EXACT, AND APPROXIMATE SOLUTION OF THE DIRAC EQUATION IN THE PRESENCE OF THE MAGNETIC FIELD WITH VARIOUS POTENTIALS

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ABSTRACT

EXACT, AND APPROXIMATE SOLUTION OF THE DIRAC EQUATION IN THE PRESENCE OF THE MAGNETIC FIELD WITH VARIOUS POTENTIALS

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Dirac equation has been studied for many years and its role in modeling physical problems is well known. In particular, Dirac equation is useful to describe properties of the spin 1/2 particles. Therefore the study of the Dirac equation has considerable impact on physics.

On the other hand the study of position dependent mass Schrödinger equation has recently attracted some interest arising from the study of the electronic properties of the semiconductors, quantum dots etc.

In this thesis, the solution of the Dirac equation and transmission probabilities of the scattering problem with a position dependent mass are studied. Thus this work consists of two parts. In the first part, exact solvability of the position dependent mass Schrödinger equation including a constant potential has been discussed and calculations of the transmission coefficients for various spatially varying effective masses have been represented. The second part covers the construction and solution of the Dirac equation including various potentials in the presence of the magnetic field. The ultimate goal of the models developed in this thesis is that the solution of the effective mass Dirac equation with constant potential.

Key words: Dirac equation, (Quasi) exactly solvable potentials

ÖZET

MANYETİK ALAN VE ÇEŞİTLİ POTANSİYELLER İÇEREN DIRAC DENKLEMİNİN TAM VE YAKLAŞIK ÇÖZÜMÜ

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Yıllardır üzerinde çalışılan Dirac denklemin modellenen fiziksel problemlerdeki rolü iyi bilinmektedir. Özellikle, parçacıkların spinlerinin özelliklerinin tanımlanması dirac denklemi ile açıklanmaktadır. Bundan dolayı dirac denkleminin çalışmaları fizikte önemli etkiye sahiptir.

Diğer taraftan yarı iletkenlerin, kuantum noktaların elektronik özelliklerin çalışmalarından, son zamanlarda konuma bağlı kütle Schröndinger denklemi ilgi çekmektedir.

Bu tezde, Dirac denkleminin çözümü ve konuma bağlı kütle ile iletim olasılığı üzerinde çalışıldı. Bundan dolayı bu çalışma iki bölümden oluşmaktadır. İlk bölümde, sabit potansiyel içeren konuma bağlı Schrödinger denkleminin tam çözülebirliği tartışıldı ve çeşitli değişken etkin kütlelerin iletim katsayılarının hesaplamaları yapıldı ve gösterildi. İkinci bölüm manyetik alan ve çeşitli potansiyeller içeren Dirac denkleminin oluşturulması ve çözümünden oluşmaktadır. Bu tezde geliştirilen modellerin son amacı sabit potansiyele sahip etkin kütle dirac denkleminin çözümüdür.

Anahtar kelimeler: Dirac denklemi, (Kısmi) tam çözülebilen potansiyeller

To Eslem

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LIST OF SYMBOLS

$[.,.]$: Commutator

$\sigma_{\pm,0}$: Standard Pauli Matrices

m : Mass of electron

m^* : Effective mass of electron

$m(x)$: Position dependent mass

E : Energy of particle

$S(x)$:Lorentz Scalar

R : Reflection coefficients

T : Transmission coefficients

$\hbar$:Planck constant

c :Speed of light

p :Momentum operator

A :Vector Potential

B :Magnetic field

α, β :The 4×4 Dirac matrices

$W(r)$:Super potential

$V_{\pm}(r)$:Partner potential

ω_L :Larmor frequency

ψ :Wave function

ϕ :Wave function

φ :Wave function

$\beta_{\gamma i}$:Pauli spin matrices

δ :Length of scale parameter

$m_{a,b,c,d}$:Mass barriers

NR :Non-relativistic

R :Relativistic

CHAPTER 1

INTRODUCTION

The Dirac equation is a relativistic quantum mechanical wave equation invented by Paul Dirac in 1928. It provides a description of elementary spin 1/2 particles, such as electrons, that is fully consistent with the principles of quantum mechanics and largely consistent with the theory of special relativity. It also accounts in a natural way for the nature of particle spin and the existence of antiparticles. Actually, the equation applies to other types of elementary spin 1/2 particles, such as neutrinos. A modified Dirac equation can be used to approximately describe protons and neutrons, which are made of smaller particles called quarks and therefore not elementary particles. The Dirac equation describes the probability amplitudes for a single electron. This single-particle theory gives a fairly good prediction of the spin and magnetic moment of the electron and explains much of the fine structure observed in atomic spectral lines. It also makes the peculiar prediction that there exists an infinite set of quantum states in which the electron possesses negative energy. This strange result led to predict, via a remarkable hypothesis known as " hole theory ", the existence of particles behaving like positively-charged electrons. This prediction was verified by the discovery of the positron in 1932. Despite these successes, the theory is flawed by its neglect of the possibility of creating and destroying particles, one of the basic consequences of relativity. This difficulty is resolved by reformulating it as a quantum field theory. Adding a quantized electromagnetic field to the this theory leads to the modern theory of quantum electrodynamics (QED).

In this thesis, before going further, we discuss the solution of the $(2+1)$-dimensional (2 dimensions of space and 1 dimension of time) Dirac equation have great importance of physical systems because of the rapid growth in nanofabrication technology that has made possible to confine laterally two-dimensional (2D) electron systems. These quantum confined electron systems are referred to as artificial atoms where the potential of the nucleus, in the non relativistic case, is replaced by an effective potential of the form $V = \frac{1}{2}r^2$ which is often used as realistic approximation[1-3]. The parabolic potential appears to be a good approximation for artificial atom structures but their modeling with various potential profiles will be interesting from the theoretical point of view as well as from its practical applications.

Dirac equation including adequate potentials is constructed to analyze relativistic effects on the spectrum of such physical systems and obtained its solution. In the relativistic case, the spectrum and properties of such systems can be determined by using two dimensional Dirac oscillator [3-5]. Relativistic extensions of the various exactly and quasi-exactly solvable (QES) potentials have also turned out to be of importance in the description of 2D phenomena and different condensed matter physics phenomena point to the existence of $(2+1)$ (2 dimensions of space and 1 dimension of time) dimensional systems whose spectrum determined by Dirac equation Hamiltonian including various potentials. As far as we know, the Dirac equation is exactly solvable only in a very restricted potentials. Our aim is to construct a Dirac equation including a class of potentials whose spectrum can exactly be determined. We transform the Dirac equation into two Schrödinger-like equation, few electron systems, most of which are tackling the problem in the framework of the Schrödinger-like equation.

We use functional approach which have been applied to solve Schrödinger equation for a exactly or QES potential profile. These are

(1) Exactly-solvable potentials: Harmonic oscillator, Coulomb Potential, Morse potential.

(2) Quasi-exactly solvable potentials: Anharmonic Oscillator Potential, Sextic Oscillator Potential, Deformed Coulomb potential.

For a QES potential it is possible to determine algebraically a part of spectrum but not whole spectrum[6-8]. Our approach also gives a hint to the solution of the problem in the framework of the SUSYQM.

The study of position dependent mass (PDM) physical systems has recently attracted a great interest arising from the study of electronic properties of semiconductors, quantum dots, liquid crystals, non-uniform materials etc. in which carrier effective mass depends on the position. Therefore solutions of the Schrödinger equations with a position-dependent mass (PDM) plays an important role in many physical problems. They appear in the energy-dependent functional approach to quantum many-body systems (e.g., nuclei, quantum liquids, ^{3}He clusters, metal clusters) and are very useful in the description of electronic properties of condensed-matter systems (e.g., compositionally-graded crystals, quantum dots, liquid crystals). The PDM presence may also reflect other unconventional effects, such as deformation of the canonical commutation relations or curvature of the underlying space or else pseudo-Hermiticity of the Hamiltonian.

Several exactly solvable, quasi-exactly solvable or conditionally exactly solvable PDM Schrödinger equations have been constructed using point canonical transformations, Lie algebraic methods or supersymmetric quantum mechanical (SUSYQM) and shape-invariance (SI) techniques . Most of them can be obtained from known constant-mass models by changes of variable and of function. As a consequence the spectrum is left unchanged although the potential is given by a complicated mass-deformed expression.

One dimensional quantum wells (QW) and their analysis have played an increasingly significant role in various applications as well as the understanding of the properties of a variety of semiconductor devices[9-12]. QW with very thin layers observes in the nanofabrication of semiconductor devices[13]. The effective mass of an electron(hole) in the thin layered QW varies with the composition rate. This systems, the mass of the electron may change with the composition rate which depends on the position. Because of this, the corresponding Schrödinger equation should be formulated in a correct form. Exact and quasi-exact solvability of the position dependent mass (PDM) Schrödinger equation has been the subject of recent interest[14-22]. This provides a useful model for the description of many physical systems [23-27]. The general solution has not yet been completed for square well potentials, although it has been solved for a number of potentials and masses.

As well as purely scientific interest, potential device applications provide the motivation for studies of the nature of the transport properties of the PDM electron through the barriers or wells. For realistic transport properties in semiconductors, the usual Schrödinger equation has to be replaced by the more general equation [28]. The abrupt heterostructures have been proven [26] that for sharp heterostructures ; otherwise the wavefunction is forced to vanish at the heterojunction boundary which is clearly an unphysical result.

Although the solution of the PDM Schrödinger equation include potentials like Coulomb, Morse, harmonic oscillator [29-32], the study of the PDM Schrödinger equation including a constant potential has not attracted much attention in the literature. This quantum systems have been found to be useful in the study of electronic properties of semiconductors. Generally, analysis of the scattering problem with PDM is based on the investigation of the simple problems. It was pointed out that the transmission probability no longer tends to unity when incoming energy goes to infinity.

When the system includes effective or position dependent mass, the usual Schrödinger equation has to be replaced by the more general equation [28]:

$$\left(\frac{1}{4}\left(m^{\alpha}pm^{\beta}pm^{\gamma}+m^{\gamma}pm^{\beta}pm^{\alpha}\right)+V\left(z\right)-E\right)\psi\left(z\right)=0$$

with the constraint over the parameters: $\alpha + \beta + \gamma = -1$. In applications, the spatial variation of m is either neglected, or, various special cases of have appeared in the literature. For instance, for abrupt heterostructures, it has been proven that $\alpha = \gamma$; otherwise the wavefunction is forced to vanish at the heterojunction boundary, which is clearly unphysical results. Although it has been solved for a large class of potentials by different methods [14-19,22,29,32-34], the ordering ambiguity of the mass and momentum operators have not yet been decided. Its effect on the exact solutions was systematically discussed in [20]. When the problem is formulated with Dirac equation the ordering ambiguity of the mass and momentum can be eliminated [35].

The practical feasibility of tunneling of relativistic particles through one-dimensional quantum well (QW) heterostructures has attracted considerable attention because of its possible application to ultra-high-speed electronic devices [36]. The motivation for studying those QW heterostructures is related to the recent developments in nanofabrication of semiconductor devices [9].

The properties of the electron (or hole) in the QW were studied usually in the context of the non-relativistic quantum mechanics by using various methods [37], to derive its energy levels and wave functions. Non-relativistic effective mass theory is a powerful and convenient method for obtaining information about the properties of semiconductors. Although it has been successful for predicting electronic and optical properties of the semiconductor heterostructures, in particular for ultra-high-speed electronic devices it needs relativistic corrections. Therefore, it is reasonable to model the physical systems including effective mass instead of Schrödinger equation, with another equation that represents the same physics as the Schrödinger equation in the low energy limit. As it is expected the corresponding equation is the *Dirac equation* in $(1+1)$ (1 dimensions of space and 1 dimension of time) dimensions. The applicability of the Dirac equation to investigate properties of the ultra-high-speed effective mass electron in QW. There are some advantages of Dirac Equation: the physical systems such as semiconductors [9] , quantum wells and dots [38] , quantum liquids [39] , graded alloys and heterostructures [40] found application in the framework of effective mass or position dependent mass Schrödinger equation.

There are a few attempts on the relativistic extension of the condensed matter problems. Recently some solid state problems were studied by using numerical methods [41] and it is applied to the Wood-Saxon potential to derive the conditions for the transmission resonance [42], and other properties of a relativistic particle in a one dimensional periodic structure have been investigated in [43]-[45]. A method for constructing exactly solvable position dependent mass relativistic particles has recently been proposed [46].

In this thesis, we deal exact and approximate solution of the Dirac equation in the presence of the magnetic field with various potentials. The structure of the study is organized as follows.

In the next chapter, we will give basic properties of the dirac equation. We briefly discuss construction of the dirac equation. We demonstrate its solution for spin 1/2 free particle.

Chapter 3 deals with introducing $(2+1)$ (2 dimensions of space and 1 dimension of time) dimensional Dirac equation and using the structures worked for the Dirac oscillator we develop a method to construct a class of exactly and QES potential profile. We transform the Dirac equation into the form of the Schrödinger equation and construct a Dirac equation including, harmonic oscillator, Coulomb and Morse potentials. Then we obtain the corresponding eigenvalues and eigenfunctions. Finally a class of QES potentials are constructed and their ground state wave functions are explicitly determined.

In Chapter 4, we discuss the construction of the Dirac sextic oscillator in polar coordinate in the presence of magnetic field. Then we solve the Dirac sextic oscillator in the context QES problem which possesses hidden sl_2-algebra.

In Chapter 5, we outline a specific formulation of the exactly solvable PDM Schrödinger equation to derive a general expression for the transmission amplitude of the wave through the square barrier. Then we apply our model to calculate the transmission coefficient of the wave through the barrier for various spatially varying effective masses.

In Chapter 6, we suggest a model of in order to obtain transmission coefficients of the position dependent mass particle through a potential well. We have shown that the model can be applicable for semiconductor heterostructures and ultra-high speed position dependent mass electrons in QW. We mention here that our model eliminate ordering ambiguity of the mass and position.

Possible generalizations of the model are discussed in chapter .

CHAPTER 2

DIRAC EQUATION

The relativistic quantum mechanical wave equation invented by Paul Dirac in 1928 is called Dirac equation. It is a useful equation to describe elementary spin-1/2 particles which is fully consistent with the principles of quantum mechanics and largely consistent with the theory of special relativity, such as electrons, positrons, neutrons etc. Additionally, this equation is required for the nature of particle spin and existence of antiparticles.

It also describes the probability amplitudes for a single electron.This single-particle theory gives a fairly good prediction of the spin and magnetic moment of the electron and explains much of the fine structure observed in atomic spectral lines. Additionally, it makes the peculiar prediction that there exists an infinite set of quantum states in which the electron possesses negative energy.

Because the Dirac equation was originally invented to describe the electron, here we will mention about "electrons". Actually, the equation applies to other types of elementary spin-1/2 particles, such as neutrinos. A modified Dirac equation can be used to approximately describe protons and neutrons, which are made of smaller particles called quarks and are therefore not elementary particles.

2.1 Construction of Dirac Equation for free particle

Lets attempt to derive a relativistic equation describing the electron, rather than starting from a non-relativistic equation and adding perturbations. As our starting point, we note that the non-relativistic Schrödinger equation, can be written in the form

$$i\hbar\frac{\partial}{\partial t}\psi = \frac{1}{2m}p^2\psi + \frac{e\hbar}{2m}(\sigma.B)\psi \tag{2.1}$$

where we have used the notation $p \to p + eA$ .There is a clever way to rewrite the two magnetic terms. Consider the following combination, which we work to simplify

$$\begin{aligned} [\overrightarrow{\sigma}.\overrightarrow{p}]^2 &= \sum_i \sigma_i p_i \sum_j \sigma_j p_j = \sum \left(\delta_{ij} + i \sum_k \varepsilon_{ijk} \sigma_k \right) p_i p_j \\ &= \overrightarrow{p}^2 + i \sum_{ijk} \varepsilon_{ijk} \sigma_k p_i p_j = \overrightarrow{p}^2 + i\sigma_x [p_y, p_z] + i\sigma_y [p_z, p_x] \\ & +i\sigma_z [p_x, p_y] \end{aligned} \tag{2.2}$$

where

$$\delta_{ij} = \begin{cases} 0 & for\ i \neq j \\ 1 & for\ i = j \end{cases}$$

$$\varepsilon_{ijk} = \begin{cases} 0 & for\ i = j = k \\ +1 & for\ (i, j, k) \in \{(1,2,3),\ (2,3,1),\ (3,1,2)\} \\ -1 & for\ (i, j, k) \in \{(1,3,2),\ (3,2,1),\ (2,1,3)\} \end{cases}$$

Pauli matrices σ satisfy the following identity $\sigma_i \sigma_j .= \delta_{ij} + i \sum_k \varepsilon_{ijk} \sigma_k$. They can be expressed in matrix form

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

When we first studied magnetic fields, we showed that

$$i [p_y, p_z] = e\hbar B_x, \qquad i [p_z, p_x] = e\hbar B_y, \qquad \text{and} \quad i [p_x, p_y] = e\hbar B_z \tag{2.3}$$

using these identities, we see that

$$[\sigma.p]^2 = p^2 + e\hbar\sigma.B \tag{2.4}$$

This allows us to rewrite the non-relativistic Schrödinger equation in the form the electromagnetic terms is dropped to help simplify our understanding. If we look at the remaining equation, we see that we have

$$i\hbar \frac{\partial}{\partial t} \psi = \frac{1}{2m} (p.\sigma)^2 \psi \tag{2.5}$$

If we interpret this classically, we see that for a plane wave, we have something like

$$E = \frac{1}{2m} (p.\sigma)^2 = \frac{p^2}{2m} \tag{2.6}$$

This is, of course, a non-relativistic equation. We would prefer to have something like the corresponding relativistic equation, namely,

$$E^2 = p^2 c^2 + m^2 c^4 \tag{2.7}$$

This suggests the following form for our equation:

$$\left(i\hbar\frac{\partial}{\partial t}\right)^2 \phi = c^2 \left(p.\sigma\right)^2 \phi + m^2c^4\phi \tag{2.8}$$

The wave function is changed from ψ to ϕ temporarily. This equation will turn out to not be exactly what we need. The problem is that it is second order in time. This violates certain basic assumption of quantum mechanics; for example, that the future of the wave function $\phi(r,t)$ depends only on the value $\phi(r,t=0)$ of the wave function at $t=0$, and not on its time derivative $\dot{\phi}(r,t=0)$.

To attempt to remedy this problem, we first bring the first operator on the right to the left side, and then we factor the difference of squares to give

$$\left(i\hbar\frac{\partial}{\partial t} + cp.\sigma\right)\left(i\hbar\frac{\partial}{\partial t} - cp.\sigma\right)\phi = m^2c^4\phi \tag{2.9}$$

Now, to eliminate the second order equation, we define a second field φ as

$$\left(i\hbar\frac{\partial}{\partial t} - cp.\sigma\right)\phi = -mc^2\varphi \tag{2.10}$$

Plugging this into our second order differential equation, we see that

$$\left(i\hbar\frac{\partial}{\partial t} + cp.\sigma\right)\varphi = -mc^2\phi \tag{2.11}$$

At present, these two equations are treated as if the first were a definition and the second derived. Think of both ϕ and φ as the given wave function, then we have two coupled differential equations for ϕ and φ . Because each of these equations is only first order in time, specifying the initial conditions for both ϕ and φ will completely determine both wave functions at future times.

To get the complete Dirac equation, we now simply combine these two equations into a single equation as follows. First we write them together like this:

$$\left[i\hbar\frac{\partial}{\partial t} - c\begin{pmatrix}\sigma & 0\\ 0 & -\sigma\end{pmatrix}.p\right]\begin{pmatrix}\phi\\ \varphi\end{pmatrix} = mc^2\begin{pmatrix}0 & -1\\ -1 & 0\end{pmatrix}\begin{pmatrix}\phi\\ \varphi\end{pmatrix} \tag{2.12}$$

We now define a four-component wave function ψ and some new matrices as follows:

$$\psi = \begin{pmatrix}\phi\\ \varphi\end{pmatrix}, \qquad \alpha = \begin{pmatrix}\sigma & 0\\ 0 & -\sigma\end{pmatrix}, \qquad \text{and} \quad \beta = \begin{pmatrix}0 & -1\\ -1 & 0\end{pmatrix} \tag{2.13}$$

the Dirac equation is

$$i\hbar\frac{\partial}{\partial t}\psi = c\alpha.p\psi + mc^2\beta\psi \tag{2.14}$$

So our relativistic Hamiltonian is given by

$$H = c\alpha.p + mc^2\beta \tag{2.15}$$

It is a good time to stop for a moment and consider the properties of the matrices α and β . They are all 4×4 Hermitian matrices, and the square of any of them is equal to one. They anticommute with each other as well. So we have

$$\begin{aligned} &\beta^\dagger = \beta, \qquad \alpha^\dagger = \alpha, \qquad \beta^2 = \alpha_i^2 = 1, \\ &\beta\alpha_i + \alpha_i\beta = 0 = \alpha_i\alpha_j + \alpha_j\alpha_i \qquad \text{if } i \neq j. \end{aligned} \tag{2.16}$$

It turns out that these properties of the α and β matrices are all you actually ever need to perform calculations. Indeed, any set of 4×4 matrices with these properties can be shown to lead to the same solutions. They differ only in that the different components of ψ will be mixed up with each other.

2.2 Solution of Dirac Equation for free particle

It is possible to get explicit solutions to the Dirac Equation. For plane wave solutions, which take the form

$$\psi = \psi_0 e^{i(p.r - Et)/\hbar} \tag{2.17}$$

Plugging this into the Dirac equation, we find

$$E\psi_0 = (c\alpha.p + mc^2\beta)\psi_0 \tag{2.18}$$

The easiest way to proceed is to let the Hamiltonian act again on both sides of the equation.

$$E^2\psi_0 = (c\alpha.p + mc^2\beta)^2\psi_0 \tag{2.19}$$

Now, the complicated expression on the right can be vastly simplified. Because all four matrices anti-commute, the cross-terms will all vanish. Because all the matrices squared are one, this simplifies to

$$E^2\psi_0 = (c^2p^2 + m^2c^4)\psi_0 \tag{2.20}$$

This leads to the following equation:

$$E = \pm\sqrt{c^2p + m^2c^4} \tag{2.21}$$

This is exactly the equation we want to except for the $\pm$ symbol. Indeed, if you study the equation more carefully, you will find that there are two solutions with positive energy, and two with negative energy, for each momentum p. The two positive energy states correspond to the two spin states of the electron, but what are we to make of the negative energy states? Dirac came up with a solution. By the time he came up with this theory, the Pauli exclusion principle was already understood, and Dirac proposed that the negative energy solutions, since they had negative energy, were already "filled up" with negative energy electrons (figure 2.1). As a consequence, any electrons that are around cannot fall into these negative energy states. The assumption here is that "empty" space is filled with countless negative electron states, and we don't notice them because that is the natural state of empty space.

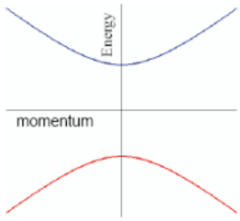

Figure 2.1: *The energy as a function of momentum for electrons. The lower curve represents the negative energy states, which Dirac assumed were all filled quantum states.*

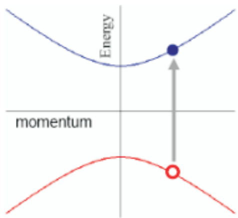

Figure 2.2: *When a negative energy electron is bumped up to a positive energy state, it creates an electron, and leaves behind a "hole" with positive charge and positive energy, which we call a positron.*

Now, the some energy is taken and use it to bump one of our negative energy electrons up to a positive energy state. The positive energy electron looks like an electron. But there is also the "hole" left over from the missing electron (figure 2.2).We would perceive this hole as an absence of negative energy (which means positive energy) with an absence of negative charge (which means positive charge). We would perceive the hole as a particle with the same rest mass as the electron, but with a positive charge. This particle is the positron. The Dirac equation predicts the existence of positrons.

In this chapter we have given basic properties of the Dirac equation for free particle. In the following chapter we will discuss solution of the Dirac equation including various potentials.

CHAPTER 3

DIRAC EQUATION INCLUDING VARIOUS POTENTIALS

In order to analyze relativistic effects on the spectrum of such physical systems one should construct Dirac equation including adequate potentials and obtain its solution. For the relativistic case, the spectrum and properties of such systems can be determined by using two dimensional Dirac oscillator [3-5]. Relativistic extensions of the various exactly and quasi-exactly solvable (QES) potentials have also turned out to be of importance in the description of 2D phenomena [47-51]. Different condensed matter physics phenomena point to the existence of $(2+1)$ dimensional systems whose spectrum determined by Dirac equation Hamiltonian including various potentials. It is well known that the dirac equation is used for the description of spin-1/2 relativistic particle. Meanwhile we mention here that the Hamiltonian in the form of the Klein-Gordon equation, so called Feshbach-Villars equation, has been constructed in a two component form for spinless particles [52] and in an eight-component form for spin-1/2 particles [53-55]. Regrettably, the Dirac equation is exactly solvable only in a very restricted potentials. It is the purpose of the present thesis to construct a Dirac equation including a class of potentials whose spectrum can exactly be determined. For this purpose we transform the Dirac equation into two Schrödinger-like equation, few electron systems, most of which are tackling the problem in the framework of the Schrödinger-like equation. A Dirac equation with an interaction linear in coordinates was considered long ago [56] and recently rediscovered in the context of the relativistic many body theories [57] .The equation is named Dirac oscillator, since in the non-relativistic limit it becomes a harmonic oscillator with a very strong spin-orbit coupling term. Dirac oscillator has attracted much attention [6,58-64]. Analogous to the Dirac equation, with a modified momentum operator,which in the non-relativistic limit turns out be the usual Schrödinger equation. As we have already noted the Dirac equation including various potentials might attract much attention because it may have some physical applications, particularly in the condensed matter physics. It seems that one can present more realistic models for the artificial atoms using the procedure given here.

3.1 Construction of Potentials

The (2+1)-dimensional Dirac equation for free particle of mass m in terms of two-component spinors ψ, can be written as

$$E\psi = \left[\sum_{i=1}^{2} c\beta\gamma_i p_i + \beta mc^2\right]\psi \tag{3.1}$$

Since we are using only two component spinors, the matrices β and $\beta_{\gamma i}$ are conveniently defined in terms of the Pauli spin matrices which satisfy the relation $\sigma_i\sigma_j = \delta_{ij} + \varepsilon_{ijk}\sigma_k$, given by

$$\beta\gamma_1 = \sigma_1; \qquad \beta\gamma_2 = \sigma_2; \qquad \beta = \sigma_3. \tag{3.2}$$

In $(2+1)$-dimensions, the momentum operator p_i is two component differential operator, $p = -i\hbar(\partial_x, \partial_y)$, for free particle. In the presence of the magnetic field it is replaced by $p \to p - eA$, where A is the vector potential, and the 2D Dirac oscillator can be constructed by changing the momentum $p \to p - im\omega\sigma_3 r\widehat{r}$. We are now seeking for a certain form of the momentum operator that can be interpreted as exactly solvable Schrödinger equation in the non-relativistic limit. For this purpose we introduce the following momentum operator

$$p \to p - eA + i\sigma_3 v(r)\widehat{r}. \tag{3.3}$$

Then Dirac equation (3.1) with the momentum operator (3.3) takes the form

$$\begin{aligned}\left[E - \sigma_0 mc^2\right]\psi = c\sigma_+\left[p_x + ip_y - e(A_x + iA_y) - i(v_x + iv_y)\right]\psi \\ + c\sigma_-\left[p_x - ip_y - e(A_x - iA_y) + i(v_x - iv_y)\right]\psi\end{aligned} \tag{3.4}$$

$$\sigma_+ = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}, \qquad \sigma_- = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}$$

where p_i, A_i, and v_i are the i^{th} components of the momentum, vector potential and the potential in Cartesian coordinate system, respectively. In polar coordinate, $x = rcos\phi$, $y = rsin\phi$, with the choices of the vector potential $A_x = -A(r)sin\phi$, $A_y = A(r)cos\phi$ and the potential $v_x = v(r)cos\phi$, $v_y = v(r)sin\phi$ the 2D Dirac equation (3.4) takes the form

$$E_-\psi_+ = ce^{i\phi}\left[-i\hbar\frac{\partial}{\partial r} + \frac{\hbar}{r}\frac{\partial}{\partial\phi} - i(eA(r) + v(r))\right]\psi_- \tag{3.5}$$

$$E_+\psi_- = ce^{-i\phi}\left[-i\hbar\frac{\partial}{\partial r} - \frac{\hbar}{r}\frac{\partial}{\partial\phi} + i(eA(r)+v(r))\right]\psi_+ \tag{3.6}$$

where $E_\pm = E \pm mc^2$ and $\psi_\pm = \psi_\pm(r,\phi)$ are the upper and lower components of the spinor ψ. The substitution of the wave functions

$$\psi_\pm(r,\phi) = \frac{e^{-i(\ell\mp\frac{1}{2})\phi}}{\sqrt{r}} f_\pm(r) \tag{3.7}$$

leads to the following set of coupled differential equations

$$E_- f_+(r) = -ic\left(\hbar\frac{\partial}{\partial r} + \frac{\hbar\ell}{r} + (eA(r)+v(r))\right) f_-(r) \tag{3.8}$$

$$E_+ f_-(r) = -ic\left(\hbar\frac{\partial}{\partial r} - \frac{\hbar\ell}{r} - (eA(r)+v(r))\right) f_+(r) \tag{3.9}$$

Our task is now to transform (3.8) and (3.9) in the form of the Schrödinger-like equation. Substitution of

$$W(r) = \frac{\ell}{r} + \frac{(eA(r)+v(r))}{\hbar}; \qquad E_\pm = \pm ic\hbar\varepsilon_\pm; \qquad \varepsilon^2 = \varepsilon_+\varepsilon_- \tag{3.10}$$

into (3.8) and (3.9), leads to the following expression

$$\varepsilon_- f_+(r) = \left(\frac{\partial}{\partial r} + W(r)\right) f_-(r) \tag{3.11}$$

$$\varepsilon_+ f_-(r) = \left(-\frac{\partial}{\partial r} + W(r)\right) f_+(r) \tag{3.12}$$

Notice that the result (3.11) and (3.12) which seem to hint at a supersymmetric treatment of the Dirac equation, because the supersymmetric operators can be expressed as $A^\pm = \left(\mp\frac{\partial}{\partial r} + W(r)\right)$. It is obvious that the functional form of the superpotential $W(r)$ and $v(r)$ are the same except that the radial function $\frac{\hbar\ell}{r}$. Thus the superpotential of the non-relativistic quantum mechanics can be recognized as the potential of the relativistic quantum mechanics. It is obvious that the expressions (3.11) and (3.12) can be written in the form of the Schrödinger-like equation, by eliminating $f_+(r)$ and/or $f_-(r)$ between (3.11) and (3.12) provides the following expressions

$$\left(-\frac{\partial^2}{\partial r^2} - W^2(r) + W'(r) + \varepsilon^2\right) f_-(r) = 0 \tag{3.13}$$

$$\left(-\frac{\partial^2}{\partial r^2} + W^2(r) + W'(r) - \varepsilon^2\right) f_+(r) = 0 \tag{3.14}$$

This is indeed an interesting result for the potentials $V_\pm = W^2(r) \pm W'(r)$ leading to a common spectrum, thus forming an isospectral system. In the following we analyze the solutions and the energy spectrum of the $(2+1)$-dimensional Dirac equation including various potentials.

3.2 Exactly Solvable Potentials

Appropriate choices of the superpotential $W(r)$ permits the construction of the equations having exactly solvable potentials. We illustrate that for a large class of potentials, the Dirac equation in the form of Schrödinger type equations of (3.13) and (3.14) possess exact solutions.

3.2.1 Harmonic Oscillator Potential

Let us start with the well known problem, namely Dirac oscillator. The Dirac oscillator can be constructed with the choices of the superpotential $W(r) = \frac{m}{\hbar}\omega_T r - \frac{\ell+1}{r}$. Thus, the Schrödinger type equations (3.13) and (3.14) takes the form:

$$\left(-\frac{\partial^2}{\partial r^2} + \frac{\ell(\ell+1)}{r^2} + \left(\frac{m}{\hbar}\omega_T\right)^2 r^2 + \frac{m}{\hbar}\omega_T(2\ell+3) - \varepsilon^2\right) f_-(r) = 0 \qquad (3.15)$$

$$\left(-\frac{\partial^2}{\partial r^2} + \frac{\ell(\ell+1)(\ell+2)}{r^2} + \left(\frac{m}{\hbar}\omega_T\right)^2 r^2 - \frac{m}{\hbar}\omega_T(2\ell+1) - \varepsilon^2\right) f_+(r) = 0 \quad (3.16)$$

In this case the vector potential $A(r)$ and scalar potential $v(r)$ are given by

$$A(r) = \frac{1}{2}Br, \qquad v(r) = \frac{m}{\hbar}wr - \frac{2\ell+1}{r}, \qquad (3.17)$$

and the frequency ω_T can be expressed in terms of the Larmor frequency as follows

$$w_T = w + w_L = w + \frac{eB}{2m} \qquad (3.18)$$

In order to solve (3.15), we change the variable $z = \frac{m}{\hbar}\omega_T r^2$, and introduce the wave function

$$f_-(z) = Cz^{\frac{\ell+1}{2}} e^{-\frac{z}{2}} g_-(z) \qquad (3.19)$$

where C is the normalization constant, then (3.15) takes the form:

$$\left[z\frac{\partial^2}{\partial z^2} + \left(\ell + \frac{3}{2} - z\right) + n\right] g_-(z) = 0 \qquad (3.20)$$

The natural number n and energy satisfy the relation

$$\varepsilon^2 = \frac{E^2 - m^2c^4}{\hbar^2 c^2} = 4n\frac{m}{\hbar}\omega_T \qquad (3.21)$$

Note that the non-relativistic limit of the energy is obtained by setting $E = E_{nr} + mc^2$ and considering $E_{nr} \ll mc^2$, we obtain the non relativistic energy

$$E_{nr} = 4n\hbar\omega_T$$

We now investigate the dependence of the energy on the spin. In order to analyze spin effects, it is worth to obtain non-relativistic form of the (3.15):

$$\left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial r^2}+\frac{\ell(\ell+1)\hbar^2}{2mr^2}+\frac{1}{2}m\omega_T^2r^2+\hbar\omega_T\left(\ell+\frac{3}{2}\right)-E_{nr}\right)f_-(r)=0 \quad (3.22)$$

The corresponding Hamiltonian is the Hamiltonian of a harmonic oscillator with an additional spin dependent term, $\hbar\omega_T\left(\ell+\frac{3}{2}\right)$. To complete our analysis we turn our attention to the normalization of the wave function. It is easy to see that the solution of (3.20) is the associated Laguerre polynomials, $L_n^{\ell+\frac{1}{2}}(z)$, then $f(z)$ can be written as

$$f_-(z)=Cz^{\frac{\ell+1}{2}}e^{-\frac{z}{2}}L_n^{\ell+\frac{1}{2}}(z) \quad (3.23)$$

The upper component, $f_+(z)$, of spinor $\psi(r)$, can be obtained from the relation (3.11) and it is given by

$$f_+(z)=-\frac{2C\sqrt{\omega_T}}{\varepsilon_-}z^{\frac{\ell+2}{2}}e^{-\frac{z}{2}}L_{n-1}^{\ell+\frac{3}{2}}(z)$$

Normalization condition in polar coordinate is given by

$$\langle\psi\psi\rangle=\int_0^\infty\left(|f_+(r)|^2+|f_-(r)|^2\right)dr=1 \quad (3.24)$$

Associated Laguerre polynomials satisfy the orthogonality condition:

$$\int_0^\infty z^\ell e^{-z}L_n^\ell(z)L_k^\ell(z)dr=\frac{\Gamma(n+\ell+1)}{n!}\delta_{nk} \quad (3.25)$$

Thus, we finally obtain an expression for the normalization constant C:

$$C=\left[\frac{\sqrt{\omega_T}\varepsilon_-^2\Gamma(n+1)}{(n\omega_T+\varepsilon_-^2\Gamma(n))\,\Gamma(n+\ell+\frac{3}{2})}\right]^{\frac{1}{2}} \quad (3.26)$$

We have solved Dirac oscillator in two dimensional space which leads to a series of interesting results. The Dirac oscillator has various physical applications particularly in semiconductor physics [65].

3.2.2 Coulomb Potential

Another well known examples of the exactly solvable Dirac equation is that relativistic Hydrogen atom. The problem can be solved exactly when the magnetic field is zero, $A(r)=0$ and in the presence of the Coulomb interaction [66, 67] $v(r)=\frac{me^2}{4\pi\varepsilon_0\hbar(\ell+1)}-\frac{\hbar(2\ell+1)}{r}$. In this case the superpotential is $W(r)=$

$\frac{me^2}{4\pi\varepsilon_0\hbar^2(\ell+1)} - \frac{(\ell+1)}{r}$, and then the Schrödinger-like equations (3.13) and (3.14) takes the form

$$\left(-\frac{\partial^2}{\partial r^2} + \frac{\ell(\ell+1)}{r^2} - \frac{me^2}{2\pi\varepsilon_0\hbar^2 r} + \left(\frac{me^2}{4\pi\varepsilon_0\hbar^2(\ell+1)}\right)^2 - \varepsilon^2\right) f_-(r) = 0 \tag{3.27}$$

$$\left(-\frac{\partial^2}{\partial r^2} + \frac{(\ell+1)(\ell+2))}{r^2} - \frac{e^2}{r} + \left(\frac{me^2}{4\pi\varepsilon_0\hbar^2(\ell+1)}\right)^2 - \varepsilon^2\right) f_+(r) = 0 \tag{3.28}$$

Following the similar developments used in the construction of the harmonic oscillator problem, the equation (3.27) can be transformed in the form:

$$\left[z\frac{\partial^2}{\partial z^2} + (2\ell + 2 - z) + n\right] g_-(z) = 0 \tag{3.29}$$

by changing the variable $r = 2\pi\varepsilon_0\hbar^2(n+\ell+1)z/me^2$ and the wave function

$$f_-(z) = Cz^{\ell+1}e^{-\frac{z}{2}}g_-(z) \tag{3.30}$$

Natural number n and energy of the Hamiltonian satisfy the relation

$$\varepsilon^2 = \frac{E^2 - m^2c^4}{\hbar^2c^2} = \left(\frac{me^2}{4\pi\varepsilon_0\hbar^2(\ell+1)}\right)^2 - \left(\frac{me^2}{4\pi\varepsilon_0\hbar^2(n+\ell+1)}\right)^2 \tag{3.31}$$

Solution of the (3.29) leads to the following expression for the wave function

$$f_-(z) = Cz^{\ell+1}e^{-\frac{z}{2}}L_n^{2\ell+1}(z) \tag{3.32}$$

and from the relation (3.11) we obtain

$$\begin{aligned} f_+(z) &= \frac{-C}{\varepsilon_-}z^{\ell+1}e^{-\frac{z}{2}} \\ &\left[2(\ell+1)L_{n-1}^{2\ell+2}(z) + (\ell+1-\frac{me^2}{2\pi\varepsilon_0\hbar^2}(2\ell+1))L_n^{2\ell+1}(z)\right] \end{aligned} \tag{3.33}$$

Using the identity

$$\int_0^\infty z^{\ell+1}e^{-z}L_n^\ell(z)L_n^\ell(z)dr = (2n+\ell+1)^{\ell+2}\frac{\Gamma(n+\ell+1)}{n!} \tag{3.34}$$

after some straight forward calculation we obtain the normalization constant

$$C = \left[\frac{2\pi\varepsilon_0\hbar^2}{me^2}\left(\frac{4(\ell+1)^2}{\varepsilon_-^2\Gamma(n)} + (2n+2\ell+2)^{2\ell+3}K\right)\Gamma(n+2\ell+2)\right]^{-\frac{1}{2}} \tag{3.35}$$

where K is given by

$$K = \left(1 + \frac{1}{\varepsilon_-^2 n!}\left(\ell+1-\frac{me^2}{2\pi\varepsilon_0\hbar^2}(2\ell+1)\right)^2\right) \tag{3.36}$$

Due to the recent interest in the 2D field theory in the condensed matter physics, the 2D Coulomb potential is physically relevant and the results obtained in 2D exhibit some new features [47, 68].

3.2.3 Morse Potential

The Morse oscillator is exactly solvable quantum mechanical problem and it is used to model the interaction of the atoms in the diatomic molecules. In order to obtain its relativistic form we apply the standard procedure. The choices of the parameters $v(r) = -\frac{\hbar\ell}{r} - \hbar a e^{-\alpha r} + \hbar b$, $A(r) = 0$ and $W(r) = b - ae^{-\alpha r}$, provides the following potential

$$\left(-\frac{\partial^2}{\partial r^2} + a^2 e^{-2\alpha r} - a\left(\alpha + 2b\right) e^{-\alpha r} + b^2 - \varepsilon^2\right) f_-\left(r\right) = 0 \tag{3.37}$$

$$\left(-\frac{\partial^2}{\partial r^2} + a^2 e^{-2\alpha r} + a\left(\alpha - 2b\right) e^{-\alpha r} + b^2 - \varepsilon^2\right) f_+\left(r\right) = 0 \tag{3.38}$$

In order to solve (3.37) we change the variable $e^{-\alpha r} = \frac{\alpha}{2a} z$ and then introduce the wave function

$$f_-\left(r\right) = z^{\frac{b}{\alpha} - n} e^{-\frac{z}{2}} g_-\left(z\right) \tag{3.39}$$

then we obtain

$$\left[z\frac{\partial^2}{\partial z^2} + \left(\frac{2b}{\alpha} - 2n + 1 - z\right) + n\right] g_-\left(z\right) = 0 \tag{3.40}$$

Energy expression for the Morse oscillator is given by

$$\varepsilon^2 = \alpha n\left(\alpha n - 2b\right)$$

The wave functions can be obtained from the equations (3.40) and (3.11) and are given by

$$f_-\left(r\right) = C z^{\frac{b}{\alpha} - n} e^{-\frac{z}{2}} L_n^{\frac{2b}{\alpha} - 2n}\left(z\right) \tag{3.41}$$

$$f_+\left(z\right) = \frac{C\alpha}{\varepsilon_-} z^{\frac{b}{\alpha} - n} e^{-\frac{z}{2}} \left[n L_n^{\frac{2b}{\alpha} - 2n}\left(z\right) + z L_{n-1}^{\frac{2b}{\alpha} - 2n + 1}\left(z\right)\right] \tag{3.42}$$

Normalization condition yields the following expression for the normalization constant

$$C = \left[\frac{\varepsilon_-^2 \Gamma\left(n\right) \Gamma\left(n-1\right)}{\Gamma\left(\frac{2b}{\alpha} + 1 - n\right)\left(\varepsilon_-^2 \Gamma\left(n\right) + 2\alpha^2 \Gamma\left(n+1\right)\right)}\right]^{-\frac{1}{2}} \tag{3.43}$$

The potentials we have derived here is significant from both physical and mathematical points of view. For instance, the relativistic quark model requires the solution of the dirac equation containing single quark potential. The potential behaving like r at a large distances and $1/r$ at a short distances has been recently treated by Muci [69]. We mention that the Morse oscillator potential can also be used as a large distance potential in some various physical systems. Consequently we have constructed relativistic version of the three well known potentials whose eigenfunctions are associated to the confluent hypergeometric functions. In the following section we construct QES potentials.

3.3 QES Potentials

In quasi-exactly solvable problems partial analytic solutions (energy spectrum and associated wavefunctions) are obtained if some potential parameters are assigned specific values. At this stage we mention that the underlying idea behind the quasi-exact solvability is the existence of a hidden algebraic structure. Our task is now to demonstrate by appropriate choices of relativistic potential we can construct QES Dirac equations. Our examples includes anharmonic oscillator potential, radial sextic oscillator potential and perturbed Coulomb potential.

3.3.1 Anharmonic Oscillator Potential

The anharmonic oscillator potential have been widely used in many physical and chemical applications. In order to construct anharmonic oscillator potential we introduce

$$v(r) = -\frac{\hbar\ell}{r} + \hbar\omega r + \hbar b r^2 + \hbar a; \quad A(r) = \hbar B r; \quad W(r) = a + \omega_T r + c r^2 \tag{3.44}$$

With these choices we obtain the following Schrödinger-like equations

$$\left(-\frac{\partial^2}{\partial r^2} + V_+ + \omega_T + a^2 + \varepsilon^2\right) f_+(r) = 0 \tag{3.45}$$

$$\left(-\frac{\partial^2}{\partial r^2} + V_- - \omega_T + a^2 + \varepsilon^2\right) f_-(r) = 0 \tag{3.46}$$

where $V_\pm$ are given by

$$V_\pm = 2(a\omega_T \pm b) r + \left(2ab + \omega_T^2\right) r^2 + 2b\omega_T r^3 + b^2 r^4 \tag{3.47}$$

and its ground state wave function is given by $f^{(0)}$

$$f_-^{(0)}(r) = \exp\left(-\frac{1}{3} b r^3 - \frac{1}{2}\omega_T r^2 - ar\right) \tag{3.48}$$

A part of the spectrum of the anharmonic oscillator potential can be obtained in the framework of the QES problem or its approximate solution can be obtained by using perturbation theory.

Another well known QES potential is the sextic oscillator potential. But we will see this at next chapter.

3.3.2 Deformed Coulomb Potential

Our last example is the deformed Coulomb potential which can be obtained by introducing

$$\begin{aligned} v(r) &= \frac{e^2}{2(\ell+1)} - \frac{\hbar(2\ell+1)}{r}; \quad A(r) = \hbar B r; \\ W(r) &= \frac{\varepsilon^2}{2(\ell+1)} - \frac{\ell+1}{r} \end{aligned} \tag{3.49}$$

In this case the equations take the forms

$$\left(-\frac{\partial^2}{\partial r^2}-\frac{(\ell+1)(\ell+2)}{r^2}+V_+-\omega_T(2\ell+1)\right.$$
$$\left.+\frac{e^4}{4(\ell+1)^2}+\varepsilon^2\right)f_+(r)=0 \tag{3.50}$$

$$\left(-\frac{\partial^2}{\partial r^2}-\frac{\ell(\ell+1)}{r^2}+V_--\omega_T(2\ell+3)+\frac{e^4}{4(\ell+1)^2}+\varepsilon^2\right)f_-(r)=0 \tag{3.51}$$

$$V_\pm=-\frac{e^2}{r}+\omega_T^2r^2+\frac{e^2\omega_T}{\ell+1}r+\frac{e^4}{4(\ell+1)^2} \tag{3.52}$$

Its ground state eigenfunction are given by

$$f_-^{(0)}=r^{\ell+1}\exp\left(-\frac{\omega_T}{2}r^2-\frac{e^2r}{2(\ell+1)}\right) \tag{3.53}$$

The non-relativistic two dimensional Hamiltonian described Coulomb interaction between charged particles, i.e. the interaction between conduction electron and donor impurity center when a constant magnetic field is applied perpendicular to the plane of motion has been discussed in the literature [66, 70, 71]. We have obtained relativistic interaction and it can be solved quasi-exactly. Recently its spectrum and wavefunction has been computed numerically [1].

We have obtained analytical solutions of the (2+1)- dimensional Dirac equation for a set of potentials in two dimensions with the hope that they could be useful in low dimensional field theory and condensed matter physics. The potentials for Dirac equation have been obtained by extending the notion of the Dirac oscillator. In the following chapter, we will construct the Dirac sextic oscillator.

CHAPTER 4

THE DIRAC SEXTIC OSCILLATOR

A Dirac equation with an interaction linear in coordinates was considered long ago [56] and recently rediscovered in the context of the relativistic many body theories [57]. The equation is named Dirac oscillator, since in the non-relativistic limit it becomes a harmonic oscillator with a very strong spin-orbit coupling term. Dirac oscillator has attracted much attention [6,58-64].

During the last years two-dimensional electron systems have become an active research subject due to the rapid growth in nanofabrication technology that has made possible to the production of low dimensional structures like quantum wells, quantum wires, quantum dots etc.[1, 2, 3]. In non-relativistic case, the two dimensional parabolic potential has often been used to describe the spectrum of the electron in confined two-dimensional systems. For the relativistic case, the spectrum and properties of the such systems can be determined by using two dimensional Dirac oscillator [3, 4, 5]. Despite their simplicity, both relativistic and non-relativistic oscillator potentials appear to be a good approximation to complicated low dimensional nanostructures.

In order to present a more realistic model we construct deformed form of the Dirac oscillator including a term qr^3. The Dirac oscillator with a deformed term becomes radial sextic oscillator potential in the non-relativistic limit. The non-relativistic sextic oscillator potential is quasi-exactly-solvable(QES) for which it is possible to determine algebraically a part of spectrum but not whole spectrum[6, 7, 8]. It will be shown that the solution of the relativistic sextic oscillator can also be treated in the context of the QES problem. We also investigate the effect of the magnetic field on the Dirac sextic oscillator. It will be shown that for a specific values of the magnetic field the Dirac sextic oscillator problem is exactly solvable.

4.1 Construction of the Dirac Sextic Oscillator

The (2+1)-dimensional Dirac equation for free particle of mass M in terms of two-component spinors ψ, can be written as equation (3.1). We introduce the following momentum operator

$$\mathbf{p} \to \mathbf{p} - i\sigma_3 \left(m\omega - qr^2\right) \mathbf{r} \tag{4.1}$$

where q is a constant and the Dirac equation takes the form

$$\begin{aligned} \left[E - \sigma_0 mc^2\right] \psi &= c\left[\sigma_+ \left(p_x - ip_y - i\left(M\omega - qr^2\right)(x - iy)\right)\right]\psi + \\ & c\left[\sigma_- \left(p_x + ip_y - i\left(M\omega - qr^2\right)(x + iy)\right)\right]\psi \end{aligned} \tag{4.2}$$

In polar coordinate, $x = r\cos\phi$, $y = r\cos\phi$, the $2D$ Dirac equation (4.2) can be written as

$$\begin{aligned} \varepsilon^2 \psi_1 &= -c^2\hbar^2 \left[\frac{\partial^2}{\partial r^2} + \frac{1}{r}\frac{\partial}{\partial r} + \frac{1}{r^2}\frac{\partial^2}{\partial \phi^2} + \frac{2i\left(M\omega - qr^2\right)}{\hbar}\frac{\partial}{\partial \phi}\right]\psi_1 \\ & +c^2\left(q^2 r^6 - 2M\omega q r^4 + \left(M^2\omega^2 - 4\hbar q\right) r^2 + 2\hbar M\omega\right)\psi_1 \end{aligned} \tag{4.3}$$

where $\psi_1 = \psi_1(r, \phi)$ is the upper component of the spinor ψ and $\varepsilon^2 = E^2 - M^2c^4$. The substitution of

$$\psi_1(r, \phi) = \frac{e^{-im\phi}}{\sqrt{r}} f(r) \tag{4.4}$$

leads to the following equation

$$\varepsilon^2 f(r) = -c^2\hbar^2 \frac{\partial^2 f(r)}{\partial r^2} + c^2\left[V(r) + 2\hbar M\omega(1 - m)\right] f(r) \tag{4.5}$$

where $V(r)$ is given by

$$V(r) = \frac{\hbar^2\left(m^2 - \frac{1}{4}\right)}{r^2} + q^2 r^6 - 2M\omega q r^4 + \left(M^2\omega^2 - 2\hbar q(2 - m)\right) r^2 \tag{4.6}$$

It is not difficult to see that in the non-relativistic limit (4.5) corresponds to the Schrödinger equation with radial sextic oscillator potential with a spin-orbit coupling term. In the presence of the symmetric gauge vector potential $A(x, y) = B/2(-y, x, 0)$, the potential (4.6) takes the form

$$\begin{aligned} V(r) &= \frac{\hbar^2\left(m^2 - \frac{1}{4}\right)}{r^2} + \hbar eB(m - 1) + q^2 r^6 - (2M\omega - eB) q r^4 + \\ & \left(\left(M\omega - \frac{eB}{2}\right)^2 - 2\hbar q(2 - m)\right) r^2 \end{aligned} \tag{4.7}$$

From now on we restrict ourselves to the solution of (4.5) and (4.6).

4.2 Method

In this section we show that the Dirac sextic oscillator (4.5) is one of the recently discovered quasi-exactly solvable operator [6, 7]. It is well known that the underlying idea behind the quasi exact solvability is the existence of a hidden algebraic structure. Let us introduce the following realization of the sl_2-algebra:

$$J_+ = \rho^2 \frac{d}{d\rho} - j\rho, \qquad J_- = \frac{d}{d\rho}, \qquad J_0 = \rho\frac{d}{d\rho} - \frac{j}{2} \tag{4.8}$$

The generators satisfy the commutation relations of the sl_2-algebra for any value of the parameter j. If j is a positive integer the algebra (4.8) possesses $j+1$-dimensional irreducible representation:

$$P_{j+1} = \langle 1, \rho, \rho^2, ..., \rho^j \rangle \tag{4.9}$$

The linear and bilinear combinations of the operators given in (4.8) are quasi exactly solvable, when the space is defined in (4.9). In order to show the Dirac sextic oscillator has a sl_2-symmetry, let us consider the following combinations of the operators 4.8:

$$T = -J_0J_- + \frac{j+2}{2}J_- + 16c^4\hbar^3 qJ_+ + 4c^2\hbar M\omega J_0 \tag{4.10}$$

Then, the eigenvalue problem can be written as

$$TP_k(\rho) = \left(\varepsilon^2 + 2Mc^2\hbar\omega\right) P_k(\rho) \tag{4.11}$$

where $P_k(\rho)$ is the k^{th} degree polynomial in ρ. Let us turn our attention to the Dirac sextic oscillator 4.5. Introducing a new function

$$f(r) = r^{m-\frac{1}{2}} e^{-\frac{m\omega}{2\hbar}r^2 - \frac{q}{4\hbar}} F(r) \tag{4.12}$$

and then changing the variable $r = 2c\hbar\sqrt{\rho}$, we obtain the following expression

$$\begin{aligned} \varepsilon^2 F(\rho) \quad = \quad & -\rho\frac{\partial^2 F(\rho)}{\partial\rho^2} + (m - 1 + 4c^2\hbar\omega M\rho - 16qc^4\hbar^3\rho^2)\frac{\partial F(\rho)}{\partial\rho} \\ & -c^2\left(4M\hbar\omega(m-1) - 16qc^2\hbar^3(m-2)\rho\right)F(\rho) \end{aligned} \tag{4.13}$$

We can show that the eigenvalue equation (4.5) and (4.11) are identical, when the following holds:

$$m = j+2, \qquad F(\rho) = P_k(\rho) \tag{4.14}$$

When the generators act on the polynomial (4.9), we can obtain the following recurrence relation

$$\begin{aligned} 16qc^4\hbar^3(k-j)P_{k+1}(\varepsilon) + (\varepsilon^2 + 4Mc^2\hbar\omega(j-k+1))P_k(\varepsilon) - & \\ k(j-k+2)P_{k-1}(\lambda) \quad = \quad & 0 \end{aligned} \tag{4.15}$$

with the initial condition $P_0(1) = 1$. If ε_i is a root of the polynomial $P_{k+1}(\varepsilon)$, the wavefunction is truncated at $k = j$ and belongs to the spectrum of the Hamiltonian T . This property implies that the wavefunction is itself the generating function of the energy polynomials. The roots of the recurrence relation (4.15) can be computed and the first few of them are given by

$$\begin{aligned}
P_1(\varepsilon) &= \varepsilon^2 + 4Mc^2\hbar\omega \\
P_2(\varepsilon) &= (\varepsilon^2 + 4Mc^2\hbar\omega)(\varepsilon^2 + 8Mc^2\hbar\omega) - 32qc^4\hbar^3 \\
P_3(\varepsilon) &= \varepsilon^6 + 8c^2\hbar(3\varepsilon^4 M\omega + 48c^4\hbar^2 M\omega(M^2\omega^2 - 3q\hbar) \\
&\quad + 2c^2\hbar\varepsilon^2(11M^2\omega^2 - 10q\hbar)) \\
P_4(\varepsilon) &= \varepsilon^8 + 40\varepsilon^6 Mc^2\hbar\omega + 80\varepsilon^4 c^4\hbar^2(7M^2\omega^2 - 6\hbar q \\
&\quad + 128\varepsilon^2 c^6\hbar^3 M\omega(25M^2\omega^2 - 69\hbar q) + 6144c^8\hbar^4(3\hbar^2 q^2 \\
&\quad - 6M^2\omega^2\hbar q + M^4\omega^4)
\end{aligned} \tag{4.16}$$

The function $P_j(\rho)$ forms a basis for sl_2-algebra and it can be written in the form

$$P_j(\rho) = \sum_{k=0}^{j} c_k P_k(\varepsilon)\rho^k \tag{4.17}$$

In the presence of the magnetic field the Hamiltonian can be solved by the same procedure given above. When the magnetic field $B = 2M\omega/e$, the Hamiltonian (4.5) takes the form

$$\begin{aligned}
\varepsilon^2 f(r) &= -c^2\hbar^2\frac{\partial^2 f(r)}{\partial r^2} + \\
&\quad c^2\left[\frac{\hbar^2(m^2 - \frac{1}{4})}{r^2} + q^2 r^6 - 2\hbar q(2-m)r^2 + 4\hbar M\omega(1-m)\right] f(r)
\end{aligned} \tag{4.18}$$

We define the wavefunction

$$f(r) = r^{\frac{1}{2}-m} e^{-\frac{qr^4}{4\hbar}} F(r) \tag{4.19}$$

and changing the variable $r = 2c\hbar\sqrt{\rho}$, we obtain the following differential equation

$$\varepsilon^2 F(\rho) = -\rho\frac{d^2}{d\rho^2} + (j + 1 - 16qc^4\hbar^3\rho^2)\frac{\partial F(\rho)}{\partial\rho} + 16jqc^4\hbar^3\rho F(\rho)$$

When $F(\rho) = P_k(\rho)$,where $P_k(\rho)$ is k^{th} degree polynomial in ρ, we obtain the following recurrence relation

$$16qc^4\hbar^3 P_{k+1}(\varepsilon) - \varepsilon^2 P_k(\varepsilon) + k(j + 2 - k)P_{k-1}(\varepsilon) = 0$$

The polynomial $P_k(\varepsilon)$ vanishes for $k = j + 1$ and the roots of $Pj(\varepsilon)$ belongs to the spectrum of the (4.18). We list the first ten of them below

$$
\begin{aligned}
P_1(\varepsilon) &= \varepsilon^2 \qquad (4.20)\\
P_2(\varepsilon) &= \varepsilon^4 - 2\eta^2\\
P_3(\varepsilon) &= \varepsilon^6 - 10\varepsilon^2\eta^2\\
P_4(\varepsilon) &= \varepsilon^8 - 30\varepsilon^4\eta^2 + 72\eta^4\\
P_5(\varepsilon) &= \varepsilon^{10} - 70\varepsilon^6\eta^2 + 712\varepsilon^2\eta^4\\
P_6(\varepsilon) &= \varepsilon^{12} - 140\varepsilon^8\eta^2 + 3820\varepsilon^4\eta^4 - 10800\eta^6\\
P_7(\varepsilon) &= \varepsilon^{14} - 252\varepsilon^{10}\eta^2 + 14796\varepsilon^6\eta^4 - 164592\varepsilon^2\eta^6\\
P_8(\varepsilon) &= \varepsilon^{16} - 420\varepsilon^{12}\eta^2 + 46380\varepsilon^8\eta^4 - 1307600\varepsilon^4\eta^6 + 4233600\eta^8\\
P_9(\varepsilon) &= \varepsilon^{18} - 660\varepsilon^{14}\eta^2 + 125004\varepsilon^{10}\eta^4 - 7250320\varepsilon^6\eta^6 + 88504707\varepsilon^2\eta^8
\end{aligned}
$$

where $\eta^2 = 16qc^4\hbar^3$. Therefore we can obtain the eigenfunction of (4.18) in the closed form. We conclude that anharmonic interaction destroys the general symmetry of the Dirac equation, but the specified magnetic field can restore the symmetries of the Dirac equation. This feature implies that for the specific values of the magnetic field $B = 2\hbar\omega/e$, analytical solutions of the roots of the polynomials are available.

Due to the interest of the lower dimensional field theory and condensed matter physics, we have constructed Dirac sextic oscillator in two-dimensional space in the presence of magnetic field. It has been shown that Dirac sextic oscillator possesses hidden sl_2-symmetry. In the next chapter, we will discuss position dependent mass hamiltonian.

CHAPTER 5

POSITION DEPENDENT MASS HAMILTONIAN

The Schrodinger equation with position-dependent mass is a very useful model in many applied branches of modern physics, e.g. semiconductors , quantum dots and ^{3}He clusters. In these cases, the envelope wavefunction actually provides a macroscopic description of the motion of carrier electrons with position-dependent (or equivalently material composition- dependent) mass. Recent interest in this field stems from extraordinary development of nanostructure technology. This sophisticated technology of semiconductor growth, like molecular beam epitaxy technique, makes production of ultrathin (nonuniform) semiconductor specimen a reality nowadays. Consequently, the study of such the equation becomes relevant for deeper understanding on the non-trivial quantum effects observed in those nanostructures. Another area, where this equation has extensive use, is the study of quantum many-body systems in solids.

We suggest a model that has been easily related to the QW structures with various PDM models. We will demonstrate a number of promising applications of the model. Potential device applications, as well as purely scientific interest, provide the motivation for studies of the nature of the transport properties of the PDM electron through the barriers or wells. For realistic transport properties in semiconductors, the usual Schrödinger equation has to be replaced by the more general equation[28]:

$$\left(\frac{1}{4}\left(m^{\alpha}pm^{\beta}pm^{\gamma}+m^{\gamma}pm^{\beta}pm^{\alpha}\right)+V\left(z\right)-E\right)\psi\left(z\right)=0 \tag{5.1}$$

with the constraint over the parameters: $\alpha+\beta+\gamma=-1$. In applications, the spatial variation of m is either neglected, or, alternatively various special cases of (5.1) have been suggested in the literature [72-74]. We focus on abrupt heterostructures. It has been proven [26] that for sharp heterostructures $\alpha=\gamma$; otherwise the wavefunction is forced to vanish at the heterojunction boundary which is clearly an unphysical result.

In contrast to the solution of the PDM Schrödinger equation including Coulomb, Morse, harmonic oscillator, etc. type potentials[29-32], the study of the PDM Schrödinger equation including a constant potential has not attracted much attention in the literature. Such quantum systems have been found to be useful in the study of electronic properties of semiconductors. Generally, analysis of the scattering problem with PDM is based on the investigation of the simple problems, and it was pointed out that the transmission probability no longer tends to unity when incoming energy goes to infinity. The fundamental question remains open: whether the behavior of the transmission probability is generic or if it depends on the properties of the mass.

5.1 Model

A typical QW structure is composed of a semiconductor thin film embedded between two semi-infinite semiconductor materials. For a compositional QW, the well material can be generated by alternate deposition of thin layers. For example, in a $GaAs/A\ell_xGa_{1-x}As$ QW there exists a wide $GaAs$ well, followed by an $A\ell_xGa_{1-x}As$ barrier and a $GaAs$ narrow well. The mole fraction x varies along the z-axis, therefore the mass of the electron may vary along the z-axis. The simplest model of the QW is that of a step potential and mass, both showing discontinuities at the same given point and constant inside and outside the well. Here we suggest a model by taking into account the spatial variation of the mass inside the barrier or well. Let us consider a potential barrier of width, d. The structure may be generated by continuously changing the alloy composition x of $A\ell_xGa_{1-x}As$ from $x = 0$ to $x = 0.32$. The relation between alloy composition x and coordinate z is given by [75, 76]:

$$x = \frac{0.32z^2}{d^2} \tag{5.2}$$

Now we turn our attention to the PDM Schrödinger equation (5.1). As we mentioned before, the continuity condition forces $\alpha = \gamma = 0$ and $\beta = -1$. With these choices the PDM Schrödinger equation (5.1), takes the form:

$$\left(p\frac{1}{2m}p + V_0 - E\right)\psi(z) = 0, \qquad d > z > 0 \tag{5.3}$$

where V_0 is the constant potential associated with the barrier height, and E is the energy of the particle. In spite of its simple appearance the Schrödinger equation (5.3) cannot be solved analytically for arbitrary m. We note here that an exact solution of (5.1) including a constant potential can be obtained when $\alpha = \gamma = -1/4$ and $\beta = -1/2$, but in this case continuity conditions can not be satisfied. We look instead at the problem from a different point of view. Instead of the potential V_0 let us introduce the following potential [31],

$$V(z) = V_0 + \frac{\hbar^2}{8m^2}\left(m'' - \frac{7m'^2}{4m}\right), \qquad d > z > 0 \tag{5.4}$$

where m is a function of z and m' and m'' denote first and second derivatives of m with respect to z. At this point it is worth mentioning that we will be interested in the potential which has a less pronounced cusp. Now, the potential resembles a square barrier or well with smooth walls. The additional term is small compared with the original potential V_0 and does not change the shape of the potential. It is obvious that the conditions are satisfied for smoothly varying mass. With the potential (5.4) the Schrödinger equation can be exactly solved with a simple coordinate transformation and the wave function is given by

$$\psi(z) = \left(C_1 e^{-ikf(z)} + C_2 e^{ikf(z)}\right) m^{\frac{1}{4}} \tag{5.5}$$

where the function $f(z)$ is defined as $f(z) = \int \sqrt{m}dz$ and $k = \frac{\sqrt{2}}{\hbar}(E - V_0)$. The results given above can easily be used to solve the Schrödinger equation including well and/or barrier potentials.

Let us illustrate our procedure on a simple example. Consider the potential barrier

$$V(z) = \begin{cases} 0 & 0 > z, \qquad z > d \\ V_0 + \frac{\hbar^2}{8m^2}\left(m'' - \frac{7m'^2}{4m}\right) & d > z > 0 \end{cases} \tag{5.6}$$

with mass barrier

$$m(z) = \begin{cases} m_0 & 0 > z, \qquad z > d \\ m(z) & d > z > 0 \end{cases} \tag{5.7}$$

We assume that the mass of the particle m_0 is constant outside the barrier. Mass of the particle inside the barrier $m(z)$ is an arbitrary function of z. The general solution of the Schrödinger equation yields:

$$\psi(z) = \begin{cases} A_1 e^{ik'z} + A_2 e^{-ik'z} & z < 0 \\ \left(A_3 e^{-ikf(z)} + A_4 e^{ikf(z)}\right) m^{\frac{1}{4}} & d > z > 0 \\ A_5 e^{ik'z} & z > d \end{cases} \tag{5.8}$$

where $k' = \sqrt{2m_0 E}/\hbar^2$ and A_i are constants. For an abrupt heterostructure the continuity conditions are given by [26]

$$m^{\alpha}\psi(z) = \text{continuous}, \; m^{\beta}\frac{d}{dz}m^{\alpha}\psi(z) = \text{continuous} \tag{5.9}$$

The transmission coefficient,T, and reflection coefficient, R, are defined by

$$T = \frac{|A_5|^2}{|A_1|^2}, \qquad R = \frac{|A_2|^2}{|A_1|^2}, \qquad T + R = 1 \tag{5.10}$$

Using elementary quantum mechanical methods, algebraic computation applying boundary conditions, will lead to the following expression which is related with the transmission coefficient:

$$\frac{A_5}{A_1} = \frac{e^{ik'd}K_+(0)K_+^*(d)e^{ik(f(0)-f(d))}}{64kk'm_0m(0)^{7/4}m(d)^{5/4}f'(d)} - \frac{e^{ik'd}K_-(0)K_-^*(d)e^{-ik(f(0)-f(d))}}{64kk'm_0m(0)^{7/4}m(d)^{5/4}f'(d)} \tag{5.11}$$

and the coefficient related with the reflection of the wave:

$$\frac{A_2}{A_1} = \frac{K_-(0)K_-^*(d)e^{2ikf(d)} - K_+(0)K_+^*(d)e^{2ikf(0)}}{K_+^*(d)K_-^*(d)e^{2ikf(d)} - K_-^*(0)K_+^*(d)e^{2ikf(0)}} \tag{5.12}$$

where $K_\pm$ are given by

$$K_\pm(a) = \left[4k'm(a)^2 \pm 4km_0m(a)f'(a) - im_0m'(a)\right] \tag{5.13}$$

$K_\pm^*$ (a) is conjugate of $K_\pm(a)$. The transmission and reflection coefficients can be computed using the relations (5.8) through (5.12). We will illustrate our model using some explicit examples.

5.2 Examples

We discuss the dependence of the transmission probability on the position dependent mass by various choices of the mass $m(z)$. We give several examples for systems with different position dependent masses. Our criterion for the selection of masses is that the shape of the original potential does not change and the square root of $m(z)$ is analytically integrable. Moreover we made an attempt to include mass functions that are frequently used in the literature. In order to demonstrate our procedure, let us begin by considering the following spatially dependent effective masses found to be useful for studying transport properties in semiconductors:

$$\begin{aligned} m_a(z) &= m_0(\sigma + \delta z^2) \\ m_b(z) &= m_0\sigma e^{\sqrt{\delta}\, z} \\ m_c(z) &= m_0(\sigma + \tanh(\sqrt{\delta} z)) \\ m_d(z) &= m_0\left(\frac{\sqrt{\sigma} + \delta z^2}{1+\delta z^2}\right)^2 \end{aligned} \tag{5.14}$$

where δ is the length scale parameter and σ is a dimensionless parameter. Through out this section the parameters are chosen $\sigma = 0.0665$, $\delta = 0.0835$, and $V_0 = 100meV$, height of the barrier and width of the barrier $d = 100^\circ A$.

It can be seen from figure 5.1, the potential (5.4) closely resembles a square barrier with smooth walls for the masses $m_a(z)$,$m_b(z)$ and $m_c(z)$. We remark that when the mass rapidly changes with position z, the shape of the potential profile has a pronounced cusp. The potential (5.4) which includes the rapidly changing mass function $m_d(z)$ can be plotted as shown in figure 5.1. We explicitly calculate transmission probability of the scattering problem employing various physically meaningful spatially varying effective masses in the following.

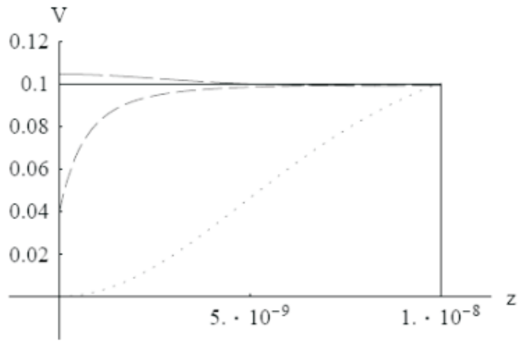

Figure 5.1: *Effect of the position dependent mass on the potential profile. The long dashed line, dashed line and dotted line show the effect of the* m_a,m_c, *and* m_d, *respectively, on the potential profile. The change in the potential profile due to* $m_b(z)$ *is plotted with long dashed lines and it is negligible.*

5.2.1 Mass Barrier: m(z)=σm_1

Consider now a simple mass barrier such that the mass changes at the potential discontinuities, but inside and outside the barrier it is a constant. In this case the potential V_0 remains the same. Since the tunneling effect is not qualitatively modified by the mass discontinuity, we have to leave aside the case where $E < V_0$. In the case $E > V_0$ the calculation for transmission coefficient can easily be done from the relation (5.11) and a plot of the transmission probability is illustrated in figure 5.2 for various mass ratios. In the plot we defined the quantities:

$$\frac{m_1}{m_0} = a, \qquad d = \frac{\pi\hbar}{\sqrt{m_o V_0}}, \qquad \omega = \frac{E}{U_0} \tag{5.15}$$

The graph shows clearly for $m_0 > m_1$ the transmission coefficient no longer tends to unity when E goes to infinity, but it becomes an oscillating function of E, as is discussed in [23, 77]. In figure 5.2, the curve denoted by $a = 1$, corresponds to the plot of transmission coefficient for $m = 0.0665 m_0$. This is the conduction band edge effective mass of the electron in the $GaAs$ structure. In the following we compute the transmission coefficients for the mass functions given in (5.14).

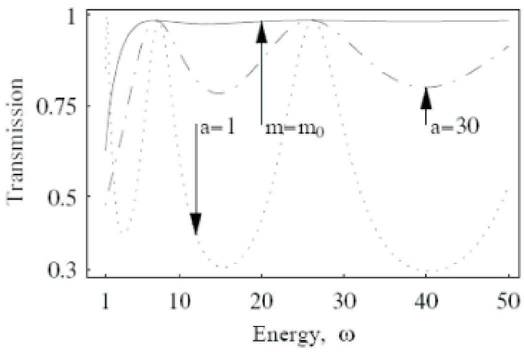

Figure 5.2: *The transmission coefficient T for a potential barrier with height V_0 and a mass discontinuities.*

5.2.2 Mass Barriers: $\mathbf{m}_a(z), m_b(z), m_c(z)$ and $m_d(z)$

The mass functions given in (5.14) are used in various fields of physics. We mention here that mass function $m_a(z)$, may be useful to analyze the structures $GaAs/A\ell_x Ga_{1-x}As$. For example the effective band mass of the electron in the barrier can be written[75, 78] as

$$m(x) = m_0(0.0665 + 0.0835x) \tag{5.16}$$

The relation between alloy composition x and the coordinate z is given in (5.2). For comparison we calculated transmission coefficients by using the relations (5.10) through (5.12) and they are illustrated in figure 5.3.

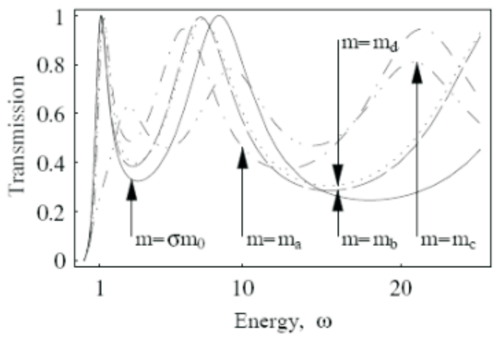

Figure 5.3: *The transmission coefficient T for a potential barrier with height V_0 and various position dependent mass discontinuities.*

In this chapter we have suggested a model that has been easily related to the non-relativistic quantum mechanical systems. We have shown that a number of important applications of the model. But the fundamental questions about the ordering ambiguity still unanswered. In the following chapter we propose a model, using Dirac equation instead of Schrödinger equation, and then we eliminate ordering ambiguity problem.

CHAPTER 6

EFFECTIVE MASS RELATIVISTIC PARTICLES IN POTENTIAL WELL IN (1 + 1) - DIMENSIONS

We propose a method of calculation to compute the transmission coefficient of the effective mass, relativistic particle through a potential well. After sketching the basis of the theory, and expressing the effective mass Dirac equation, the simplest problem, namely transmission through a square potential is treated and its novel aspects are presented. We discuss applications for semiconductor heterostructures and the applicability of the Dirac equation to investigate properties of the ultra-high-speed effective mass electron in QW. We also mention here some advantages of Dirac Equation: the physical systems such as semiconductors [9] , quantum wells and dots [38], quantum liquids [39], graded alloys and heterostructures found application in the framework of effective mass or position dependent mass Schrödinger equation [40]. When the system includes effective or position dependent mass, the usual Schrödinger equation has to be replaced by the more general equation (5.1).

Although it has been solved for a large class of potentials by different methods [14-19,22,29,32-34], the ordering ambiguity of the mass and momentum operators have not yet been decided. Its effect on the exact solutions was systematically discussed in [20]. When the problem is formulated with Dirac equation the ordering ambiguity of the mass and momentum can be eliminated [35].

6.1 The Model

The Dirac equation is a relativistically invariant first order differential equation in 4-dimensional space-time for a four-component wavefunction ψ. However we consider a particle with mass $m(x)$ that is subjected to a one-dimensional potential well. In this case the Dirac equation has been expressed by Pauli matrices, resulting in a two-component wavefunction ψ. One-dimensional, time-independent Dirac equation can be written as

$$\left[c\sigma_2 p + \sigma_0(mc^2 + S(x)) + V(x)\right]\psi = E\psi \tag{6.1}$$

where $p = -i\hbar\partial_x$ is the momentum operator, σ_2 and σ_0 are Pauli matrices, m is the rest mass of the free particle, c is the velocity of light, and E is the energy of the particle. The function $S(x)$ is a Lorentz scalar and $V(x)$ is zeroth order component of the Lorentz vector. The quantity $m + S(x)/c^2$ can be regarded as an effective mass m^* or position dependent mass $m(x)$.

Let the upper and lower components of the wavefunction ψ be ψ_+ and ψ_-, respectively, then the one dimensional Dirac equation (6.1) takes the form

$$\hbar c\frac{\partial\psi_-}{\partial x} + (m^*c^2 + V - E)\psi_+ = 0 \tag{6.2}$$

$$\hbar c\frac{\partial\psi_+}{\partial x} + (m^*c^2 - V + E)\psi_- = 0 \tag{6.3}$$

Meanwhile, we conclude that the Dirac equation (6.2) and (6.3) is invariant under charge conjugation: that is under the transformation $\psi_+ \longrightarrow \psi_-$; $\psi_- \longrightarrow \psi_+$; $E \longrightarrow -E$; and $V \longrightarrow -V$: The expressions (6.2) and (6.3) can be written in the form of the Schrödinger like equation by eliminating ψ_+ or ψ_- between (6.2) and (6.3), the resulting equation takes the form

$$\hbar^2c^2\frac{\partial^2\psi_\pm}{\partial x^2} + (V - E - m^*c^2)(V - E + m^*c^2)\psi_\pm = 0 \tag{6.4}$$

We will investigate the features brought in the behavior of a relativistic quantum particle by an effective mass in a quantum well. The square well potential is given by and the mass barrier is given by

$$V = \begin{cases} 0 & -a > x, \quad x > a \\ -V_0 & a > x > -a \end{cases} \tag{6.5}$$

and the mass barrier is given by

$$m^* = \begin{cases} m_0 & -a > x, \quad x > a \\ m & a > x > -a \end{cases} \tag{6.6}$$

We assume that mass of the particle m_0 is the rest mass of the particle outside the well and the mass of the particle is m inside the well. Based on the effective mass theory there exist such a potential and mass wells/barriers in the $GaAs - Al_xGa_{1-x}$ structures, as well as the other semiconductor structures [79].

6.1.1 Scattering States: $E > m_0c^2$

We now solve the equation (6.4) for a particle scattering by the potential (6.5) and the mass (6.6). We take the particle incident from left, so that the solution can immediately be written down:

$$\psi_+ = \begin{cases} e^{ikx} + re^{-ikx} & x < -a \\ Ae^{iqx} + Be^{-iqx} & a > x > -a \\ te^{ikx} & x > a \end{cases} \tag{6.7}$$

It is obvious that the reflection and transmission coefficients are given by $R = |r|^2$ and $T = |t|^2$, respectively, with $T + R = 1$. The wave numbers k and q are defined as

$$k = \frac{\sqrt{E^2 - m_0^2c^4}}{\hbar c}; \qquad q = \frac{\sqrt{2m_0(\varepsilon + V_0)}}{\hbar c} \tag{6.8}$$

We can easily check that the relativistic wave numbers are identical to those non-relativistic wave numbers which hold in the standard case $m = m_0$ and when we define $E = \varepsilon + m_0c^2$, which leads to the expressions

$$k = \frac{\sqrt{2m_0\varepsilon}}{\hbar}; \qquad q = \frac{\sqrt{2m_0(\varepsilon + V_0)}}{\hbar} \tag{6.9}$$

Our task is now to derive an expression for the transmission coefficient of a relativistic particle through the well potential (6.5) and the mass barrier (6.6). The solution (6.7) must satisfy the appropriate boundary conditions across the interface, (at $x = \pm a$), namely, that

$$\psi_{+1}(-a) = \psi_{+2}(-a); \qquad -\frac{1}{m_0}\psi'_{+1}(-a) = \frac{1}{m}\psi'_{+2}(-a); \tag{6.10}$$

$$\psi_{+2}(a) = \psi_{+3}(a); \quad \frac{1}{m}\psi'_{+2}(a) = \frac{1}{m_0}\psi'_{+3}(a) \tag{6.11}$$

Here $\psi_{+i}(x), (i = 1, 2, 3)$ show the values of the wave function in the three regions of interest. A straightforward calculation leads to an expression for the transmission coefficient

$$T = \left[1 + (q^2 - b^2k^2)^2(2bkq)^{-2}\sin^2(2aq)\right]^{-1} \tag{6.12}$$

where $b = m/m_0$ is the mass ratio. To demonstrate the validity and usefulness of (6.12) we sketch the graph of T versus energy. Let us define the energy in terms of a dimensionless quantity ω and the well width in terms of the V_0 such that

$$E = \sqrt{m_0c^2(V_0\omega^2 + m_0c^2)}; \quad a = \frac{\pi\hbar}{\sqrt{m_0V_0}}. \tag{6.13}$$

To make comparison between the transmission of the effective mass and constant mass particles through the well we plot figures (6.1) and (6.2), T versus energy ratio, for a well of depth $V_0 = 1.42\ eV$, well width $2a = 14.5\ A^0$. The graphs exhibits most clearly the essential difference between the case $m = m_0$ and $m \neq m0$: When $m < m_0$ the transmission coefficient no longer tends to unity for large values of the energy but it reaches unity for a specific values of the energy.

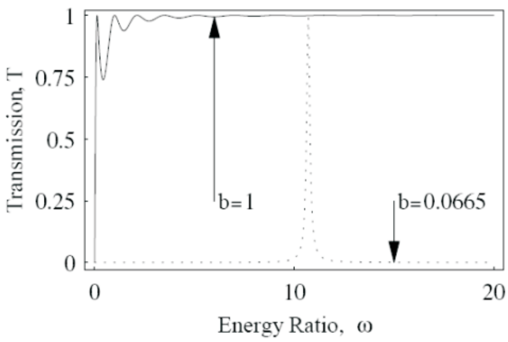

Figure 6.1: *The transmission coefficient T for a well of potential with height $V_0 = 1.42\ eV$: Solid line corresponds the plot of transmission without mass discontinuities and dotted line corresponds transmission with a mass discontinuities.*

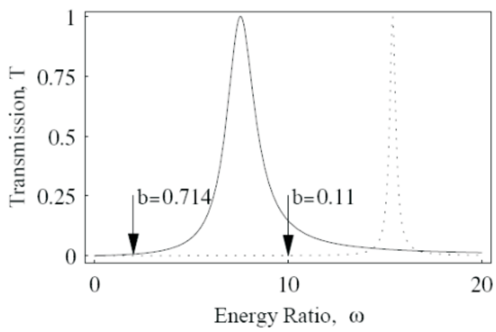

Figure 6.2: *The transmission coefficient T for a well of potential with height $V_0 = 1.42\ meV$ for different mass discontinuities.*

To make a comparison between relativistic and non-relativistic theory we plot both of them in figure (6.3). In non-relativistic case one can observe the similar features of the transmission: when $m \neq m_0$ the transmission coefficient reaches to an asymptotic value for large values of energy. But in the relativistic case the transmission almost zero except that some specific values of the energy and it becomes oscillating function of energy [40,77]. The mass ratio $b = 0.0665$, used here corresponds to the conduction band edge effective mass of the electron in $GaAs$ structure. NR is the non-relativistic, R is the relativistic.

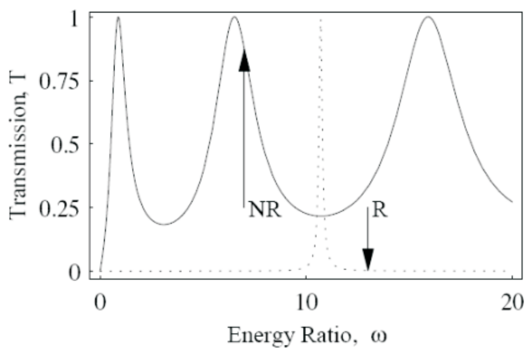

Figure 6.3: *The transmission coefficient T for a well of potential with height $V_0 = 100$ meV and a mass discontinuities.*

6.1.2 Solution for $E < m_0c^2$

In this case k is imaginary and q is real. The permitted bound solutions are given by

$$\psi_{\pm} = \begin{cases} Ce^{kx} & x < -a \\ Ae^{iqx} + Be^{-iqx} & a > x > -a \\ De^{kx} & x > a \end{cases} \tag{6.14}$$

From the boundary conditions we obtain the dispersion relation

$$\left(\tan(aq) - \frac{bk}{q}\right)\left(\tan(aq) + \frac{q}{bk}\right) = 0 \tag{6.15}$$

The bound state energies can be obtained from the solution of (6.15). To bound the electron in the well the potential barrier should be $V_0 > E + m^*c^2$. The condition for a semiconductor heterostructure gives us a large V_0 value for the barrier height. We can notice that it is not possible to obtain that values of potential for heterostructures.

In this chapter, we have discussed solution of the effective mass Dirac equation including constant potential and obtained a general expression for the transmission coefficient of the wave through the square potential well. We have presented calculations of the transmission of the particle through the well for various mass barriers.

CHAPTER 7

CONCLUSION

In this thesis, we have discussed the exact solvability of the PDM Schrödinger equation including a constant potential and recovered a general expression for the transmission coefficient of the wave through the square potential barrier. After that we presented calculations of transmission coefficients for various spatially varying effective masses.

Within the framework of the effective mass approximation, in some previous works the electron was assumed to be confined in a square infinitely high potential well. In fact, a finite height potential well model is more realistic for describing the motion of the electron in the QW. It is obvious that the model described in this thesis can easily be modified to study QW structures and superlattices.

Then we have represented construction and solution of dirac equation.

We obtained analytical solutions of the $(2+1)$- dimensional Dirac equation for a set of potentials in two dimensions with the hope that they could be useful in the low dimensional field theory and condensed matter physics. The potentials for Dirac equation have been obtained by extending the notion of the Dirac oscillator. In a similar manner one can construct the exactly and QES Dirac equation including hyperbolic and trigonometric potentials. It has been shown that the $(2+1)$-dimensional Dirac equation can be transformed in the form of a Schrödinger-like equation and for all exactly and QES Schrödinger equations one can find potentials of the Dirac equation which are also exactly solvable or QES.

Therefore, besides its importance as a new treatment of the construction of the various potentials for Dirac equation,the potentials obtained here might be relevant to model some physical problems. Before ending this studying a remark is in order. It is expected that the models presented here to construct Dirac equation including various potentials may provide a good starting point for the study of more realistic models for the low dimensional of field theory and condensed matter physics.

We have constructed Dirac sextic oscillator in two-dimensional space in the presence of the magnetic field. Then we have given eigenstates of the corresponding equation in terms of the orthogonal polynomials.

Finally, solution of the effective mass Dirac equation including constant potential have been discussed. We have obtained a general expression for the transmission coefficient of the wave through the square potential well and presented calculations of transmission of particle through the well for various mass barriers.

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