Kronig-Penney and Delta-Potential Models in Quantum Mechanics

Mohamed Em. F. Ali

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Assoc. Prof. Dr. Ali Hakan Ulusoy
Acting Director

I certify that this thesis satisfies the requirements as a thesis for the degree of Master of Science in Physics.

Prof. Dr. İzzet Sakallı
Chair, Department of Physics

We certify that we have read this thesis and that in our opinion it is fully adequate in scope and quality as a thesis for the degree of Master of Science in Physics.

Assoc. Prof. Dr. S. Habib Mazharimousavi
Co-Supervisor

Prof. Dr. Mustafa Halilsoy
Supervisor

Examining Committee

1. Prof. Dr. Ayhan Bilsel
2. Prof. Dr. Mustafa Halilsoy
3. Prof. Dr. Omar Mustafa
4. Assoc. Prof. Dr. S. Habib Mazharimousavi
5. Asst. Prof. Dr. Mustafa Riza

ABSTRACT

Kronig-Penney model is applicable to quantum mechanical study of electrons in confined periodic potentials. Exact solution for a single-well potential can easily be generalized to many-wells through the Bloch theorem. In this study for a single-well potential eigenfunctions/eigenvalues are solvable numerically and forbidden energy gaps are identified. We consider next the potential with double-delta functions for which stationary states and energy levels are found. For this purpose, a transcendental algebraic equation is studied numerically. Reflection and transmission coefficients are determined appropriately. Finally, we propose that the distributional functions must find more applications in quantum mechanical problems.

Keywords: Kronig-Penney, delta-potential, allowed energies, gap regions.

ÖZ

Krönig–Penney modeli sınırlı, periyodik potansiyellerde elektron alanlarını kuantumsal olarak inceler. Tek çukur potansiyelinde bulunan kesin çözüm Bloch teoremi sayesinde çok sayıda çukur problemine genellenir. Bu çalışmada birim hücre için fonksiyonun uygun değerleri sayısal yöntemle elde ediliyor ve yasak enerji kesitleri bulunuyor. İkinci olarak Dirac delta potansiyeli ele alınıyor. Çift delta potansiyeli için durağan dalga ve enerji değerleri bulunuyor. Bunun için transendent cebirsel bir denklemi incelemek gerekiyor. Dalga fonksiyonunun yansıma ve geçirgenlik katsayıları hesaplanıyor. Son olarak distribütasyonların Kuantum Mekaniğinde daha geniş bir kullanım alanı olması gerektiğini öneriyoruz.

Anahtar kelimeler: Krönig-Penney, delta-potansiyeli, enerji seviyeleri, aralık bölgeleri.

DEDICATION

To My Parents

ACKNOWLEDGEMENT

I would like to express my sincere gratitude to my supervisor Prof. Dr. Mustafa Halilsoy and my co-supervisor Assoc. Prof. Dr. S. Habib Mazharimousavi and Asst. Prof. Dr. Mustafa Riza for their kind help, motivation, guidance during the process of this thesis study.

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INTRODUCTION

The potentials in quantum mechanics are commonly represented by an idealized function which is piecewise constant with discontinuities. Step barriers and square wells for scattering calculations are the most common potentials among others such as distributions. The mathematical convenience is the reasoning behind choosing such potentials, e.g., solutions of Schrödinger equations can easily be obtainable than the most real-life potentials.

The discontinuous potentials resulting in the solutions of Schrödinger equation proceeded by evaluating those solutions within each certain region where the potential is continuous. Then, determining the allowed energies and the wavefunction explicitly evaluated by applying and matching the most common quantum mechanics boundary conditions. The Dirac delta function is the better example for such discontinuous potentials, which specifically have extreme usage in molecules and solid's atomic modelling [10].

Basically, obtaining the solutions of Schrödinger equation for any properties of an electron influenced by such a potential is supplemented by two conditions, i.e., the continuity of wavefunction, which is one of the most fundamental constraints on the wavefunction of any physical entity, which ought be to observed even though at boundaries of an infinite discontinuous potentials (for probabilistic interpretation of the wavefunction the continuity is urgently required and willingly defined at every point) . The continuity of the derivative of the wavefunctions, in turn, has applied, just except at an infinite discontinuous potential, which means that the infinite discontinuity in the first derivative implies an infinite discontinuity in the second derivative as well, which leads to an infinite discontinuity in the kinetic energy, which in turn is physically unrealistic.

There are three factors that the electronic properties of crystalline solids are determined. Firstly, the periodicity of the potential of the atoms in solids. Secondly, the electrostatic interactivity between electron and nuclei and among the electrons themselves. Thirdly, the occupancy of electronic states (Pauli principle).

Felix Bloch is regarded as the most important contributor ever, who had considered the effectiveness of the periodicity of crystalline solids as a form of a wave function due to the movement of electrons in a potential - now the so-called Bloch Function - and how the energy bands are being structured. As a result, many realistic calculations of the crystalline metals had been carried out. However, a more fundamental and practical approach for research-level activity is still an active part in quantum mechanics.

The second chapter is devoted to studying a quantum particle interacting with a one-dimensional structure of equidistant scattering centres, with the presence of Bloch theorem. This generalizes the well-known solid-state physics textbook result which is called the Kronig-Penney model. In metals, ions arrange themselves in a way that exhibit a spatial periodicity as a general case for those have a crystalline structure. The motion of the free electrons in the metal are affected by such a periodicity, this effectiveness is being exhibited in a simple model that we will now discuss. Followed by a discussion of energy bands, gap energies and wavefunctions. However, presence of different kinds of atomic states give rise to a different type of energy band.

The δ-potential spikes as a limit of the gaussian helps to simulate states in which a particle can be able to move freely in two regions of space with presence of a barrier allocated in the midpoint between the two regions. For instance, in a conducting metal the electron can almost move with freedom, but, if we suppose two-conducing surfaces are closely overlapped, the interface between them works as a barrier for the electron that can be regarded as a δ-potential. The calculations presented by using the δ-potential might seem unrealistic at the outset and practically hard to use. However, it has proved to be a convenient model for many of the real-life applications. Another significant point about the Dirac δ-potential is that it is exactly solvable which makes it also suitable and useful for teaching purposes.

The δ-function model according to the dimensional scaling approach is a one-dimensional version of the Hydrogen atom. Particularly, with the double δ-model, a delta function approach becomes extremely useful, it can be presented as a one-dimensional version of the Hydrogen molecule ion [12].

The third chapter is dedicated to discussing about a double Dirac delta potential well case, where a symmetry of the potential (the potential is symmetric with respect to $x = 0$) is to be considered when the bound state solutions are calculated.

In the fourth chapter we consider the general role of distributional potentials in physics. We concentrate mainly on the Dirac Delta and Heaviside distributions since these are used mostly in physics. In particular we give the example of second order differential equations which admit a series of delta functions and give its exact solution. That's of course corresponds to the zero-energy eigenvalue case of the Schrödinger equation. To proceed with the non-zero energy solution of the Schrödinger equation we have to make use again the local regional solutions and apply the boundary conditions as in the *2*-δ-potential case. Let us add that at a higher level there are green's function methods [5] to tackle the same problem which lies beyond the scope of the present thesis.

Chapter 2

KRONIG-PENNEY MODEL

2.1 Preview

Kronig-Penney Model is a unique model which exhibits many of basic characteristics of the electronic structure of real crystals, generally regarded as an idealized and a one-dimensional model of a crystal. It is among the simplest possible models to describe electrons in a periodic lattice. It has been proved that a band gaps and hence energy bands are possibly yielded for a one-dimensional periodic potential. The mathematics is a bit involved, but this model will allow us to discuss qualitatively several important concepts. The potential energy which is considered is $V(x)$ of an electron with an infinite sequence of potential wells of depth $-V_0$ and width a, arranged with evenly spacing. Furthermore, it is a more interesting when solving the time-independent Schrödinger equation, the band structure and hence allowable and forbidden energies for a periodic potential can easily be obtained and calculated, respectively. While this model is an oversimplification of *3-d* potential and band structure, it is also extended to include the effects of the impurity atoms.

2.2 Bloch Wave

If the effect of the symmetry on the wave function is utilized from the outset of the solution of the Schrödinger equation for an electron in a periodic potential this will be extremely simplified. Consider a potential has the form $V(x+a) = V(x)$, and let the effect of translating by a, that is, changing to $(x+a)$ instead of x, so the second derivative will not be affected, because a is a constant, and the potential will not have changed because of its periodicity. Similarly, E will not be affected by this translation either, because it is a constant. So, Schrödinger equation transformed to the new form

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2}(x+a)+V(x)\psi(x+a)=E\psi(x+a) \tag{2.1}$$

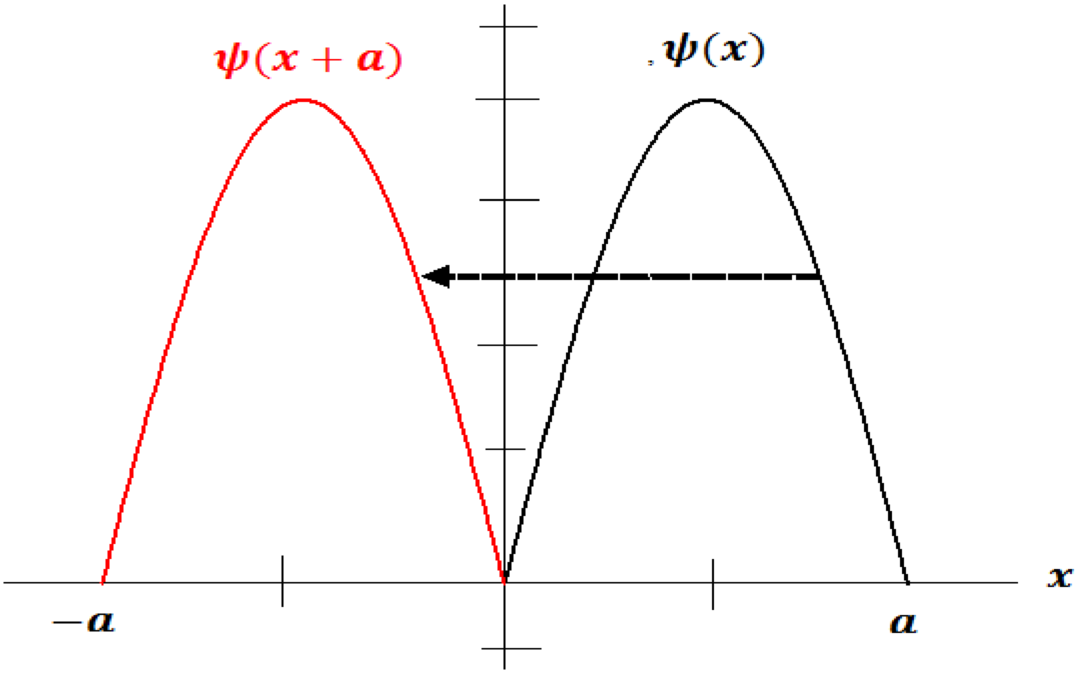

Figure 2.1: A plot of a periodic wave function: $\psi(x+a)=\psi(x)$.

Since, $\psi(x)$ and $\psi(x+a)$ satisfy the same Schrödinger equation, the new forms with $\psi(x)$ and $\psi(x+a)$ are the same (Fig.2.1). Therefore, for any observable such as probability density associated with $\psi(x)$, must also embody this invariance. Explicitly, $\psi(x+a)$ can be written as

$$\psi(x+na)=e^{i\mu(a)}\psi(x) \tag{2.2}$$

where $\mu(a)$ is an a-dependent phase.

This means that $\psi(x)$ and $\psi(x+a)$ only differ by a pure phase. It is worthwhile to notice that, the functional form of μ can be determined if we take into consideration that the probability density will not be affected by n number of translations by a, that is:

$$|\psi(x+na)|^2 = |\psi(x)|^2 \tag{2.3}$$

The state of $\psi(x+na)$ can be evaluated in two different ways, by a single (na) and by a sequence of n individual (each by a) translations as mentioned by the expressions below:

$$\psi(x+na) = e^{i\mu(na)}\psi(x) \tag{2.4}$$

$$\psi(x+na) = e^{i\mu(a)}\psi(x+(n-1)a)$$

$$= e^{2i\mu(a)}\psi(x+(n-2)a) = \cdots = e^{in\mu(a)}\,\psi\,(x) \tag{2.5}$$

So, equating them yields

$$\mathrm{e}^{\mathrm{i}\mu(\mathrm{na})} = \mathrm{e}^{\mathrm{in}\mu(\mathrm{a})} \tag{2.6}$$

which implies that $\mu(a) \propto\ (a)$.

So, differentiate Eq. (2.6) with respect to n, setting $n = 1$ and cancelling the common factor, we get

$$a\frac{d\mu}{da} = \mu \tag{2.7}$$

To obtain a solution in the form of $\mu(a) = ka$, just integrate this equation either by separation of variables or by a trial solution.

Equation (2.2) can be reduced to one form of Bloch Theorem. So, a more explicit form for $\psi(x)$ can be obtained by solving (2.1) for $\psi(x)$, if the both sides of the resulting equation are multiplied by the factor e^{-ikx} we get:

$$e^{-ikx}\psi(x) = e^{-ikx}e^{-ika}\psi(x+a) = e^{-ik(x+a)}\psi(x+a) \tag{2.8}$$

Let, $u(x) = e^{-ikx}\psi(x)$, which is the periodic function with period a, or alternatively:

$$\psi(x) = e^{ikx}\,u(x) \tag{2.9}$$

where $u(x+a) = u(a)$. This is known as Bloch function (Fig. 2.2).

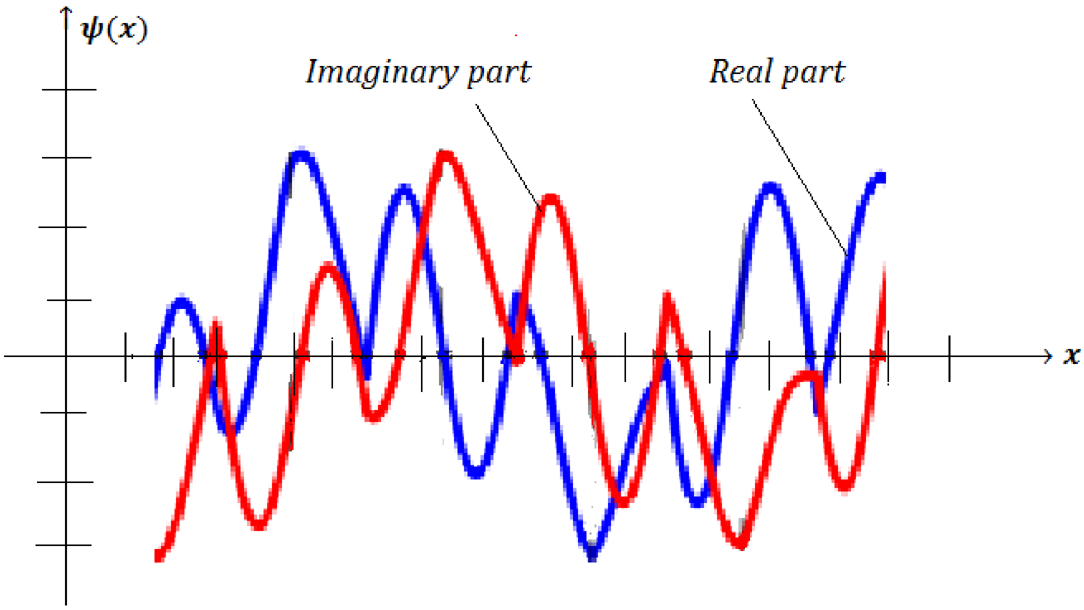

Figure 2.2: A plot depicts the Bloch wave: $\psi(x) = u(x)\, e^{ikx}$.

We would like to mention that the solution of the free particle is being that exponential factor, while the periodic function, can be said that it is a direct consequence of a periodic potential. This is one of the major results for describing electrons in crystalline solids.

2.3 Formulation and Solution of Kronig-Penney Model

When infinite square wells are being placed side-by-side with each other, the resulting is a potential $V(x)$ for the electrons in a periodic potential array as introduced by Kronig-Penney model. We are concerned with solving a stationary and single particle of independent-time Schrödinger equation:

$$\frac{-\hbar^2}{2m}\frac{\partial^2\psi(x)}{\partial x^2} + V_{(kp)}\psi(x) = E\psi(x) \tag{2.10}$$

Here $V_{(kp)}$ denotes the Kronig-Penney potential, it is describing a potential with infinite spatial support, and spatial periodicity $(a+b)$ which can be formulated to the functional shape as follows (Fig. 2.3).

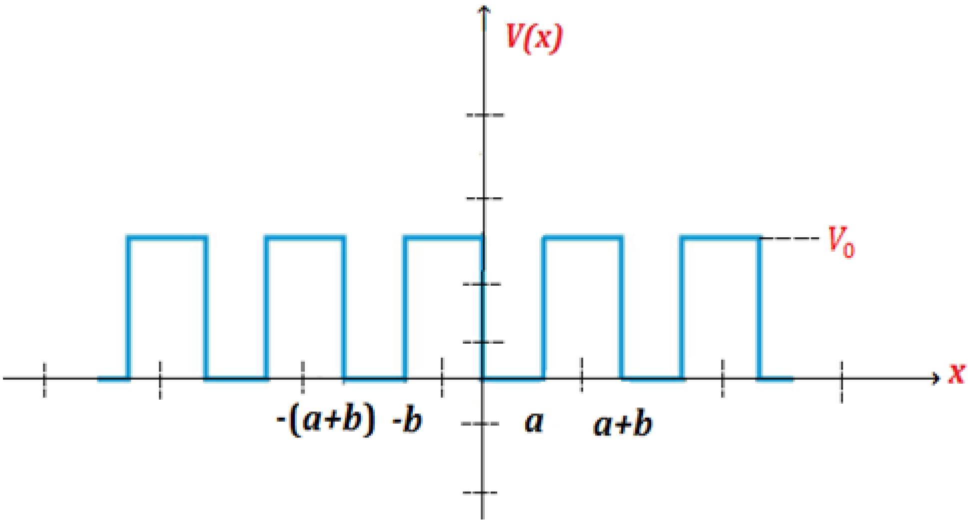

Figure 2.3: The periodic Kronig-Penney potential in one dimension.

$$V_{(kp)}(x) = \sum_{n=-\infty}^{\infty} V_{(well)}[x - n(a+b)] \qquad (2.11)$$

Where $V_{(well)}$ is the potential well, that is

$$V_{(well)}(x) = \begin{cases} 0 & for \quad 0 < x < a \\ V_0 & for \quad a < x < a+b \end{cases} \qquad (2.12)$$

Now we can say that each primitive cell in the lattice consists of a repulsive barrier of strength V_0, width b and inter-spacing barrier a. The approach that we now seek to solve by utilizing Bloch's Theorem is completely descriptive of both eigenfunctions and eigenvalues of the time-independent Schrödinger Equation.

When the eigenfunctions of Schrödinger equation is being subjected to such a periodic potential as it had introduced by Bloch's Function, then $V_{(periodic)}(x)$ strictly are constrained as follows

$$\psi_{(\boldsymbol{k})}(\boldsymbol{r}) = e^{i\boldsymbol{k}.\boldsymbol{r}} u_{(\boldsymbol{k})}(\boldsymbol{r}) \qquad (2.13)$$

The eigenfunction is a linear combination, which belongs to a region where $V = 0$,

$$\psi(x) = Ce^{iKx} + De^{-iKx} \qquad 0 < x < a \qquad (2.14)$$

so, these plane waves are travelling in opposite directions (to left and to right) whose energy is

$$E(K) = \frac{\hbar^2 K^2}{2m} \tag{2.15}$$

The solution in the region where the barrier exists is a linear combination of an eigenfunction:

$$\psi(x) = Fe^{Qx} + Ge^{-Qx} \qquad -b < x < 0 \tag{2.16}$$

with

$$E(Q) = V_0 - \frac{\hbar^2 Q^2}{2m} \tag{2.17}$$

To get the Bloch form (2.13), a complete solution must be obtainable, i.e., the solutions in both regions *(* $a < x < a + b$ and $-b < x < 0$) must be related, thus

$$\psi(a < x < a + b) = \psi(-b < x < 0)e^{i\boldsymbol{k}(\boldsymbol{a}+\boldsymbol{b})} \tag{2.18}$$

is serving to determine k as index labelling the solution. At $x = a$ and $x = 0$, (the usual quantum mechanical boundary conditions in such problems involving square potential wells) of ψ and $\frac{d\psi}{dx}$ will be applied so that the constants *C, D, F, G* have been conveniently chosen.

At $x = 0$

$$C + D = F + G \tag{2.19}$$

$$iK(C - D) = Q(F - G) \tag{2.20}$$

similarly, at $x = a$, using the relation (2.18) under the barrier in terms of $\psi(-b)$ for $\psi(a)$ we obtain

$$Ce^{i\boldsymbol{Ka}} + De^{-i\boldsymbol{Ka}} = e^{i\boldsymbol{k}(\boldsymbol{a}+\boldsymbol{b})}(Fe^{-Qb} + Ge^{Qb}) \tag{2.21}$$

and

$$iK(Ce^{i\boldsymbol{Ka}} - De^{-i\boldsymbol{Ka}}) = e^{i\boldsymbol{k}(\boldsymbol{a}+\boldsymbol{b})}(Fe^{-Qb} - Ge^{Qb})Q \tag{2.22}$$

Resolving the constraints (2.19), (2.20), (2.21) and (2.22) into a linear system is of course possible:

$$\begin{pmatrix} 1 & 1 & -1 & -1 \\ iK & -iK & -Q & Q \\ e^{iKa} & e^{-iKa} & -e^{ik(a+b)-Qb} & -e^{ik(a+b)+Qb} \\ iKe^{iKa} & -iKe^{-iKa} & -Qe^{ik(a+b)-Qb} & Qe^{ik(a+b)+Qb} \end{pmatrix} \begin{pmatrix} C \\ D \\ F \\ G \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \end{pmatrix} \tag{2.23}$$

If the determinant of the coefficients *C*, *D*, *F*, *G* on the left-hand side is vanishing, then this system of equations will only admit non-zero (non-trivial) solution. If just doing some rather tedious algebraic manipulations, we can derive a constraint on k in terms of the model parameters from such determinant.

$$\frac{Q^2-K^2}{2QK} sinh(Qb)\, sin(Ka) \;+\; cosh(Qb)cos(Ka) = cos[k(a+b)] \tag{2.24}$$

If the model parameter a, b, and V_0 have fixed values, for a given value of k, we look for values of K that will give a solution to this transcendental equation. The stationary states of energy $E(K)$ associated to these values of K is $\frac{\hbar^2 K^2}{2m}$.

Intuitively, there will be values of K for which there are no real values of k that satisfy the solution of this equation, in such a case a gap in the spectrum of energies will take place. The periodicity of delta function would be employed to get a more simplified result, i.e., passing to the limit $b \rightarrow 0$ and $V_0 \rightarrow \infty$ in such a way that $\frac{Q^2 ba}{2} = P$ is a finite quantity. In the limit $cosh\, Qb \rightarrow 1,$ also $sinh\, Qb \rightarrow Qb\ \ll 1$ and $Q \gg K$. So,

$$Q^2 \propto V_0$$

$$\lim_{v_0 \rightarrow \infty} (Q^2 - k^2) \cong Q^2$$

Then the Eq. (2.24) can be reduced to a more concise form:

$$P\left[\frac{sin\, Ka}{Ka}\right] + cos\, Ka = cos\, ka \tag{2.25}$$

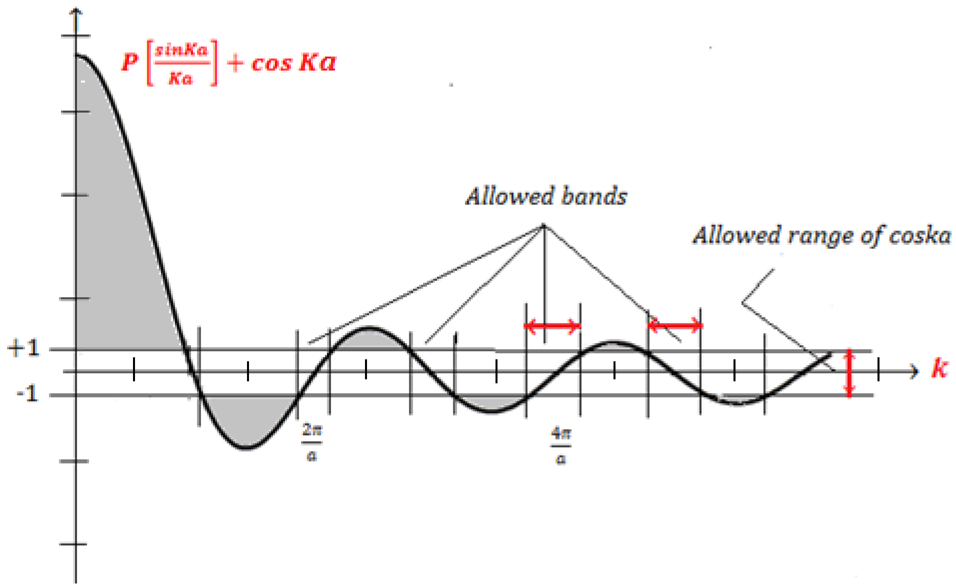

Figure 2.4: The function $(\frac{P}{Ka})\ \sin Ka\ +\ \cos Ka$ versus k is plotted. For the ranges of $k = \sqrt{2mE\ /\ \hbar^2}$, the allowed permissible values of E are determined.

It becomes more constructive to consider the solution graphically of Eq. (2.25), in which the left-hand side as a function of (Ka) can be plotted when the right-hand side - the ranges of $cos(ka)$ - are between -1 and 1, a solution for values of k exist. However, for non-real values of K, no energy eigenfunction exists, i.e., the spectrum of solutions will then have a gap in the admissible energies. It means that no proper solutions for certain energies for this model can be found. Figures (2.4) and (2.5) show the domains of K for which the Eq. (2.25) has solutions. Here, the Bloch function wavevector index k is more significant than K, which has a relevant relation to the energy Eq. (2.15).

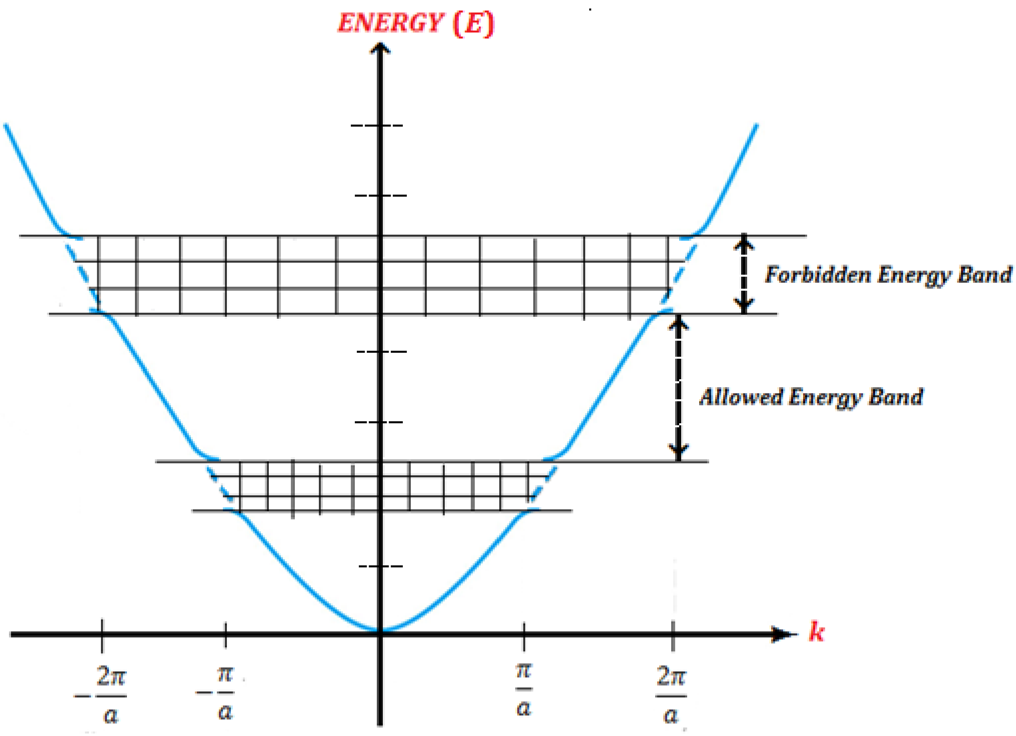

Figure 2.5: This plot depicts *E*-*k* graph. The zones or regions extending from $k = -\frac{\pi}{a}$ $to\ k = +\frac{\pi}{a}$ (first Brillouin zone) and from $k = \pm\frac{\pi}{a}$ $to\ k = \pm\frac{2\pi}{a}$ (second Brillouin zone) and so on, in which an allowed energy values for the electron has clearly marked.

Chapter 3

DOUBLE DIRAC δ-POTENTIAL SCHRÖDINGER EQUATION

3.1 Double Dirac δ-Potential Well

A double Dirac δ-function potential to be considered here is in the form

$$V(x) = -\beta[\delta(x + a) + \delta(x - a)] \tag{3.1}$$

Where β and a are positive constants.

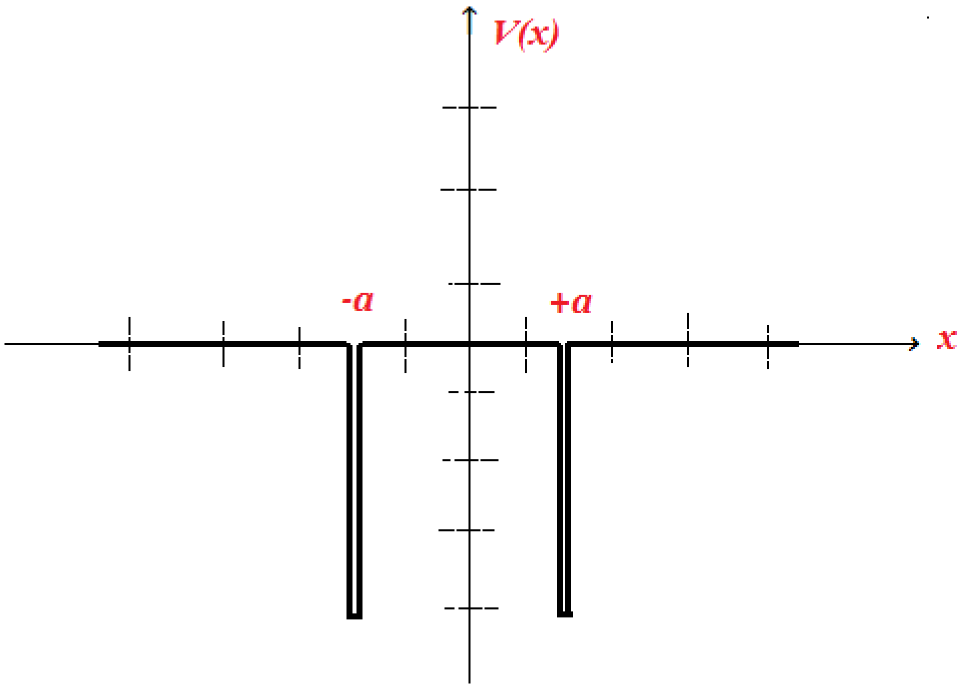

Figure 3.1: A double Dirac δ-potential well.

We wish to investigate how many bound states does it possess and to find the possible allowed energies for $\beta = \frac{\hbar^2}{ma}$ *and* $\beta = \frac{\hbar^2}{4ma}$.

The potential $V(-x)$ is an even function i.e., $V(-x) = V(x)$, then $\psi(x)$ can always be taken to be either even or odd. For a given energy E, if $\psi(x)$ satisfies the time-independent Schrödinger equation so does $\psi(-x)$ and hence also the even and odd linear combination $\psi(x) = \psi(-x)$. The δ-potential show above is called a delta-potential well if β is negative and a δ-potential barrier if β is positive.

3.1.1 Even Solution of Double Dirac δ-Potential Well

In regions away from the δ-potential, where $V(-x) = 0$ (Fig. 3.1 and Fig.3.2).

$$\hat{H}\psi = E\psi \tag{3.2}$$

$$\kappa = \frac{\sqrt{2m(-E)}}{\hbar} \tag{3.3}$$

E is negative, so κ is real.

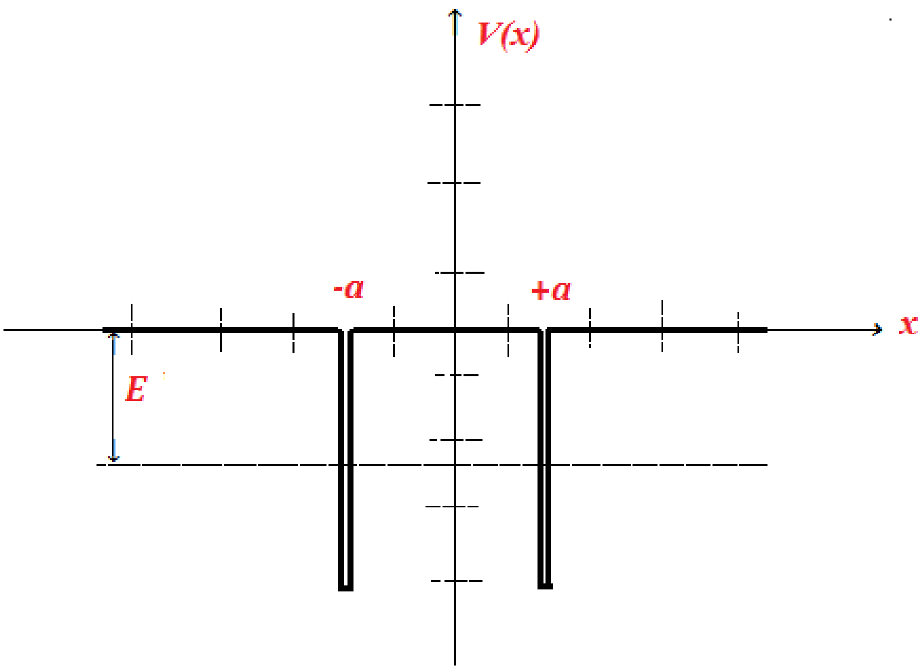

Figure 3.2: A double Diract δ-potential well ($E<0$).

The most general even solution of $\psi_{(even)}(x)$ is

$$\psi_{(even)}(x) = \begin{cases} Ae^{-\kappa x} & x > a \\ Be^{-\kappa x} + Ce^{\kappa x} & 0 < x < a \\ Be^{\kappa x} + Ce^{-\kappa x} & -a < x < 0 \\ Ae^{\kappa x} & x < -a \end{cases} \tag{3.4}$$

Where, in the region $x > a$ the wavefunction becomes $\psi(x) = Be^{\kappa x} + Ae^{-\kappa x}$, *as* $x \longrightarrow \infty$, ψ will blow up, so *B* must be *zero*. And similarly, for the region $x < -a$, where as $x \longrightarrow -\infty$, ψ will blow up as well, so *B* must again be *zero*.

Since $\psi(x)$ is a well-behaved wavefunction, then Born's conditions would be applied to narrow down of constants. The wave function must be continuous at all points, so applying this condition at $(x = a)$ yields

$$Ae^{-\kappa x} \quad |_{x=a} = Be^{-\kappa x} + Ce^{\kappa x} \quad |_{x=a} \tag{3.5}$$

then

$$A = B + Ce^{2ka} \tag{3.6}$$

It is obvious that no information would be extracted if the continuity condition has been applied at $(x = 0)$, and $(x = -a)$ is just repeating $(x = a)$. Another condition that must be applied is the derivative of the wavefunction, when the potential is finite, the continuity must be at all points, so at $(x = 0)$

$$\left.\frac{\partial\psi}{\partial x}\right|_{(x=0;\ 0<x<a)} = \left.\frac{\partial\psi}{\partial x}\right|_{(x=0;\ -a<x<a)} \tag{3.7}$$

$$B = C \tag{3.8}$$

Plugging Eq. (3.6) and Eq. (3.8) into Eq. (3.4), we obtain

$$\psi_{(even)}(x) = \begin{cases} B(1 + e^{2\kappa a})\, e^{-\kappa x} & x > a \\ B(e^{-\kappa x} + e^{\kappa x}) & -a < x < a \\ B(1 + e^{2\kappa a})\, e^{\kappa a} & x < -a \end{cases} \tag{3.9}$$

Since the form of the double δ-potential is $V(x) = -\beta[\delta(x + a) + \delta(x - a)]$. So, plugin this into time-independent Schrödinger becomes

$$\frac{-\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} - \beta[\delta(x + a) + \delta(x - a)]\psi(x) = E\psi(x) \tag{3.10}$$

The idea is to integrate Eq. (3.10) from $-\boldsymbol{\epsilon}$ to $+\boldsymbol{\epsilon}$ and then take the limit as $\boldsymbol{\epsilon}$ goes to a. That is,

$$\int_{-\varepsilon}^{+\varepsilon} \frac{-\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2}dx \; - \beta\int_{-\varepsilon}^{+\varepsilon}[\delta(x+a)+\delta(x-a)]\psi(x)dx = \; E\int_{-\varepsilon}^{+\varepsilon}\psi(x)dx \tag{3.11}$$

$$\frac{-\hbar^2}{2m}\;\frac{\partial\psi}{\partial x}\Big|_{+\varepsilon} - \frac{\partial\psi}{\partial x}\Big|_{-\varepsilon} - \lim_{\epsilon\longrightarrow a}\beta\int_{-\varepsilon}^{+\varepsilon}\delta(x+a)\psi(x)\,dx - \lim_{\epsilon\longrightarrow a}\int_{-\varepsilon}^{+\varepsilon}\delta(xa)\psi(x)\,dx$$

$$= E\lim_{\epsilon\longrightarrow a}\int_{-\varepsilon}^{+\varepsilon}\psi(x)dx. \tag{3.12}$$

Note that at the limit the last term in the left-hand side and the term in the right-hand side are identically *zeros*, so that we are left with

$$\frac{\partial\psi}{\partial x}\Big|_{+\varepsilon} - \frac{\partial\psi}{\partial x}\Big|_{-\varepsilon} = \frac{-2m\beta}{\hbar^2}\psi(a) \tag{3.13}$$

Now letting $\boldsymbol{\epsilon}$ goes to a

$$\psi_{(even)}(x) = B(1+e^{2\kappa a})\,e^{-\kappa x} \qquad\qquad x > a \tag{3.14}$$

$$\frac{\partial\psi}{\partial x}\Big|_{(+a)} = -\kappa B(1+e^{2\kappa a})\,e^{-\kappa a} \tag{3.15}$$

And, for

$$\psi_{(even)}(x) = B(e^{-\kappa x}+e^{\kappa x}) \qquad\qquad -a < x < a \tag{3.16}$$

$$\frac{\partial\Psi}{\partial x}\Big|_{(-a)} = B(-\kappa e^{-\kappa a}+e^{\kappa a})$$

$$= -\kappa B(1-e^{2\kappa a})\,e^{-\kappa a} \tag{3.17}$$

Discontinuous derivative at a gives

$$\Delta\left(\frac{\partial\psi}{\partial x}\right) = \frac{-2m\beta}{\hbar^2}\psi(a) \tag{3.18}$$

$$\kappa B(1+e^{2\kappa a})\,e^{-\kappa a} + \kappa B(1-e^{2\kappa a})\,e^{-\kappa a} = \frac{-2m\beta}{\hbar^2}\psi(a) - 2\kappa B e^{-\kappa a}$$

$$= \frac{-2m\beta}{\hbar^2}\psi(a) \tag{3.19}$$

But, we have

$$\psi(a) = B(e^{-\kappa a}+e^{\kappa a}) \tag{3.20}$$

$$-2\kappa B e^{-\kappa a} = \frac{-2m\beta}{\hbar^2} B(e^{-\kappa a} + e^{\kappa a})$$

$$\frac{\hbar^2\kappa}{m\beta} - 1 = e^{-2\kappa a} \tag{3.21}$$

To obtain a condition on the energy we need κ, Eq. (3.21) is a transcendental equation in κ, so solving it numerically is the only way we could do. We can see the solution graphically by plotting the right and the left-hand side and look for the intersections. If we introduce an auxiliary variable (say, $y \equiv 2\kappa a$ and $\xi \equiv \frac{\hbar^2}{2ma\beta}$) this makes it easier to deal with, so we left with

$$\xi y - 1 = e^{-y} \tag{3.22}$$

We plot both sides and look for intersections. From the Figs. $(3.3 - 3.5)$ we see that ξ and y are both positive and there is one and only one solution for even ψ.

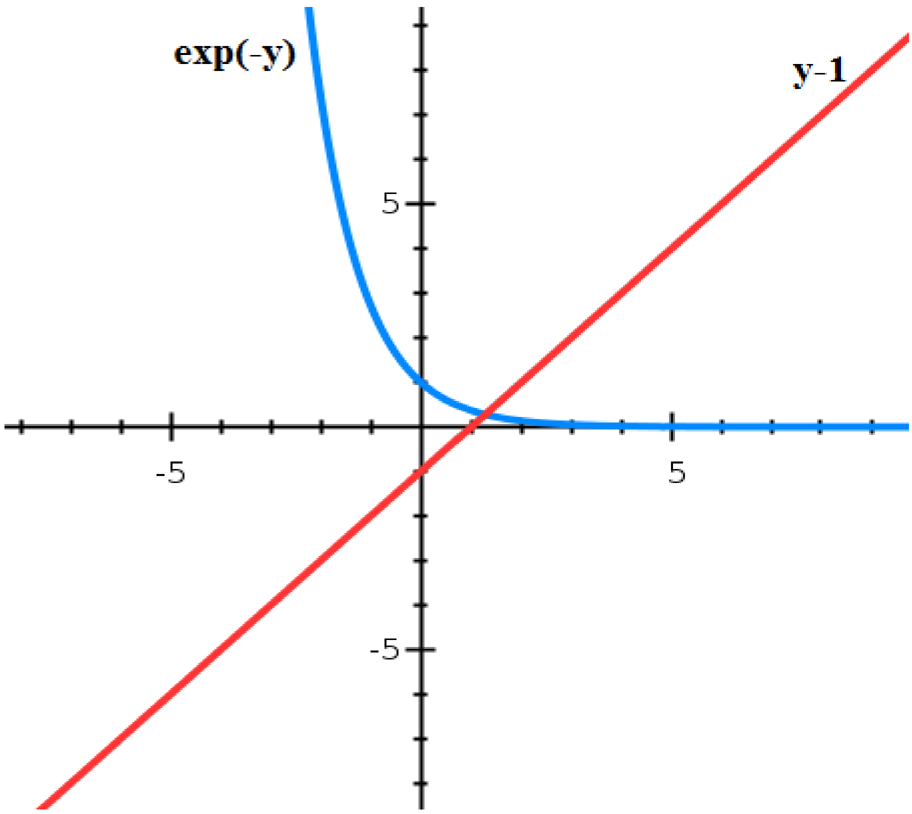

Figure 3.3: A plot of $y - 1$ *and* e^{-y} versus y on the same frame to find the solution for the equation $y - 1 = e^{-y}$.

If $\beta = \frac{\hbar^2}{2ma}$, so $\xi = 1$ (the solution can be seen around $\xi = 1$ but to see this more clearly, we can use a software to solve this equation numerically).

So, y =1.27846 (Fig. 3.3). Since

$$\kappa^2 = \frac{-2mE}{\hbar^2} = \frac{y^2}{(4a^2)} \tag{3.23}$$

Then the energy

$$E = -\frac{(1.278)^2}{8}\left(\frac{\hbar^2}{ma^2}\right) = -\,0.204\left(\frac{\hbar^2}{ma^2}\right) \tag{3.24}$$

If $\beta = \frac{\hbar^2}{ma}$, so $\xi = \frac{1}{2}$. (Fig. 3.4);

$$e^{-y} = \frac{1}{2}y - 1 \;\Rightarrow\; y = 2.21772 \tag{3.25}$$

So, the energy

$$E = -0.615\left(\frac{\hbar^2}{ma^2}\right) \tag{3.26}$$

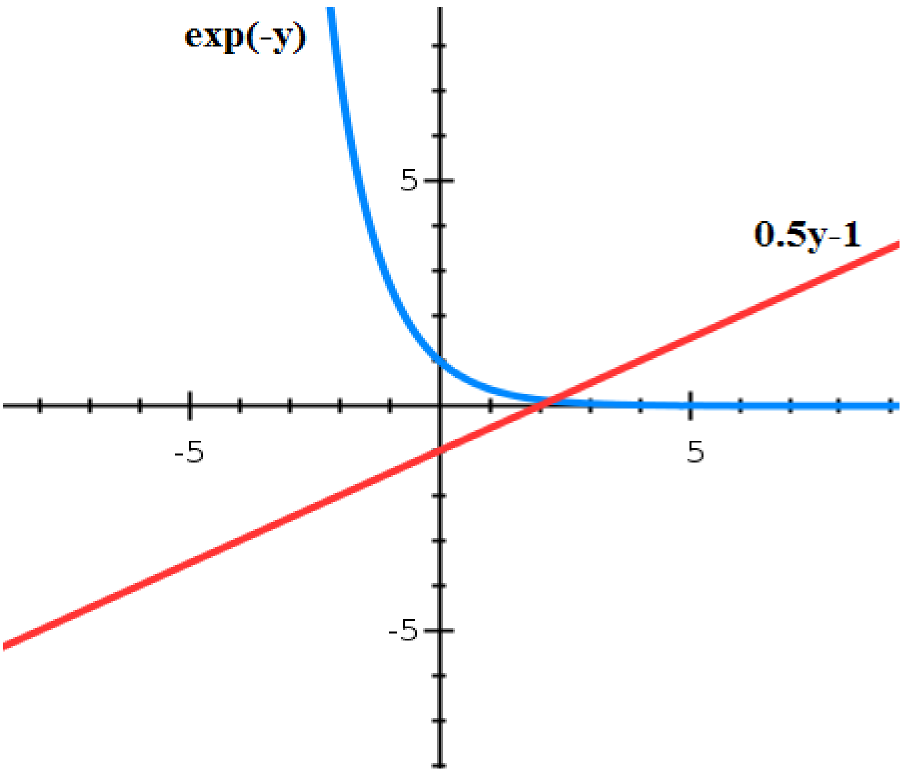

Figure 3.4: The plot of the straight line $\frac{1}{2}y - 1$ and the curve e^{-y} with their intersection.

If $\beta = \frac{\hbar^2}{4ma}$, so $\xi = 2$ (Fig. 3.5);

$$\text{Only even: } e^{-y} = 2y - 1 \Rightarrow y = 0.738835 \tag{3.27}$$

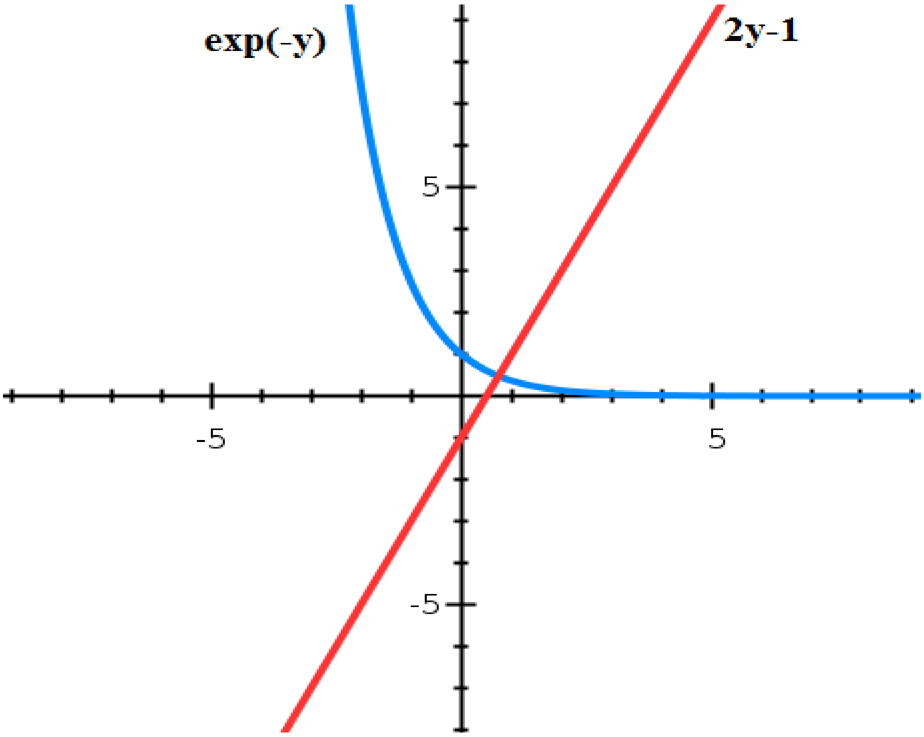

Figure 3.5: The plot of $2y - 1$ *and* $e^{-y}$and their intersection.

Then, the energy is

$$E = -\,0.0682\left(\frac{\hbar^2}{ma^2}\right) \tag{3.28}$$

3.1.2 Odd Solution of Double Dirac δ-Potential Well

The most general odd solution of $\psi_{(odd)}(x)$ is

$$\psi_{(odd)}(x) = \begin{cases} Ae^{-\kappa x} & x > a \\ Be^{-\kappa x} - Ce^{\kappa x} & 0 < x < a \\ -Be^{\kappa x} + e^{-\kappa x} & -a < x < 0 \\ -Ae^{\kappa x} & x < -a \end{cases} \tag{3.29}$$

As before, at $(x = a)$ the continuity condition gives

$$\psi_{(odd)}(x)|_{(x=a;x>a)} = \psi_{(odd)}(x)|_{(x=a;-a<x<a)} \tag{3.30}$$

$$Ae^{-\kappa a} = Be^{-\kappa a} - Ce^{\kappa a}$$

$$A = B - Ce^{-2\kappa a} \tag{3.31}$$

This time the continuity of the derivative at (*x* = *0*) gives us nothing new, but the continuity of the wave function itself gives us

$$\psi_{(0dd)}(x)|_{(x=0;\, for\ 0<x<a)} = \psi_{(odd)}(x)|_{(x=0;\, for\ -a<x<0)} \tag{3.32}$$

$$Be^{-\kappa(0)} - Ce^{\kappa(0)} = -Be^{\kappa(0)} + Ce^{-\kappa(0)}$$

$$B - C = -B + C$$

$$B = C \tag{3.33}$$

Thus, the wave function is

$$\psi(x) = \begin{cases} B(1 - e^{2\kappa a})\, e^{-\kappa x} & x > a \\ B(e^{-\kappa x} - e^{\kappa x}) & -a < x < a \\ -B(1 - e^{2\kappa a})\, e^{\kappa x} & x < -a \end{cases} \tag{3.34}$$

Now, we follow the same argument as before to obtain

$$\left.\frac{\partial\psi}{\partial x}\right|_{(x=+a;\, for\ x>a)} = \left.\frac{\partial\psi}{\partial x}\right|_{(x=-a;\, for\ -a<x<a)} \tag{3.35}$$

$$-\kappa B(1 - e^{2\kappa a})\, e^{-\kappa a} = -B\kappa(1+e^{2\kappa a})\, e^{-\kappa a} \tag{3.36}$$

$$\Delta\left(\frac{\partial\psi}{\partial x}\right)_{(odd)} = \left(\frac{\partial\psi}{\partial x}\right)_{(a+)} - \left(\frac{\partial\psi}{\partial x}\right)_{(a-)} \tag{3.37}$$

$$= -\kappa B(1 - e^{2\kappa a})\, e^{-\kappa a} + B\kappa(1+e^{2\kappa a})\, e^{-\kappa a}$$

$$= 2\kappa B e^{\kappa a} \tag{3.38}$$

As in the even solution, last term in the left-hand side and the term in the right-hand side in the Eq. (3.12) are identically *zeros* at the limit, so that we are left with

$$\left.\frac{\partial\psi}{\partial x}\right|_{+\varepsilon} - \left.\frac{\partial\psi}{\partial x}\right|_{-\varepsilon} = \frac{-2m\beta}{\hbar^2}\psi(a) \tag{3.39}$$

$\Delta\left(\frac{\partial\psi}{\partial x}\right)_{(odd)} = \frac{-2m\beta}{\hbar^2}\psi(a)$, where is, $\psi(a) = B(e^{-\kappa x} - e^{\kappa x})$

$$\Delta\left(\frac{\partial\psi}{\partial x}\right)_{(odd)} = 2\kappa B e^{\kappa x} \tag{3.40}$$

$$2\kappa B e^{\kappa x} = \frac{-2m\beta}{\hbar^2}\, B(e^{-\kappa x} - e^{\kappa x})$$

$$\kappa = \frac{m\beta}{\hbar^2}(1 - e^{-2\kappa a}) \tag{3.41}$$

$$e^{-2\kappa a} = 1 - \frac{\hbar^2 \kappa}{m\beta} \tag{3.42}$$

Introducing the auxiliary variables ($y \equiv 2\kappa a$ and $\xi \equiv \frac{\hbar^2}{2ma\beta}$) the Eq. (3.42) is converted to:

$$e^{-y} = 1 - \xi y \tag{3.43}$$

This time there may or may not be a solution. Both graphs have their y-intercepts at 1. However, if ξ is smaller there will be an intersection, whereas if ξ is too large (β too small), there may not be. Note that $y = 0 \Rightarrow \kappa = 0$ is not a solution, since ψ is non-normalizable. The slope of $(1- \xi y)$ is $-\xi$; and the slope of at $y = 0$ is -1. So, there is an odd solution $\Rightarrow y < 1$ or $\beta > \frac{\hbar^2}{2ma}$. We conclude that one bound state occurs if $\beta \le \frac{\hbar^2}{2ma}$; and two bound states if $\beta > \frac{\hbar^2}{2ma}$ (Fig. 3.7).

For $\beta = \frac{\hbar^2}{ma} \Rightarrow \xi = \frac{1}{2}$ (Fig. 3.6), then

$$e^{-y} = 1 - \frac{1}{2}y \Rightarrow y = 1.59362 \tag{3.44}$$

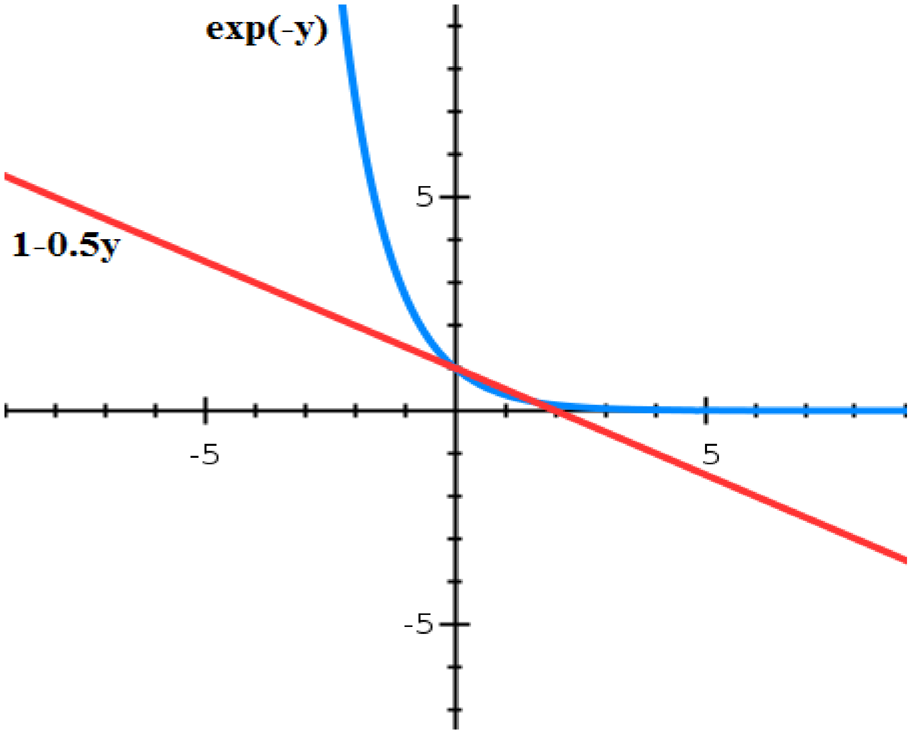

Figure 3.6: The plot of $1 - \frac{1}{2}y \; and \; e^{-y}$ and their two-point intersection.

Then energy is

$$E = -0.317 \left(\frac{\hbar^2}{ma^2}\right) \tag{3.45}$$

For $\beta = \frac{\hbar^2}{4ma}$, in this case, there is intersection except the non-physical one at $\xi = 0$. So for this value of β, there is no bound state with an odd wave function (Fig. 3.8).

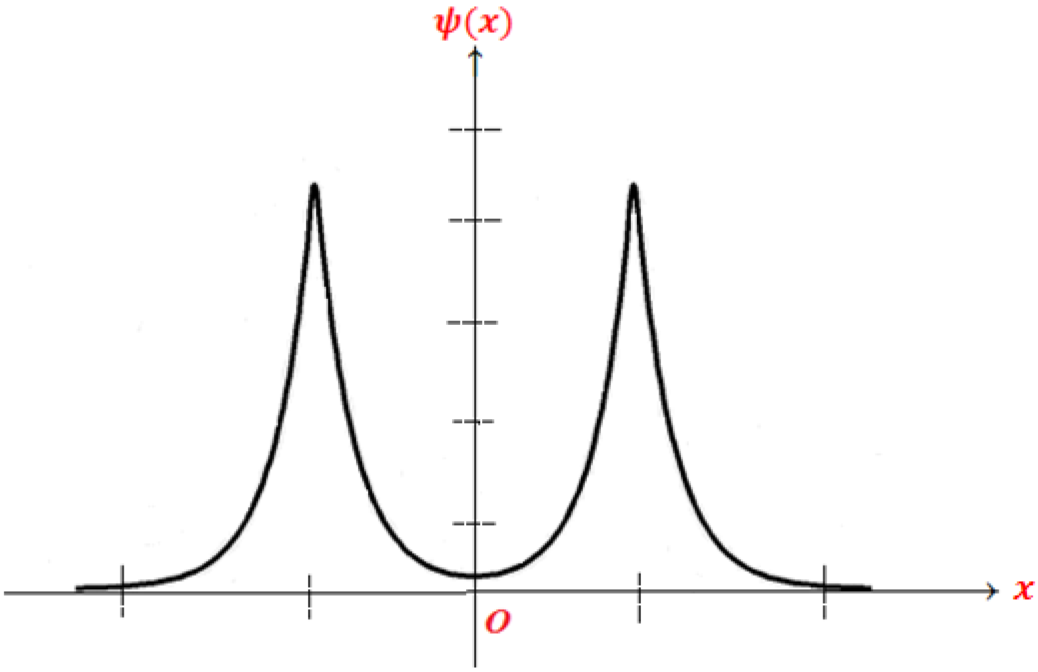

Figure 3.7: Typical symmetric eigenstate of an electron in a double δ-potential well.

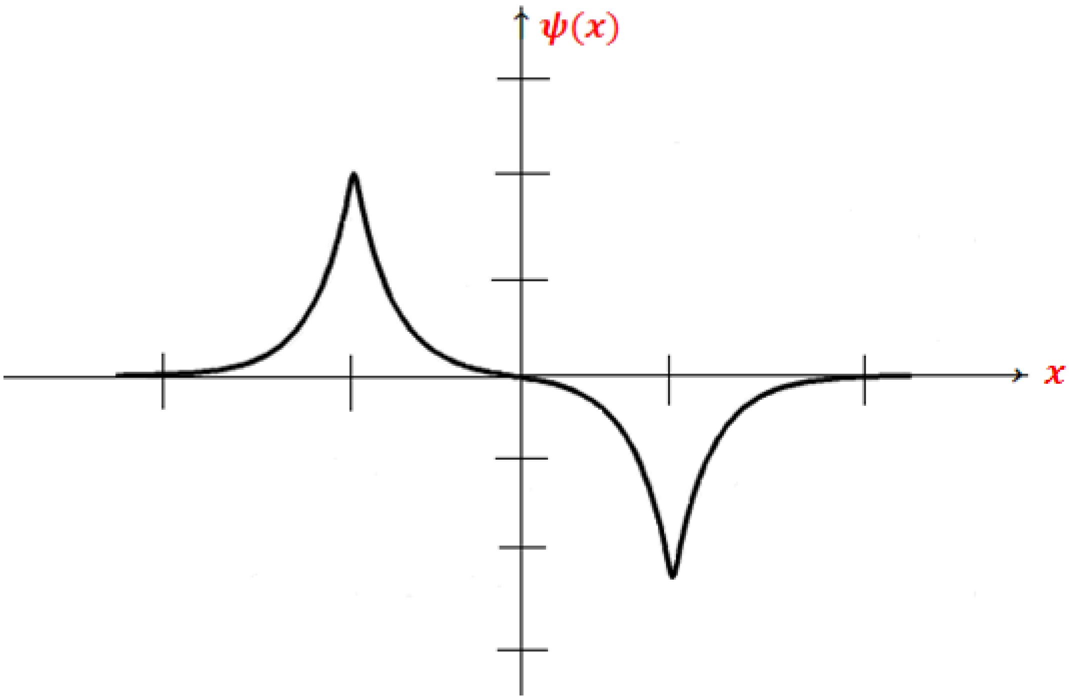

Figure 3.8: Typical antisymmetric eigenstate of an electron in a double δ-potential.

3.2 Double Dirac δ-Potential Well Scattering States

In the previous sections we had a look at the bound states of the double δ-potential. In this section, we'll look at the scattering states of this potential. At first glance, this problem seemed to be a trivial extension of the single δ-function potential case. For a surge of particles incident from the left, then a part will get transmitted, with the remainder being reflected at the first δ-function. Of those that being transmitted, another fraction will be reflected at the second δ-function, and those left will be transmitted to move in the right to infinity.

Again, those particles that are reflected at the second δ-function will go back the left and some fraction will be reflected to right-hand side once more when they faced the first δ-function. The process will be infinitely repeated bouncing back and forth between the two δ-functions, i.e., an infinite of reflections and transmissions. The best way to handle this problem is to confront the mathematical procedure and see where it leads us. Since we have considered that the particles enter from the left, so there is not any stream travelling from the right. In this case, the solution is asymmetric, i.e., we cannot consider an even and an odd solution to such problem.

This most general solution of $\psi(x)$ in this problem is

$$\psi(x) = \begin{cases} Ae^{ikx} + Be^{-ikx} & x < -a \\ Ce^{ikx} + De^{-ikx} & -a < x < a \\ Fe^{ikx} & x > a \end{cases} \tag{3.46}$$

Some constants will be eliminated by applying boundary conditions. The continuity of the wavefunction at $(x = -a)$ yields

$$\psi(x)|_{(x=-a;\, for\, x<-a)} = \psi(x)|_{(x=-a;\, for\, -a<x<a)} \tag{3.47}$$

$$Ae^{-ika} + Be^{ika} = Ce^{-ika} + De^{ika} \tag{3.48}$$

Also, the continuity at $(x = a)$ gives

$$\psi(x)|_{(x=a;\, for\, -a<x<a)} = \psi(x)|_{(x=a;\, for\, x>a)} \tag{3.49}$$

$$Ce^{ika} + De^{-ika} = Fe^{ika} \tag{3.50}$$

We can be guided by a single δ-function at $(x = 0)$, where the same condition to the change of derivative of $\psi(x)$ across the delta function will be now applied except for the former at $(x = \pm a)$ is being satisfied.

$$\Delta\left(\frac{\partial\psi}{\partial x}\right) = \frac{-2m\,\beta}{\hbar^2}\,\psi(\pm a) \tag{3.51}$$

At $(x = -a)$

$$\Delta\left(\frac{\partial\psi}{\partial x}\right) = ik[Ce^{-ika} - De^{ika} - Ae^{-ika} + Be^{ika}]$$

$$= \frac{-2m\,\beta}{\hbar^2}(Ae^{-ika} + Be^{ika}) \tag{3.52}$$

Similarly, at $(x = a)$ we have

$$\Delta\left(\frac{\partial\psi}{\partial x}\right) = ik[Fe^{ika} - Ce^{ika} + De^{-ka}]$$

$$= \frac{-2m\,\beta}{\hbar^2}(Fe^{ika}) \tag{3.53}$$

We are left with four equations in five unknowns which are *A*, *B*, *C*, *D*, and *F*. The system of equations which is constituted in the constants can be expressed in terms of the constant *A*. So, it is algebraically straightforwardly manipulated and solved. Using a software to do this will save us from a laborious work. The results are

$$B = \frac{-iy[2y\,sin(2ka) - 4k\,cos(2ka)]}{y^2(e^{i4ka} - 1) + 4k(k - iy)}A \tag{3.54}$$

$$C = \frac{-i2k(y + i2k)}{y^2(e^{i4ka} - 1) + 4k(k - iy)}A \tag{3.55}$$

$$D = \frac{i2kye^{i2ka}}{y^2(e^{i4ka} - 1) + 4k(k - iy)}A \tag{3.56}$$

$$F = \frac{4k^2}{y^2(e^{i4ka} - 1) + 4k(k - iy)}A \tag{3.57}$$

Where $y = \frac{2m\beta}{\hbar^2}$.

The reflection coefficient (R) relation is

$$R = \frac{|B|^2}{|A|^2} = \frac{2y^4(2k\cos(2ka) - y\sin(2ka))^2}{8k^4 + 4k^2y^2 + y^4 - 4ky^3\sin(4ka) + y^2\cos(4ka)[4k^2 - y^2]} \tag{3.58}$$

Similarly, the transmission coefficient (T) is

$$T = \frac{|F|^2}{|A|^2} = \frac{8k^4}{8k^4 + 4k^2y^2 + y^4 - 4ky^3\sin(4ka) + y^2\cos(4ka)[4k^2 - y^2]} \tag{3.59}$$

It is easy to check that

$$R + T = 1 \tag{3.60}$$

The internal reflection and transmission rates can be calculated in the same fashion

$$T_{(internal)} = \frac{|C|^2}{|A|^2} = \frac{2y^2k^2 + 8yk^4}{8k^4 + 4k^2y^2 + y^4 - 4ky^3\sin(4ka) + y^2\cos(4ka)[4k^2 - y^2]} \tag{3.61}$$

$$R_{(internal)} = \frac{|D|^2}{|A|^2} = \frac{2y^2k^2}{8k^4 + 4k^2y^2 + y^4 - 4ky^3\sin(4ka) + y^2\cos(4ka)[4k^2 - y^2]} \tag{3.62}$$

In fact,

$$R_{(internal)} + T = T_{(internal)} \tag{3.63}$$

which means that the sum of probabilities of that being reflected from the second well and that being transmitted through it is equal to the probability of being transmitted pass the first well. The first ratio represents the flow to the right direction after the first δ-function, whereas the second represents the flow to the left, which is obviously a smaller than the first one.

This approach makes sense, since as we would expect that the main stream incident from the left, and of that which gets transmitted pass the first well, partial fractions will get transmitted past the second well and escaped, while some will get reflected towards the first well.

Chapter 4

THE ROLE OF DISTRIBUTIONS IN PHYSICS

From the inception of quantum mechanics (QM), almost a century ago distributional functions have been indispensable. The most famous among these distributions is known to be the Dirac delta function, $\delta(x)$, called at the same time the Dirac distribution whose support is defined at a point. For this reason, point sources such as mess or change can be expressed in terms of the delta function. Closely related with the delta function is the Heaviside step function, which have a large but discontinuous support. We define the step function by

$$\theta(x) = \begin{cases} 1, & x > 0 \\ 0, & x < 0 \end{cases} \tag{4.1}$$

So that we have the relation

$$\delta(x) = \frac{d}{dx}\theta(x) \tag{4.2}$$

The one-dimensional Green function satisfies the second order differential equation given by

$$\frac{d^2G}{dx^2} = \delta(x) \tag{4.3}$$

Whose solution is expressed in the terms of the absolute value function

$$G(x) = \frac{1}{2}|x| \tag{4.4}$$

This can be easily checked by integrating both side from $-\infty$ to $+\infty$.

As a matter of fact, any sourceful second order equation can be constructed from a Green function whose source is a delta function. In particular the basic equation of

QM, the Schrödinger equation, is a second order equation whose solution can be constructed from Green functions. More generally, any impulsive event such as an impulse wave, explosion of a source, jets, supernova events etc. can be formulated mathematically only with the help of the delta function. Not need to mention that orthogonality, orthonormality, complementary and many other mathematical events / processes are defined by the delta function.

As an example, we consider the following second order differential equation

$$F'' = h(x)F \tag{4.5}$$

Where a prime means $\frac{d}{dX}$, and $h(x)$ stands for a potential of the form

$$h(x) = \pm\delta(x) \mp \delta(x - x_0) \tag{4.6}$$

Clearly this potential represents two spikes located at $x = 0$ and $x = x_0$.

Our aim is to integrate this equation provided we have the proper boundary conditions. The method is to apply Laplace transform, use selected boundary conditions and then at the end to invert the transform and obtain $F(x)$. We multiply both sides of the differential equation by e^{-sx} when s is the Laplace transform parameter and integrate with respect to x from $x = 0$ to $x = \infty$.

We have

$$\mathcal{L}[1] = \frac{1}{s} \tag{4.7}$$

$$\mathcal{L}[x\theta(x)] = \frac{1}{s^2} \tag{4.8}$$

$$\mathcal{L}[(x - x_0)\theta(x - x_0)] = \frac{e^{-sx_0}}{s^2} \tag{4.9}$$

And so on.

We obtain as a result of the inverse Laplace transform $\mathcal{L}^{-1}[\quad]$, the solution for *F(x)* as

$$F(x) = 1 + x\theta(x)[F'(0) \pm 1] \mp F(x_0)(x - x_0)\theta(x - x_0) \tag{4.10}$$

So that by initial condition

$$F'(0) = 0 \tag{4.11}$$

$$F(x_0) = 1 + x_0 \tag{4.12}$$

One finds

$$F(x) = 1 + \ x\theta(x) - \ (1 + x_0)(x - x_0)\theta(x - x_0) \tag{4.13}$$

One can easily check that by direct substitution of this expression into the differential equation with the given potential the equation will be satisfied. We stress once more that all derivations are taken in the sense of distributions. Another example is the one that makes of the Heaviside step function, namely

$$F'' = -\theta(x)F(x) \tag{4.14}$$

By applying the Laplace Transform once more to this equation and integrating appropriately it will not be difficult to show that the solution is given by

$$F(x) = F_0\, cos\big(x\theta(x)\big), (F_0 = constant) \tag{4.15}$$

The first derivative

$$F'(x) = -F_0\theta(x)\, sin\big(x\theta(x)\big) \tag{4.16}$$

And the second derivative

$$F''(x) = -\theta(x)F_0\, cos(x\theta(x)) \tag{4.17}$$

$$F''(x) = -\ \theta(x)F \tag{4.18}$$

Which shows that $F(x)$ is a solution. Note that the distributional conditions such as

$$x\delta(x) = 0 \tag{4.19}$$

$$\theta^2(x) = \theta(x) \tag{4.20}$$

are used whenever necessary.

Interestingly not only *2*-delta function differential equation but *N*-number of delta function equation is also solvable. That means, take

$$F''(x) = h(x)F \tag{4.21}$$

where

$$h(x) = \delta(x) + \sum_{i=0}^{N} A_i \delta(x - x_0) \tag{4.22}$$

Solution for *F(x)* follows through the inverse Laplace transform which is

$$F(x) = \mathcal{L}^{-1}\left[\frac{1}{s^2} + \frac{1}{s} + \sum_{i=0}^{N} A_i \frac{e^{-sx_i}}{s^2} F(x_i)\right] \tag{4.23}$$

Here the constants $F(x_i)$ are defined by

$$F(x_N) = 1 + x_N + \sum_{i=0}^{N-1} A_i (x_N - x_i) F(x_i) \tag{4.24}$$

Note that for $N = 0$, we have $F(x_0) = 1 + x_0$.

The general solution for *F(x)* is given by [8].

$$F(x) = 1 + x\theta(x) - 2\sum_{i=0}^{N}(-1)^{\ell}(x - x_\ell)\theta(x - x_\ell)$$

$$\times \prod_{n=0}^{\ell}\left(\frac{1+(-1)^{n-1}x_{n-1}}{1-(-1)^{n}u_n}\right) \tag{4.25}$$

Can Schrödinger equation be integrated exactly in the presence of delta functions?

Let us take the Schrödinger equation in the following form

$$\psi'' - \frac{\lambda}{a_0}\sum_{N=0}^{\infty} \delta(x - Na_0)\,\psi = \frac{-2mE}{\hbar^2}\psi \tag{4.26}$$

For simplicity we choose $\lambda = 1$ and $E_0 = \frac{-2mE}{\hbar^2}$ and $N = 0$, which implies that

$$\psi'' - \frac{1}{a_0}\delta(x)\psi(x) = E_{\grave{o}}\psi \tag{4.27}$$

By the Laplace transform we obtain

$$(s^2 - E_0)\mathcal{L}[\psi] - s\psi(0) - \psi'(0) = \frac{1}{a_0}\psi(0) \tag{4.28}$$

Take now the case $E_0 > 0$ $(or\ E < 0)$. We obtain for $(s > 0)$ for the Cauchy integral

$$\psi(x) = \frac{1}{2\sqrt{\frac{-2mE}{\hbar^2}}} e^{\sqrt{\frac{-2mE}{\hbar^2}}x} \left[\left(\sqrt{\frac{-2mE}{\hbar^2}} + \frac{1}{a_0} \right) \psi(0) + \psi'(0) \right] \tag{4.29}$$

This becomes meaningful only in case we impose the initial conditions $\psi(0)$ and $\psi'(0)$. Going to higher number of delta potentials, however, becomes rather tedious so that the Laplace transform technique is not applicable to the Schrödinger equation with non-zero eigenvalue, i.e., $E_0 \neq 0$.

Chapter 5

CONCLUSION

In this thesis, we considered first the quantum model known as the Kronig-Penney model. The periodic potential is modeled by a series of infinite square wells potentials. Whose limit goes to delta-function to replace the broad barrier. However, we are proceeded with a bit harder calculation. By applying the continuity and the discontinuity of the derivative of the wave function when passing through a barrier, the Bloch's theorem was used.

The aim of the approach is to have a look at what restrictions is for an electron in a periodic potential can be found. A relation between the wave function and k in Bloch wave are obtained. From this model we have the condition (2.25). Both left and right-hand sides of this condition are bounded by 1 and $1 + P\left[\frac{\sin Ka}{ka}\right]$, respectively. Thus, this equality does not hold for some regions. However, these forbidden band are given by the onset of forbidden regions. As a result, allowed and forbidden values of k are yielded. Moreover, a delta-potentials are still valid for such model.

The double-function potential in one dimension is a problem of considerable interest in that it allows us to study the influence on a primary potential. We have studied both bound-state energies of two different strengths of delta-function ($\beta = \frac{\hbar^2}{ma}$ and $\beta = \frac{\hbar^2}{4ma}$) and the scattering states. For the former case, the even and odd solutions have been separately studied. The transcendental equation (3.22) has been graphically solved by the right and the left-hand side plot, the intersections for a different value of (ξ) is graphed and labelled. For each graph, the energy has been determined. We used a software to see the solution more clearly. We concluded that the even solution has a bound state for both strengths of the delta-function. The odd solution is as well considered. Like the even solution case, the transcendental equation (3.43) is obtained. We concluded that either, one bound state occurs if $\beta \leq \frac{\hbar^2}{2ma}$; and two bound states if $\beta > \frac{\hbar^2}{2ma}$. However, for $\beta = \frac{\hbar^2}{4ma}$, there is no intersection except for the non-physical case at $\xi = 0$. In other words, no bound states arise with such an odd wave function.

The double delta-function well scattering case is as well covered. We are left with four equations in five unknowns (*A*, *B*, *C*, *D*, and *F*) in such away that the constants are expressed in terms of a constant *A*. A software has been used to solve these equations. The relations of both reflection and transmission coefficients are obtained. We concluded that the relation of the internal scattering is that the probability of being transmitted pass the first well is equal to the sum of probabilities of that being reflected from the second well and that transmitted through it.

The role of the distributions is discussed briefly in general, hoping that more ground of applications will be available in quantum-well problems.

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