center. It is monotonically increasing with distance, i.e. attracting. When using the Schrödinger equation to find the energy levels of nucleons subjected to the Woods Saxon potential, the problem cannot be solved analytically, and must be treated numerically.

A.7 Yukawa potential

Many properties of nuclear forces can be explained quantitatively by the potential proposed by Yukawa in 1939 [64]:

$$V(r) = -\frac{a}{r} e^{-\lambda r}, \tag{A.15}$$

with a the coupling constant and $\lambda = 1/r_0$, where the range r_0 of the force is the Compton wavelength $\hbar/\mu c$ of the exchanged particle of mass μ. Yukawa noticed that the range of nuclear forces $r_0 \approx 1.4$ fm corresponds to the exchange of a particle of mass $\mu \approx 140$ MeV. This is how he predicted the existence of the π meson[1].

As the mass μ of the exchange particle approaches zero, the exponential term goes to one, and the Yukawa potential becomes equivalent to a Coulomb potential, and the range is said then to be infinite.

---

[1] For this insight, Hideki Yukawa received the 1949 Nobel Prize in Physics.