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Quantum Mechanics With a Quartic Dispersion Law

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QUANTUM MECHANICS WITH A QUARTIC DISPERSION LAW

A Thesis Presented

by

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ABSTRACT

QUANTUM MECHANICS WITH A QUARTIC DISPERSION LAW

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Creation of three-dimensional matter waves, the three-dimensional analog of one-dimensional solitons, has been a goal of experimental physics for some time. A recent proposal has suggested that changing the dispersion law from quadratic to quartic for ultra cold atoms in a shaken lattice should allow for the creation of these objects. In this thesis, we develop the theoretical basis for quantum mechanics with a quartic dispersion law. The probability current functional is constructed from the corresponding time-dependent Schrödinger equation, and used to derive the junction conditions that connect the derivatives of the wavefunction on one side of a potential discontinuity to the ones on the other side. Reflection and transmission amplitudes are determined for scattering problems concerning both step potentials and rectangular barriers/wells. For sufficiently narrow barriers/wells, we show that a δ-potential constitutes a simple but reliable model for the scatterer. The scattering properties of wide barriers/wells are consistent with the predictions of the classical theory. Finally, we find the eigenstates and eigenenergies of a particle in an infinitely deep well. A simple approximate expression for the high-energy spectrum is obtained; it is found to be fully consistent with Weyl's law. Our results should aid in the development of experimental systems capable of creating and sustaining self-supporting, mobile, three-dimensional matter waves.

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CHAPTER 1

INTRODUCTION

This thesis constitutes an integral part of a project aimed at an experimental creation of three-dimensional solitary matter waves of cold bosonic atoms. While one-dimensional solitons have been experimentally realized [1, 2], their three-dimensional analogs remain experimentally elusive. Creation of a mobile, self-supporting three-dimensional matter wave remains a goal of physics of ultracold gases [3].

The difficulty in creating these self-supporting matter waves in three dimensions comes from the need to balance collapse and dissipation forces acting on the atoms. In fact, three-dimensional Bose-Einstein solitons in continuum space can be shown to be unstable [3]. A number of strategies have been employed to circumvent this problem, including utilization of optical lattices to create discrete solitons which are stable for specific sets of parameters [4–6], use of time-dependent non-linearities [7], and spatial variation of nonlinearity strength [8]. However, none of these strategies fully reach the goal: either the soliton suggested is not mobile, filling a large fraction of the whole dispersion curve [4–6], or its scheme requires losses [7], thus limiting its life-time, or the scheme lacks the translational invariance [8].

It has been suggested that instead of attempting to avoid the problem, a natural way to create a stable large three-dimensional soliton is to change the atomic dispersion law, from quadratic to quartic [3]. Dispersion laws have been already successfully altered in numerous previous experiments [9, 10] using a variety of methods, including shaken lattices [9, 11, 12].

Before making any concrete experimental suggestions that uses quartic dispersion, however, it is necessary to form an understanding of quantum mechanics with a quartic dispersion law. The name of the game here is to shut the acquired intuition off and diligently redo all the standard scattering and bound value problems with piece-wise-constant potential to gain a new one. Even the deceivingly familiar reflection from a hard wall exhibits a nontrivial energy dependence of the phase of the reflected wave, instead of the familiar sign-flip. In the world with quartic dispersion, nothing should be taken for granted, and it won't be. As in the conventional quantum mechanics, our first line of attack is the problems with piece-wise-constant potentials.

To formulate the rules for relating the wavefunction on one side of a potential discontinuity to the one on another we request the continuity of the probability current. To this end, we re-derive the probability current functional afresh. Armed with these rules, we solve scattering problems with a rectangular step, with localized rectangular potentials, both a hill and a well, and with a δ-potential, both repulsive and attractive; we proceed, using some of our scattering results, to quantization of particle motion in an infinitely deep well. We compare our results with a formula produced by Weyl's law, that we successfully adapt to the quartic dispersion.

CHAPTER 2

CONVENTIONAL DISPERSION

Before approaching problems in one-dimensional quantum mechanics with a quartic dispersion law, it is necessary to have an understanding of conventional one-dimensional quantum mechanics. The strategies used to solve the problems in conventional quantum mechanics outlined here will be similar to the strategies used to solve the analogous problems in quantum mechanics problems with quartic dispersion. These concepts and problems are standard for any introductory course in quantum mechanics, and are considered to summarize the important main ideas of quantum mechanics.

2.1 Probability Current

In conventional quantum mechanics in one dimension, wavefunctions of normalizable states are normalized such that

$$\int \Psi^* \Psi dx = 1 \tag{2.1}$$

where Ψ is a wavefunction that is a solution to the Schrödinger equation, and Ψ^* is its complex conjugate. The amplitude $|\Psi|^2$ is interpreted as a probability, specifically the probability of finding the particle described by wavefunction Ψ in the interval of integration.

The time-dependent one-dimensional Schrödinger equation reads

$$i\hbar\frac{\partial}{\partial t}\Psi(x,t) = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\Psi(x,t) + V(x)\Psi(x,t) \tag{2.2}$$

where m is the mass of the particle, and $\hbar$ is the reduced Planck's constant, defined as $\hbar = \frac{h}{2\pi}$. In operator notation, this can be expressed as

$$i\hbar\frac{\partial}{\partial t}\Psi(x,t) = \hat{H}\Psi \tag{2.3}$$

where $\hat{H}$ is the Hamiltonian operator $[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)]$. One can then write

$$i\hbar\frac{\partial}{\partial t}\left(\Psi^*\Psi\right) = \Psi^*\hat{H}\Psi - \Psi\hat{H}\Psi^* \tag{2.4}$$

so that the $V(x)$ terms cancel, being real. The expression can then be re-written as

$$\frac{\partial}{\partial t}\left(\Psi^*\Psi\right) = \frac{\partial}{\partial x}\frac{i\hbar}{2m}\left(\Psi^*\frac{\partial}{\partial x}\Psi - \frac{\partial}{\partial x}\Psi^*\Psi\right) \tag{2.5}$$

independent of potential. This has the form of an equation of continuity, indicating a conservation law [13].

Let

$$J(x) = \frac{\hbar}{2m}\,\mathrm{Im}[\Psi^*\frac{\partial}{\partial x}\Psi]\,. \tag{2.6}$$

Then if both sides of (2.5) are integrated over the interval x_1 to x_2, one obtains

$$\frac{\partial}{\partial t}\int_{x_1}^{x_2}\Psi^*\Psi dx = J(x_1) - J(x_2)\,. \tag{2.7}$$

According to (2.1), however, the left-hand side is simply the time derivative of the probability, and so $J(x)$ is identified as the probability current, which then must be a conserved quantity [13]. This will be used to determine the connection between the values of the wavefunction derivatives to the right and to the left of the potential discontinuity; also the spatial constancy of current allows for an efficient consistency check in scattering problems.

2.2 Scattering Problems

Scattering is a major experimental tool in many branches of physics, and scattering theory provides the framework to design and interpret those experiments. Scattering problems are concerned with free particles, which come from asymptotically large distances away, interact with an object or potential, and return to a large distance from the potential. In other words, these problems deal with unbound particles, which can be found at continuum many energy levels, colliding with objects and continuing on as unbound particles. Here we will review the most common introductory conventional quantum mechanics scattering problems in one dimension: scattering of a wave incident on a potential step, and scattering of a wave incident on a rectangular barrier.

2.2.1 Step potential

In these problems, consider the time-independent Schrödinger equation and a potential with a discontinuous jump at $x = 0$. That is,

$$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\Psi(x) + V(x)\Psi(x) = E\Psi(x) \tag{2.8}$$

where

$$V(x) = \begin{cases} 0, & x < 0 \\ U_0, & x > 0\,. \end{cases} \tag{2.9}$$

There are two possibilities for a wave with incoming energy E encountering this potential; that the incoming wave is above the potential, i.e. $E > U_0$, or that the incoming wave is below the potential, i.e. $E < U_0$. Each of these is diagrammed in Figure 2.1. In both cases, to the left of the barrier the wavefunction is

$$\psi(x < 0) = \alpha e^{ikx} + \beta e^{-ikx} \tag{2.10}$$

where α is the amplitude of the incoming wave, and β is the amplitude of the reflected wave. To the right of the barrier, the wavefunction must be

$$\psi(x > 0) \begin{cases} \gamma e^{ik'x}, & E > U_0 \\ \eta e^{-k'x}, & E < U_0 \end{cases} \tag{2.11}$$

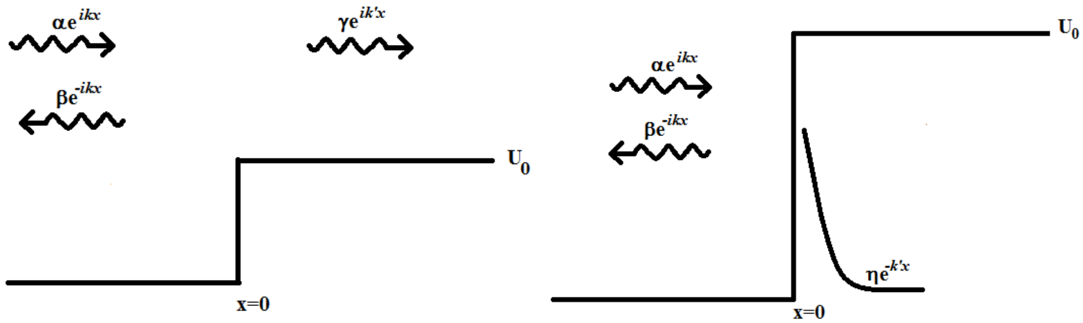
where $k = \sqrt{\frac{2mE}{\hbar^2}}$ and $k' = \sqrt{\frac{2m|E-U_0|}{\hbar^2}}$ [14].

Conservation of probability demands continuity of both $\psi(x)$ and its first derivative at the boundary $x = 0$. For $E > U_0$, this yields the conditions

$$\begin{cases} \alpha + \beta = \gamma \\ ik(\alpha - \beta) = ik'\gamma \end{cases} \tag{2.12}$$

with solutions

$$\beta = \tfrac{k-k'}{k+k'}, \qquad \gamma = \tfrac{2k}{k+k'} \tag{2.13}$$



(a) Scattering from a step potential with incident wave having $E > U_0$

(b) Scattering from a step potential with incident wave having $E < U_0$

Figure 2.1: Conventional scattering in one dimension of an incident wave on a potential step.

assuming the wavefunction has been normalized such that $|\alpha|^2 = 1$ [14]. The probabilities of reflection and transmission are then the square magnitude of β and γ respectively.

Conservation of the probability current in this case is fulfilled when

$$k(1 - |\beta|^2) = k'|\gamma|^2 \tag{2.14}$$

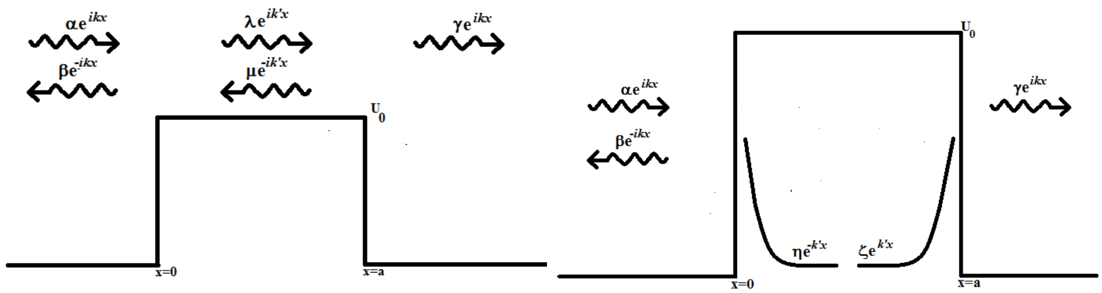
where $|\cdot|^2$ indicates the absolute square value, the product of the variable and its complex conjugate. Algebraic manipulation of (2.13) shows these values to be consistent [14].

In the case where $E < U_0$, there is no transmitted wave, only an evanescent decay inside the barrier [14]. Asymptotically far from the barrier, then, $|\beta|^2 = 1$, the wavefunction undergoes total reflection.

2.2.2 Rectangular barrier

For rectangular potential barrier problems, consider a potential with two discontinuous jumps, such that

$$V(x) = \begin{cases} 0 & x < 0 \\ U_0 & 0 < x < a \\ 0 & x > a\,. \end{cases} \tag{2.15}$$



(a) Scattering off a rectangular potential barrier with incident wave having $E > U_0$

(b) Scattering off a rectangular potential barrier with incident wave having $E < U_0$

Figure 2.2: Conventional scattering in one dimension of an incident wave on a rectangular potential barrier.

Here again it is possible to have an incoming wave with either $E > U_0$ or $E < U_0$. Both cases are diagrammed in Figure 2.2. In these problems, continuity of the wavefunction and its derivative are required not only at the $x = 0$ boundary, but also at the $x = a$ boundary [15]. For $E > U_0$, the wavefunction is

$$\psi(x) = \begin{cases} \alpha e^{ikx} + \beta e^{-ikx}, & x < 0 \\ \lambda e^{ik'x} + \mu e^{-ik'x}, & 0 < x < a \\ \gamma e^{ikx}, & x > a \end{cases} \tag{2.16}$$

with k and k' defined as before. This yields the following conditions:

$$\begin{cases} \alpha + \beta = \lambda + \mu \\ ik(\alpha - \beta) = ik'(\lambda - \mu) \\ \gamma e^{ika} = \lambda e^{ik'a} + \mu e^{-ik'a} \\ ik\gamma e^{ika} = ik'(\lambda e^{ik'a} - \mu e^{-ik'a}) \end{cases} \tag{2.17}$$

which, when solved result in a transmission amplitude

$$\gamma = \frac{2kk'e^{-ika}}{2kk'\cos(k'a) - i(k^2 + k'^2)\sin(k'a)} \tag{2.18}$$

and transmission probability

$$|\gamma|^2 = \frac{1}{1 + \frac{1}{4}(\frac{k}{k'} - \frac{k'}{k})^2 \sin^2(k'a)} \tag{2.19}$$

assuming α has been normalized to 1 [15]. The transmission amplitude, and therefore the probability the wave will be totally transmitted, becomes 1 when $U_0 = 0$, i.e. there is no potential barrier present, and when $k' = n\pi$ where n is an integer. This is in contrast to classical mechanics, where any wave above the barrier is completely transmitted. From conservation probability, the reflection probability is simply

$$|\beta|^2 = 1 - |\gamma|^2\,. \tag{2.20}$$

[15].

For the case where $E < U_0$, the plane waves in the region $0 < x < a$ are replaced by evanescent waves and the wavefunction becomes

$$\psi(x) = \begin{cases} \alpha e^{ikx} + \beta e^{-ikx}, & x < 0 \\ \eta e^{-k'x} + \zeta e^{k'x}, & 0 < x < a \\ \gamma e^{ikx}, & x > a \end{cases} \tag{2.21}$$

which yields the system of equations

$$\begin{cases} \alpha + \beta = \eta + \zeta \\ ik(\alpha - \beta) = k'(\zeta - \eta) \\ \gamma e^{ika} = \eta e^{-k'a} + \zeta e^{k'a} \\ ik\gamma e^{ika} = k'(\zeta e^{k'a} - \eta e^{-k'a}) \end{cases} \tag{2.22}$$

which results in a transmission probability

$$|\gamma|^2 = \frac{1}{1 + \frac{1}{4}(\frac{k}{k'} + \frac{k'}{k})^2 \sinh^2(k'a)} \tag{2.23}$$

in contrast to classical mechanics, where the transmission probability of an incoming wave below the barrier is zero. The classical result is recovered in the limit where the height of the barrier becomes infinite [15]. These results can be extended to the case of scattering from a potential well if $U_0 < 0$.

2.3 Bound Value Problems

While scattering problems describe free particles with continuous energies, bound value problems, as the name suggests, deal with bound particles, i.e. those that are confined by a potential to have finite, non-zero probability of being found in a particular region of space. These problems also explicitly show quantization of allowed energies for the bound particles.

2.3.1 Infinite potential well

The infinite potential well is an idealization of a well with perfectly impenetrable walls that allows easy calculations leading to energy quantization. For the infinite well, consider a potential such that

$$V(x) = \begin{cases} 0 & -a < x < +a \\ +\infty & \text{otherwise}\,. \end{cases} \tag{2.24}$$

Outside the region $-a$ to $+a$ the wavefunction must be zero, while inside this region it has the form of a standing wave [16]

$$\psi(x) = \alpha e^{ikx} + \beta e^{-ikx} \tag{2.25}$$

where

$$k = \sqrt{\frac{2mE}{\hbar^2}}\,. \tag{2.26}$$

Since the wavefunction must vanish at the boundary, the boundary constraints are

$$\psi(-a) = \psi(+a) = 0 \tag{2.27}$$

which, when applied to (2.25), results in the linear equations

$$\begin{cases} \alpha e^{ika} + \beta e^{-ika} = 0 \\ \alpha e^{-ika} + \beta e^{ika} = 0\,. \end{cases} \tag{2.28}$$

The only non-trivial solution is the eigenvalue condition

$$\sin(2ka) = 0 \tag{2.29}$$

where

$$k_n = \tfrac{\pi}{2a} n, \quad n = \pm 1, \pm 2, \ldots \quad . \tag{2.30}$$

The value $k = 0$ is excluded because it violates the normalization condition [16]. Substituting the value of k in (2.30) into the definition (2.26), it is easily shown that energies in the infinite potential well are restricted to

$$E_n = \frac{\hbar^2 \pi^2}{8ma^2} n^2 \tag{2.31}$$

and a continuous spectrum of energies is no longer available [16].

Furthermore, by substituting the k expression from (2.30) into (2.28), it is easily shown that the exponential reduces to i^n. This means that for odd integer values of n, $\alpha = \beta$ while for even integer values, $-\alpha = \beta$ [16]. This results in the solutions separating into even parity and odd parity eigenfunctions, specifically

$$\begin{aligned} \psi_{even}(x) &= \tfrac{1}{\sqrt{a}} \cos(\tfrac{n\pi x}{2a}) \qquad n = \pm 1, \pm 3, \ldots \\ \psi_{odd}(x) &= \tfrac{1}{\sqrt{a}} \sin(\tfrac{n\pi x}{2a}) \quad n = \pm 2, \pm 4, \ldots \quad . \end{aligned} \tag{2.32}$$

2.3.2 *Finite potential well*

In the finite well, the walls of the potential are no longer completely impenetrable, and there is a finite, non-zero probability the particle will be found outside the well. Energy is still quantized, but wavefunction is no longer zero at the barrier. Instead, boundary conditions must be matched for the wavefunction and its derivative.

Instead of a potential barrier, consider now a rectangular potential hole such that

$$V(x) = \begin{cases} 0 & x < -a \\ -U_0 & -a < x < +a \\ 0 & x > +a \end{cases} \tag{2.33}$$

for some arbitrary width, a, and $U_0 > 0$. In this case, bound states will occur for energies $-U_0 < E < 0$. Since the potential is symmetric, and invariant with respect to inversion, solutions will again separate into those with even parity and those with odd parity [17]. These solutions are

$$\begin{aligned} \text{even} \quad \psi(x) &= \begin{cases} \alpha \cos(kx) & 0 \le x \le +a \\ \alpha \cos(ka) e^{\kappa(a-x)} & x > a \end{cases} \\ \text{odd} \quad \psi(x) &= \begin{cases} \beta \sin(kx) & 0 \le x \le +a \\ \beta \sin(ka) e^{\kappa(a-x)} & x > a \end{cases} \end{aligned} \tag{2.34}$$

where $k = \sqrt{\frac{2m(E+U_0)}{\hbar^2}}$ and $\kappa = \sqrt{-\frac{2mE}{\hbar^2}}$. Continuity of the wavefunction and its derivative are again required at the boundary. This time, however, instead of an analytic expression, the resulting systems of equations give the following conditions

$$\begin{aligned} &\text{even} \quad \tfrac{\kappa}{k} = \tan(ka) \\ &\text{odd} \quad \tfrac{-\kappa}{k} = \cot(ka) \end{aligned} \tag{2.35}$$

which are transcendental and must be solved numerically to find allowed energy values [17].

CHAPTER 3

CONSTRUCTION OF THE PROBABILITY CURRENT FUNCTIONAL

To begin the study of quantum mechanics with a quartic dispersion law, it is first necessary to determine the form of the probability current functional. Because it is a fundamental conserved quantity, the probability current can be used to test results for consistency, and will determine boundary conditions in bound value and scattering problems in quantum systems with quartic dispersion. This problem will again consider wavefunctions in one dimension, but results should easily generalize to higher dimensions.

The wavefunction is still normalized as in (2.1), and the interpretation of this integral is still a probability. With an artificially designed quartic dispersion law, achieved by shaking an optical lattice along the grand diagonal, the Schrödinger equation becomes

$$i\hbar\frac{\partial}{\partial t}\Psi(x,t) = \varkappa\hbar^4\frac{\partial^4}{\partial x^4}\Psi(x,t) + V(x)\Psi(x,t) \tag{3.1}$$

where $\varkappa$ is a real constant, dependent on mass. The Hamiltonian operator is then

$$\hat{H} = \varkappa\hbar^4\frac{\partial^4}{\partial x^4} + V(x) \tag{3.2}$$

To again obtain an expression independent of the potential, write

$$i\hbar\frac{\partial}{\partial t}\left(\Psi^*\Psi\right) = \Psi^*\hat{H}\Psi - \Psi\hat{H}\Psi^* \tag{3.3}$$

similar to (2.4). This can also be written as

$$\frac{\partial}{\partial t}\left(\Psi^{*}\Psi\right) = -i\varkappa\hbar^{3}\left(\Psi^{*}\frac{\partial^{4}}{\partial x^{4}}\Psi - \frac{\partial^{4}}{\partial x^{4}}\Psi^{*}\Psi\right) . \tag{3.4}$$

We again integrate both sides with respect to x, which again shows that the left-hand side is nothing more than the time derivative of the probability, and so the right hand side must again be difference between the incoming and outgoing probability currents, $J(x_2) - J(x_1)$.

$$\frac{\partial}{\partial t}\int_{x_1}^{x_2} dx\,\Psi^{*}\Psi = J(x_2) - J(x_1)\,. \tag{3.5}$$

Performing the integration yields the probability current functional

$$J(x) = 2\varkappa\hbar^{3}\,\mathrm{Im}[\frac{\partial^{3}}{\partial x^{3}}\Psi^{*}\Psi + \frac{\partial}{\partial x}\Psi^{*}\frac{\partial^{2}}{\partial x^{2}}\Psi] \tag{3.6}$$

which defines conservation of probability for quantum mechanics with a quartic dispersion law.

CHAPTER 4

SCATTERING PROBLEMS

Scattering problems provide important methods for studying low energy systems. By developing an understanding of scattering problems with the quartic dispersion law, it is possible to determine reflection and transmission probabilities, and develop boundary conditions for the infinite square well which lead to explicit energy quantization. In this chapter we will re-analyze the standard scattering problems of one-dimensional quantum mechanics using the quartic dispersion law. Results will be tested for consistency using asymptotic conservation of the probability current constructed in the previous chapter.

Solving these problems is procedurally similar to the solving of the conventional one-dimensional scattering problems outlined in Chapter 2. However, where in the conventional problems the boundary conditions require only continuity of the wavefunction and its derivative, under the quartic dispersion law continuity of the wavefunction, and its first, second, and third derivatives are required to fully determine all coefficients.

4.1 Step Potential

As in conventional quantum mechanics, the step potential is the simplest scattering problem, and so will be treated first. There are again two regimes for the step potential scattering problem; incoming energy above the step, and incoming energy below the step. Each of these cases will be treated in the following sections.

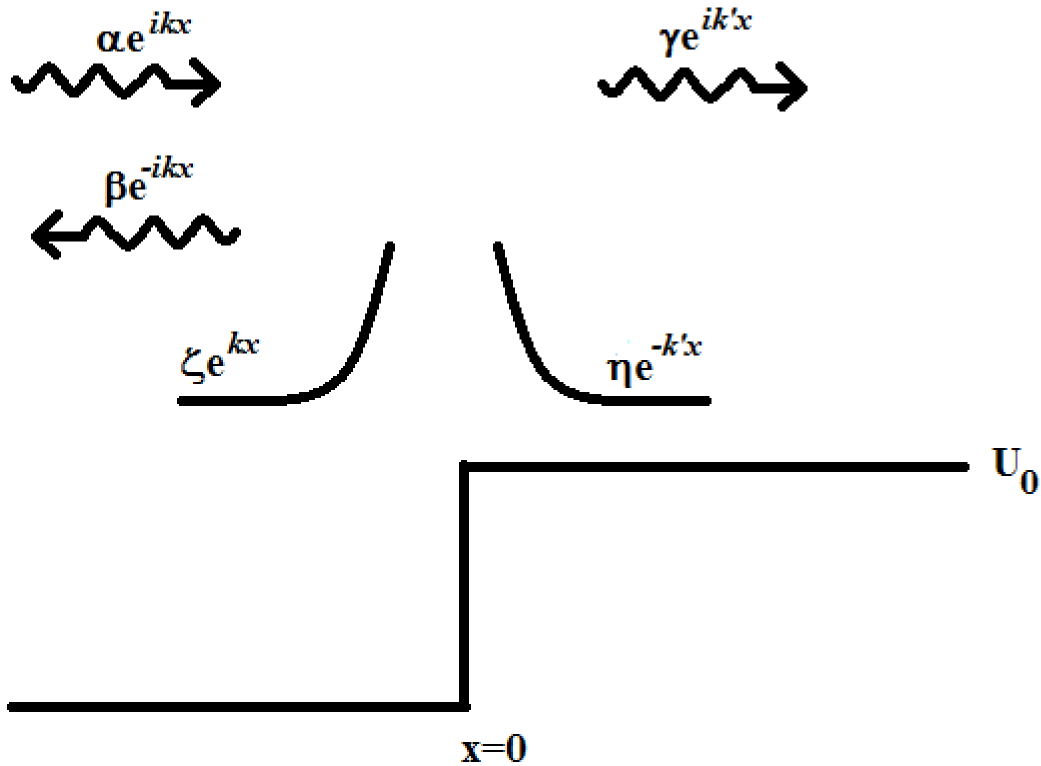


Figure 4.1: Scattering from a step potential of an incoming plane wave with $E > U_0$ and quartic dispersion.

4.1.1 Incoming energy above the barrier

For the case where the incoming wave has energy greater than the potential energy, consider the potential

$$V(x) = \begin{cases} 0 & x < 0 \\ U_0 & x > 0 \end{cases} \tag{4.1}$$

and plane wave solutions of the form e^{ikx}.

As shown in Figure 4.1, the incoming wave has amplitude α, the reflected and transmitted waves have amplitudes β and γ respectively, the back propagating evanescent wave at the barrier has amplitude ζ, and the forward propagating evanescent wave at the barrier has amplitude η. The wave function, then, is

$$\Psi(x) = \begin{cases} \alpha e^{ikx} + \beta e^{-ikx} + \zeta e^{kx} & x < 0 \\ \gamma e^{ik'x} + \eta e^{-k'x} & x \geq 0 \end{cases} \tag{4.2}$$

where $k = (\frac{E}{\varkappa})^{\frac{1}{4}}$ and $k' = (\frac{E-U_0}{\varkappa})^{\frac{1}{4}}$.

Requiring continuity of the wave function and its first, second, and third derivatives at $x = 0$ where the step potential begins means that

$$\begin{aligned} &\Psi(x<0) = \Psi(x>0)|_{x=0} \\ &\tfrac{\partial}{\partial x}\Psi(x<0) = \tfrac{\partial}{\partial x}\Psi(x>0)|_{x=0} \\ &\tfrac{\partial^2}{\partial x^2}\Psi(x<0) = \tfrac{\partial^2}{\partial x^2}\Psi(x>0)|_{x=0} \\ &\tfrac{\partial^3}{\partial x^3}\Psi(x<0) = \tfrac{\partial^3}{\partial x^3}\Psi(x>0)|_{x=0} \end{aligned} \tag{4.3}$$

which, for the wave function specified in (4.2), yields the system of simultaneous equations

$$\begin{cases} \alpha + \beta + \zeta = \gamma + \eta \\ ik\alpha - ik\beta + k\zeta = ik'\gamma - k'\eta \\ -k^2\alpha - k^2\beta + k^2\zeta = -k'^2\gamma + k'^2\eta \\ -ik^3\alpha + ik^3\beta + k^3\zeta = -ik'^3\gamma - k'^3\eta\,. \end{cases} \tag{4.4}$$

Assuming the amplitude of the incoming wave, α, has been normalized to 1, and solving for the reflection and transmission amplitudes gives a reflection amplitude

$$\beta = \frac{(k-k')(ik+k')}{(k+k')(k+ik')} \tag{4.5}$$

and a transmission amplitude

$$\gamma = \frac{2k^2}{k'(k+k')} \, . \tag{4.6}$$

Conservation of probability demands that the incoming probability current be equal to the outgoing probability current. In order to test the consistency of these expressions, the asymptotic values of the probability current are compared. Using equation (3.6) derived in Chapter 3, and the wavefunction specified in (4.2), the condition for probability current to be conserved is

$$k^3|\alpha|^2 = k^3|\beta|^2 + k'^3|\gamma|^2 \tag{4.7}$$

where, as usual, $|\cdot|^2$ denotes the product of the variable and its complex conjugate. Substituting (4.5) and (4.6) into (4.7), and again taking the incoming wavefunction to be normalized to 1, the equality holds, and the values obtained for the reflection and transmission amplitudes are shown to be consistent.

4.1.2 Incoming energy below the barrier

The second case for the step potential is the one where the incoming wave has energy which is less than the energy of the potential barrier. The potential to be considered here is again the one specified in (4.1). In contrast to the conventional quantum mechanics case, where a single evanescent wave penetrates the barrier, in the quartic dispersion case,

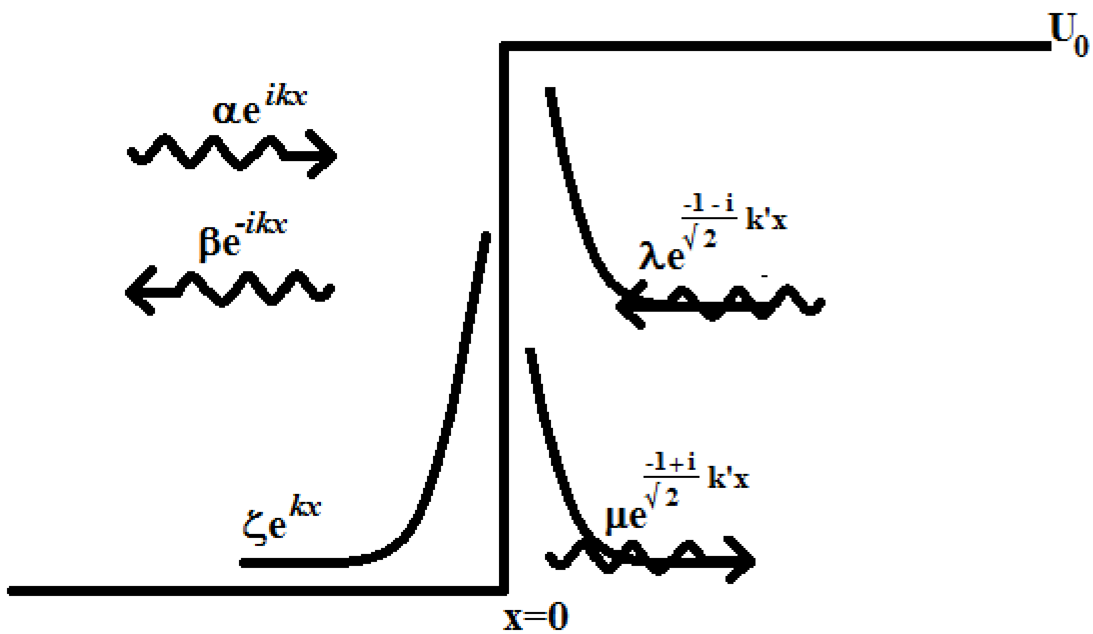


Figure 4.2: Scattering from a step potential of an incoming plane wave with $E < U_0$ and quartic dispersion.

an evanescent wave occurs to the left of the barrier in the zero potential region, and inside the barrier two waves propagate as $e^{\frac{-1\pm i}{\sqrt{2}}k'x}$ as shown in Figure 4.2.

The incoming wave again has amplitude α, and transmitted wave has amplitude β. The evanescent wave has amplitude ζ, while the waves inside the region of non-zero potential have amplitudes λ and μ. The wavefunction in this case is then

$$\Psi(x) = \begin{cases} \alpha e^{ikx} + \beta e^{-ikx} + \zeta e^{kx} & x < 0 \\ \lambda e^{\frac{-1-i}{\sqrt{2}}k'x} + \mu e^{\frac{-1+i}{\sqrt{2}}k'x} & x \geq 0\,. \end{cases} \tag{4.8}$$

Again requiring continuity of the wavefunction and its first, second, and third derivatives at the barrier, as in (4.3) now yields the following system of equations:

$$\begin{cases} \alpha + \beta + \zeta = \lambda + \mu \\ ik\alpha - ik\beta + k\zeta = \frac{-1-i}{\sqrt{2}}k'\lambda + \frac{-1+i}{\sqrt{2}}k'\mu \\ -k^2\alpha - k^2\beta + k^2\zeta = ik'^2\lambda - ik'^2\mu \\ -ik^3\alpha + ik^3\beta + k^3\zeta = \frac{1-i}{\sqrt{2}}k'^3\lambda + \frac{1+i}{\sqrt{2}}k'^3\mu\,. \end{cases} \tag{4.9}$$

Again assuming α has been normalized, solving for the amplitude of the reflected wave gives the result

$$\beta = i\frac{k^2 - k'^2 - i\sqrt{2}kk'}{k^2 - k'^2 + i\sqrt{2}kk'}\,. \tag{4.10}$$

Since there is no transmitted wave, conservation of probability current requires only that

$$|\beta|^2 = |\alpha|^2 = 1\,.$$

Some algebra with the value of β given in (4.10) shows that this is indeed the case. Furthermore, it is expected that as the height of the barrier increases, the sum of the incoming, reflected, and evanescent wave amplitudes should converge to zero, to ensure that the wave function before the barrier wall is continuously connected to its vanishing counterpart in the forbidden (even quantum-mechanically) zone under the barrier. Solving (4.9) for ζ gives the result

$$\zeta = (1+i)\frac{k - rk'}{k + rk'} \tag{4.11}$$

where $r = e^{\frac{i\pi}{4}}$. It can be shown that

$$\lim_{k' \to \infty} \alpha + \beta + \zeta = 0$$

as required.

4.2 Rectangular Potential Barrier

Next we will examine scattering problems with a rectangular potential barrier and quartic dispersion. Again, the incoming wave can have energy greater than that of the potential barrier, or below that of the potential barrier. These two cases will again be treated separately below. As was the case in Chapter 2, the rectangular barrier has two boundaries, where the step potential has only one, so continuity of the wavefunction and its first, second, and third derivatives is required not only at the position $x = 0$ where the incoming wave first encounters the potential, but also at $x = a$ when the potential barrier again drops to zero.

4.2.1 Incoming energy above the barrier

First we will consider the case where the incoming energy is greater than that of the potential barrier. We will consider a general potential barrier of the form

$$V(x) = \begin{cases} 0 & x < 0 \\ U_0 & 0 < x < a \\ 0 & x > a \end{cases} \tag{4.12}$$

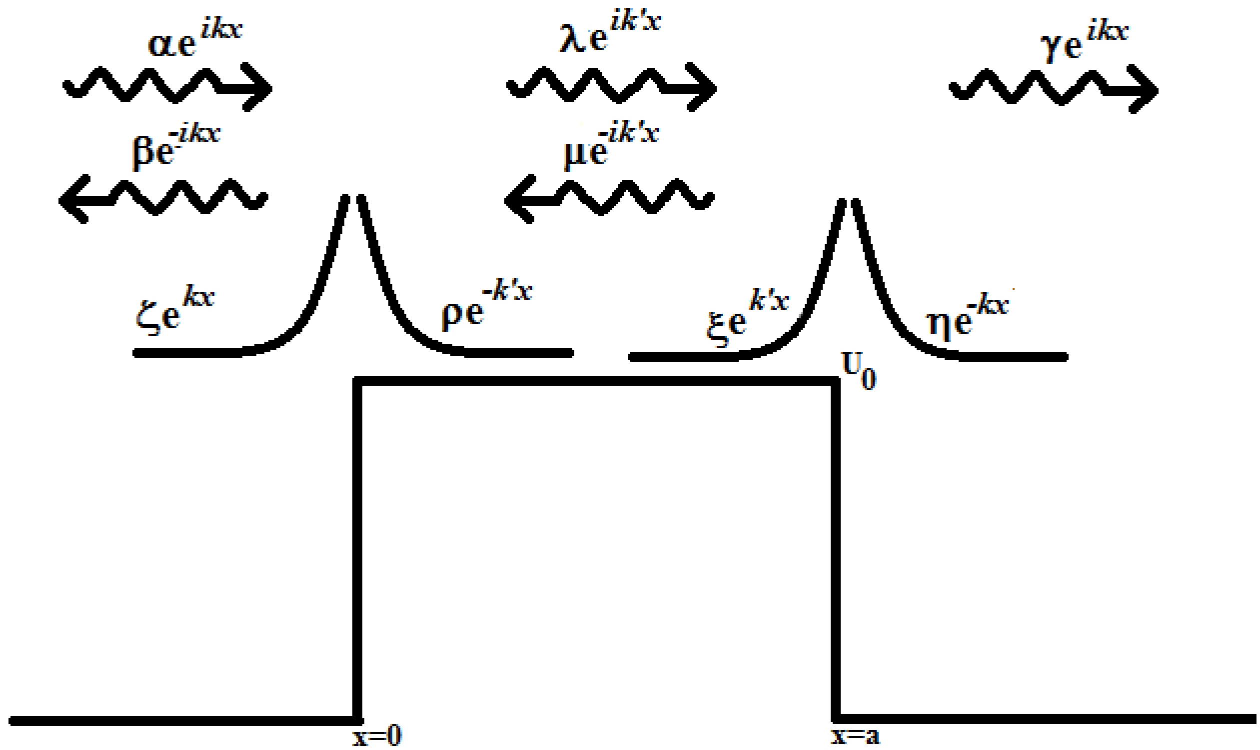


Figure 4.3: Scattering from a rectangular potential barrier of an incoming plane wave with $E > U_0$ and quartic dispersion.

where a is the arbitrary width of the barrier. As with the step potential, we will also be considering plane wave solutions of the form e^{ikx}.

As Figure 4.3 shows, to the left of the barrier the incoming wave has amplitude α, the reflected wave has amplitude β, and the back propagating evanescent wave has amplitude ζ. In the region above the potential barrier, the forward propagating wave has amplitude λ, the back propagating wave has amplitude μ, and the forward and back propagating evanescent waves have amplitudes ρ and ξ respectively. Finally, to the right of the barrier, the transmitted wave has amplitude γ, and there is a final forward evanescent wave with amplitude η. This then gives the wavefunction

$$\Psi(x) = \begin{cases} \alpha e^{ikx} + \beta e^{-ikx} + \zeta e^{kx} & x < 0 \\ \lambda e^{ik'x} + \mu e^{-ik'x} + \xi e^{k'x} + \rho e^{-k'x} & 0 \leq x \leq a \\ \gamma e^{ikx} + \eta e^{-kx} & x > a\,. \end{cases} \tag{4.13}$$

The boundary conditions require the conditions in (4.3), and additionally

$$\begin{aligned} &\Psi(x < a) = \Psi(x > a)|_{x=a} \\ &\tfrac{\partial}{\partial x}\Psi(x < a) = \tfrac{\partial}{\partial x}\Psi(x > a)|_{x=a} \\ &\tfrac{\partial^2}{\partial x^2}\Psi(x < a) = \tfrac{\partial^2}{\partial x^2}\Psi(x > a)|_{x=a} \\ &\tfrac{\partial^3}{\partial x^3}\Psi(x < a) = \tfrac{\partial^3}{\partial x^3}\Psi(x > a)|_{x=a}\,. \end{aligned} \tag{4.14}$$

This yields the following system of equations:

$$\begin{cases} \alpha + \beta + \zeta = \lambda + \mu + \xi + \rho \\ ik\alpha - ik\beta + k\zeta = ik'\lambda - ik'\mu + k'\xi - k'\rho \\ -k^2\alpha - k^2\beta + k^2\zeta = -k'^2\lambda - k'^2\mu + k'^2\xi + k'^2\rho \\ -ik^3\alpha + ik^3\beta + k^3\zeta = -ik'^3\lambda + ik'^3\mu + k'^3\xi - k'^3\rho \\ \gamma e^{ika} + \eta e^{-ka} = \lambda e^{ik'a} + \mu e^{-ik'a} + \xi e^{k'a} + \rho e^{-k'a} \\ ik\gamma e^{ika} - k\eta e^{-ka} = ik'\lambda e^{ik'a} - ik'\mu e^{-ik'a} + k'\xi e^{k'a} - k'\rho e^{-k'a} \\ -k^2\gamma e^{ika} + k^2\eta e^{-ka} = -k'^2\lambda e^{ik'a} - k'^2\mu e^{-ik'a} + k'^2\xi e^{k'a} + k'^2\rho e^{-k'a} \\ -ik^3\gamma e^{ika} - k^3\eta e^{-ka} = -ik'^3\lambda e^{ik'a} + ik'^3\mu e^{-ik'a} + k'^3\xi e^{k'a} - k'^3\rho e^{-k'a}\,. \end{cases} \tag{4.15}$$

When solved, this system gives a reflected wave amplitude

$$\beta = \frac{i(k^4 - k'^4)[-k^4 + k'^4 + A(k,k',a)B(k,k',a)]}{-(k^4 - k'^4)^2 + C(k,k',a)D(k,k',a)} \tag{4.16}$$

where

$$\begin{aligned}
A(k,k',a) &= (k-k')(k+k')\cos(ak') - 2kk'\sin(ak') \\
B(k,k',a) &= (k^2 + k'^2)\cosh(ak') + 2kk'\sinh(ak') \\
C(k,k',a) &= ((k^4 - 4ik^2k'^2 - k'^4)\cos(ak') - (2+2i)kk'(k^2 - ik'^2)\sin(ak') \\
D(k,k',a) &= (k^4 + 4ik^2k'^2 - k'^4)\cosh(ak') + (2+2i)kk'(k^2 + ik'^2)\sinh(ak')
\end{aligned} \tag{4.17}$$

and a transmitted wave amplitude

$$\gamma = \frac{e^{-a(ik+k')}kk'\{(k^2+k'^2)^2[k-k'+e^{ak'}(k+k')][-k+k'+e^{ak'}(k+k')] + G(k,k',a)\}}{-(k^4 - k'^4)^2 + C(k,k',a)D(k,k',a)} \tag{4.18}$$

where $C(k,k',a)$ and $D(k,k',a)$ are as specified in (4.17) and

$$G(k,k',a) = 2e^{ak'}(k^2 - k'^2)^2[-2kk'\cos(ak') + (-k^2 + k'^2)\sin(ak')] \,. \tag{4.19}$$

Because the wavenumber is the same for the incoming, reflected, and transmitted waves, unlike in the step potential problems, the conservation of probability current requirement is the familiar

$$|\alpha|^2 = |\beta|^2 + |\gamma|^2 \,. \tag{4.20}$$

Making the appropriate substitutions for β and γ, and assuming α has been normalized to 1, the equality holds, and the results are consistent with conservation of probability current.

Further checks are possible by changing the height of the potential barrier. The limit where $U_0 = 0$ corresponds to free space with no potential barrier. In this case $k = k'$. When this substitution is made to (4.16) and the square magnitude of the reflection coefficient calculated, it can be shown that $|\beta|^2 = 0$ as expected. If there is no barrier, the wave is simply propagating in free space, and no portion of it should be reflected. Similarly, setting $k = k'$ and evaluating $|\gamma|^2$ returns a value of 1. Since there is no barrier, the incoming wave is wholly transmitted, as expected.

4.2.2 *Incoming energy below the barrier*

The remaining scattering problem with quartic dispersion is that of an incoming wave incident on a rectangular barrier with $E < U_0$. In this section we will again consider the potential specified in (4.12), but with incoming energy below the barrier. These results will then be extended to find the unbound scattering states from a potential well. Bound states will be addressed in the next chapter.

As Figure 4.4 shows, the waves to the left and right of the potential are defined the same way as in the previous case where $E > U_0$. In the region of the potential barrier, the wavefunction propagates as modified plane waves with exponents dependent on $\sqrt[4]{-1}$. The total wavefunction then is

$$\Psi(x) = \begin{cases} \alpha e^{ikx} + \beta e^{-ikx} + \zeta e^{kx} & x < 0 \\ \lambda e^{\frac{1+i}{\sqrt{2}}k'x} + \mu e^{\frac{-1-i}{\sqrt{2}}k'x} + \xi e^{\frac{-1+i}{\sqrt{2}}k'x} + \rho e^{\frac{1-i}{\sqrt{2}}k'x} & 0 \le x \le a \\ \gamma e^{ikx} + \eta e^{-kx} & x > a \end{cases} \tag{4.21}$$

and imposing the same boundary conditions stated in (4.3) and (4.14), gives the following system of equations:

$$\begin{cases} \alpha+\beta+\zeta = & \lambda+\mu+\xi+\rho \\ ik\alpha-ik\beta+k\zeta = & \frac{1+i}{\sqrt{2}}k'\lambda+\frac{-1-i}{\sqrt{2}}k'\mu+\frac{-1+i}{\sqrt{2}}k'\xi+\frac{1-i}{\sqrt{2}}k'\rho \\ -k^2\alpha-k^2\beta+k^2\zeta = & ik'^2\lambda+ik'^2\mu-ik'^2\xi-ik'^2\rho \\ -ik^3\alpha+ik^3\beta+k^3\zeta = & \frac{-1+i}{\sqrt{2}}k'^3\lambda+\frac{1-i}{\sqrt{2}}k'^3\mu+\frac{1+i}{\sqrt{2}}k'^3\xi+\frac{-1-i}{\sqrt{2}}k'^3\rho \\ \gamma e^{ika}+\eta e^{-ka} = & \lambda e^{\frac{1+i}{\sqrt{2}}k'a}+\mu e^{\frac{-1-i}{\sqrt{2}}k'a}+\xi e^{\frac{-1+i}{\sqrt{2}}k'a}+\rho e^{\frac{1-i}{\sqrt{2}}k'a} \\ ik\gamma e^{ika}-k\eta e^{-ka} = & \frac{1+i}{\sqrt{2}}k'\lambda e^{\frac{1+i}{\sqrt{2}}k'a}+\frac{-1-i}{\sqrt{2}}k'\mu e^{\frac{-1-i}{\sqrt{2}}k'a} \\ & +\frac{-1+i}{\sqrt{2}}k'\xi e^{\frac{-1+i}{\sqrt{2}}k'a}+\frac{1-i}{\sqrt{2}}k'\rho e^{\frac{1-i}{\sqrt{2}}k'a} \\ -k^2\gamma e^{ika}+k^2\eta e^{-ka} = & ik'^2\lambda e^{\frac{1+i}{\sqrt{2}}k'a}+ik'^2\mu e^{\frac{-1-i}{\sqrt{2}}k'a}-ik'^2\xi e^{\frac{-1+i}{\sqrt{2}}k'a} \\ & -ik'^2\rho e^{\frac{1-i}{\sqrt{2}}k'a} \\ -ik^3\gamma e^{ika}-k^3\eta e^{-ka} = & \frac{-1+i}{\sqrt{2}}k'^3\lambda e^{\frac{1+i}{\sqrt{2}}k'a}+\frac{1-i}{\sqrt{2}}k'^3\mu e^{\frac{-1-i}{\sqrt{2}}k'a} \\ & +\frac{1+i}{\sqrt{2}}k'^3\xi e^{\frac{-1+i}{\sqrt{2}}k'a}+\frac{-1-i}{\sqrt{2}}k'^3\rho e^{\frac{1-i}{\sqrt{2}}k'a}. \end{cases} \tag{4.22}$$

This results in a reflected wave amplitude

$$\beta = \frac{i\Theta\{-2\Theta+H\cos(\sqrt{2}ak')+L\cosh(\sqrt{2}ak')+2\sqrt{2}k'[M(k,k',a)+N(k,k',a)]\}}{-2\Theta^2+P(k,k',a)+Q(k,k',a)+4(-1)^{\frac{1}{4}}kk'[R(k,k',a)+S(k,k',a)]} \tag{4.23}$$

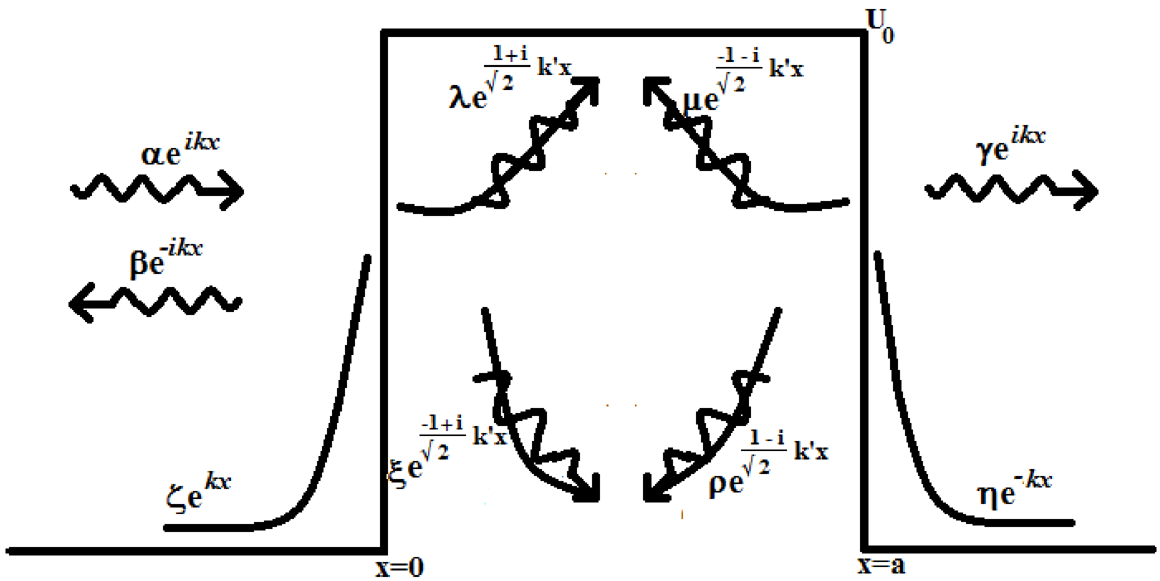


Figure 4.4: Scattering from a rectangular potential barrier of an incoming plane wave with $E < U_0$ and quartic dispersion.

where

$$
\begin{aligned}
&\Theta = k^4 + k'^4 \\
&H = (k^4 - 4k^2k'^2 + k'^4) \\
&L = (k^4 + 4k^2k'^2 + k'^4) \\
&M(k,k',a) = k(-k^2 + k'^2)\sin(\sqrt{2}ak') \\
&N(k,k',a) = k(k^2 + k'^2)\sinh(\sqrt{2}ak') \\
&P(k,k',a) = (k^2 - ik'^2)^2(k^4 - 6ik^2k'^2 - k'^4)\cos(\sqrt{2}ak') \\
&Q(k,k',a) = (k^2 + ik'^2)^2(k^4 + 6ik^2k'^2 - k'^4)\cosh(\sqrt{2}ak') \\
&R(k,k',a) = -(k^2 - ik'^2)^3\sin(\sqrt{2}ak') \\
&S(k,k',a) = (k^2 + ik'^2)^3\sinh(\sqrt{2}ak')
\end{aligned}
\tag{4.24}
$$

and a transmitted wave amplitude

$$\gamma = \frac{-4e^{-iak}kk'\{\cosh(\frac{ak'}{\sqrt{2}})[W(k,k',a) + X\sin(\frac{ak'}{\sqrt{2}})] + Y(k,k',a)\sinh(\frac{ak'}{\sqrt{2}})\}}{-2\Theta^2 + P(k,k',a) + Q(k,k',a) + 4(-1)^{\frac{1}{4}}kk'[R(k,k',a) + S(k,k',a)]} \tag{4.25}$$

where

$$\begin{aligned} W(k,k',a) &= 8k^3k'^3\cos(\tfrac{ak'}{\sqrt{2}}) \\ X &= \sqrt{2}(k-k')(k+k')L \\ Y(k,k',a) &= -\sqrt{2}\{k^2 + k'^2 H\cos(\tfrac{ak'}{\sqrt{2}}) + 4kk'[k^4 - k'^4\sin(\tfrac{ak'}{\sqrt{2}})]\} \end{aligned} \tag{4.26}$$

and $H, L, P(k,k',a), Q(k,k',a), R(k,k',a)$, and $S(k,k',a)$ are as defined in (4.24). These coefficients can again be tested for consistency using conservation of probability current, and it can be shown that $|\beta|^2 + |\gamma|^2 = 1$, the square magnitude of the normalized incoming wave.

Potential well

The results for the rectangular barrier with incoming energy below the barrier also describe scattering from a potential well. If one takes $U_0 < 0$ for the potential described in (4.12), the potential becomes a well, while boundary conditions and the wave function remain the same, and the results from the previous section describe the scattering of unbound particles. Since $k' = (\frac{E-U_0}{\varkappa})^{\frac{1}{4}}$, deeper wells correspond to higher values of k'. It is expected that as the depth of the well increases, the probability of reflection increases. Since for a given energy the velocity in a deep well is high, the current conservation will require a drop in density. For an infinitely deep well, the wave function must fall to zero completely, thus emulating an infinitely high wall. Indeed, the system exhibits a total reflection,

$$\lim_{k'\to\infty} |\beta|^2 = 1 \ ,$$

consistent with a wall.

4.2.3 Comparison to delta potential theory

The behavior of the scattering solutions for the rectangular barrier divide into two distinct regimes, dependent on the height and width of the barrier. As the potential barrier becomes large compared to the de-Broglie wavelength, the reflection coefficient approaches purely classical behavior. When the barrier is small, however, the best approximation is δ-potential scattering.

The one-dimensional Schrödinger equation with quartic scattering and a δ-potential reads

$$\hbar^4 \varkappa \frac{\partial^4}{\partial x^4}\Psi + g\delta(x)\Psi = E\Psi \tag{4.27}$$

where g is a parameter quantifying the strength of the interaction. The δ-potential is compared to a rectangular barrier with the same area with

$$V(x) = \begin{cases} U_0 & 0 < x < a \\ 0 & \text{otherwise} \, . \end{cases} \tag{4.28}$$

This implies

$$\begin{gathered} \tfrac{\partial^3}{\partial x^3}\Psi(0+) - \tfrac{\partial^3}{\partial x^3}\Psi(0-) = -\tfrac{g}{\hbar^4 \varkappa}\Psi(0) \\ \text{when} \\ \tfrac{1}{\hbar}(\tfrac{U_0}{\varkappa})^{\frac{1}{4}} a \ll 1 \end{gathered} \tag{4.29}$$

i.e. the δ-potential model applies when the size of the potential becomes less than the de-Broglie wavelength associated with its height. As with conventional δ-potential scattering, the scattered wave amplitudes have either even or odd parity. It can be shown by summing the scattering amplitudes of the incoming, transmitted, and reflected waves that the odd-wave scattering amplitude is zero, and the even-wave scattering amplitude is $-\frac{(1-i)g}{\varkappa(\frac{2g}{\varkappa}-(4+4i)k^3)}$. Using this, it is possible to make a comparison between scattering from a δ-potential and scattering from a rectangular barrier of the same area using the results from the previous section.

Figure 4.5 compares the probability amplitude of the reflected wave as a function of wavenumber for the scattering off a rectangular potential well with the one for a δ-potential, for different sets of the well parameters. Narrow wells are well described by the δ-potentials, except at very low values of the incoming wavevector. As $k \to 0$, scattering from the δ-potential acts as a 50-50 beam splitter, while scattering from the rectangular well behaves classically with the reflection coefficient going to unity.

Similar behavior is seen in Figure 4.6, which shows the probability amplitude of the reflected wave as a function of wavenumber for the δ-potential scattering, and scattering from a rectangular potential barrier for a repulsive potential with different interaction strengths. Here again it is seen that for narrow potentials, the scattering behavior is the same for both potentials, with the same exception that as $k \to 0$, scattering from the δ-potential acts as a 50-50 beam splitter, while scattering from the rectangular barrier behaves classically with the reflection coefficient going to unity. Again, as the width of the barrier becomes larger, the scattering behavior of the rectangular barrier diverges from that of the $k \to 0$, the δ-potential scattering.

In fact, for even broader barriers, the scattering becomes close to classical. Here classical behavior is defined as total reflection if the incoming wavevector is below the barrier,

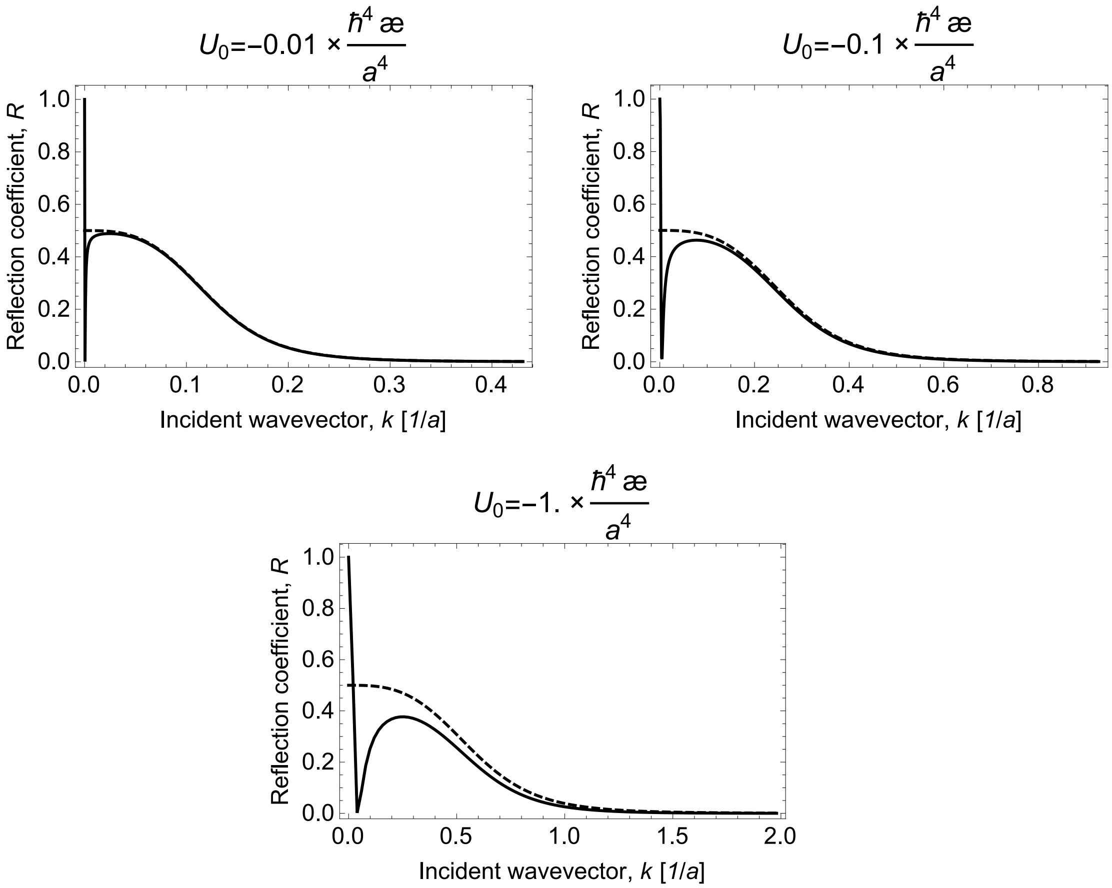


Figure 4.5: Scattering off a rectangular well, "δ-potential" regime and beyond: *ab initio* calculation (solid line), δ-potential model (dashed line).

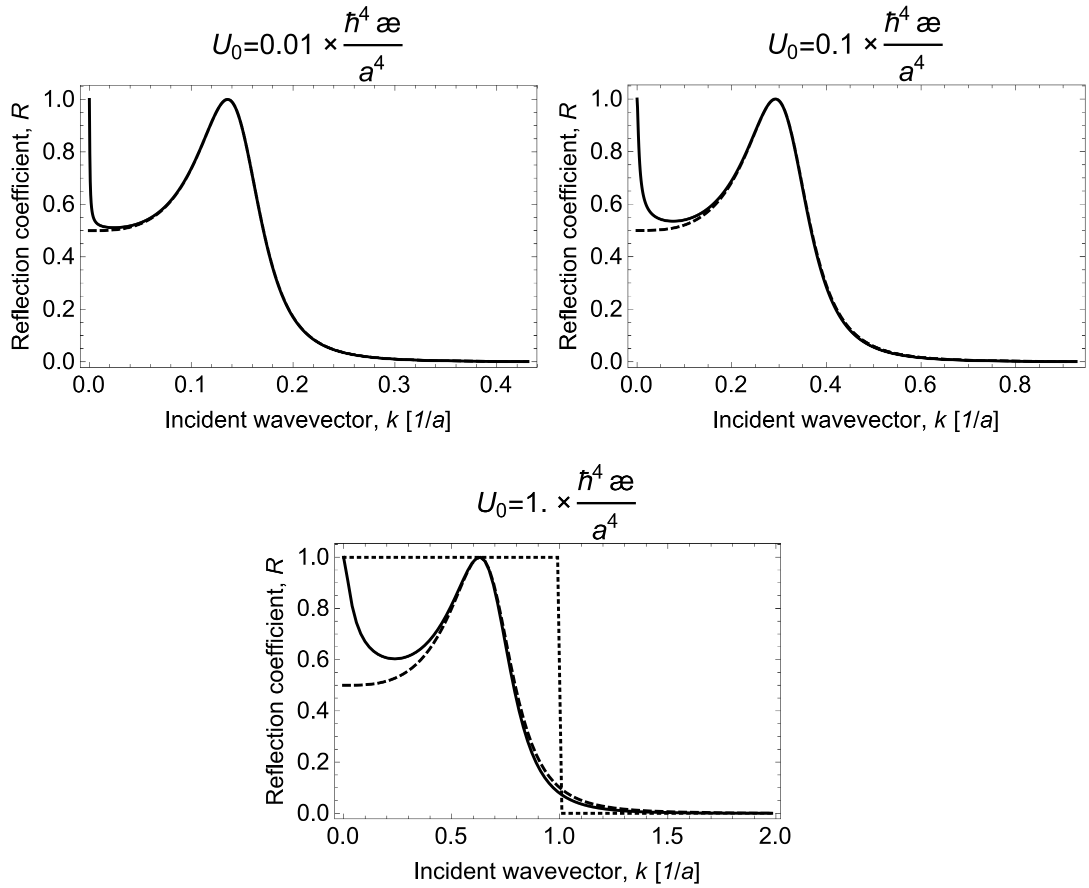


Figure 4.6: Scattering off a rectangular barrier, "δ-potential" regime: *ab initio* calculation (solid line), δ-potential model (dashed line), classical model (dotted line).

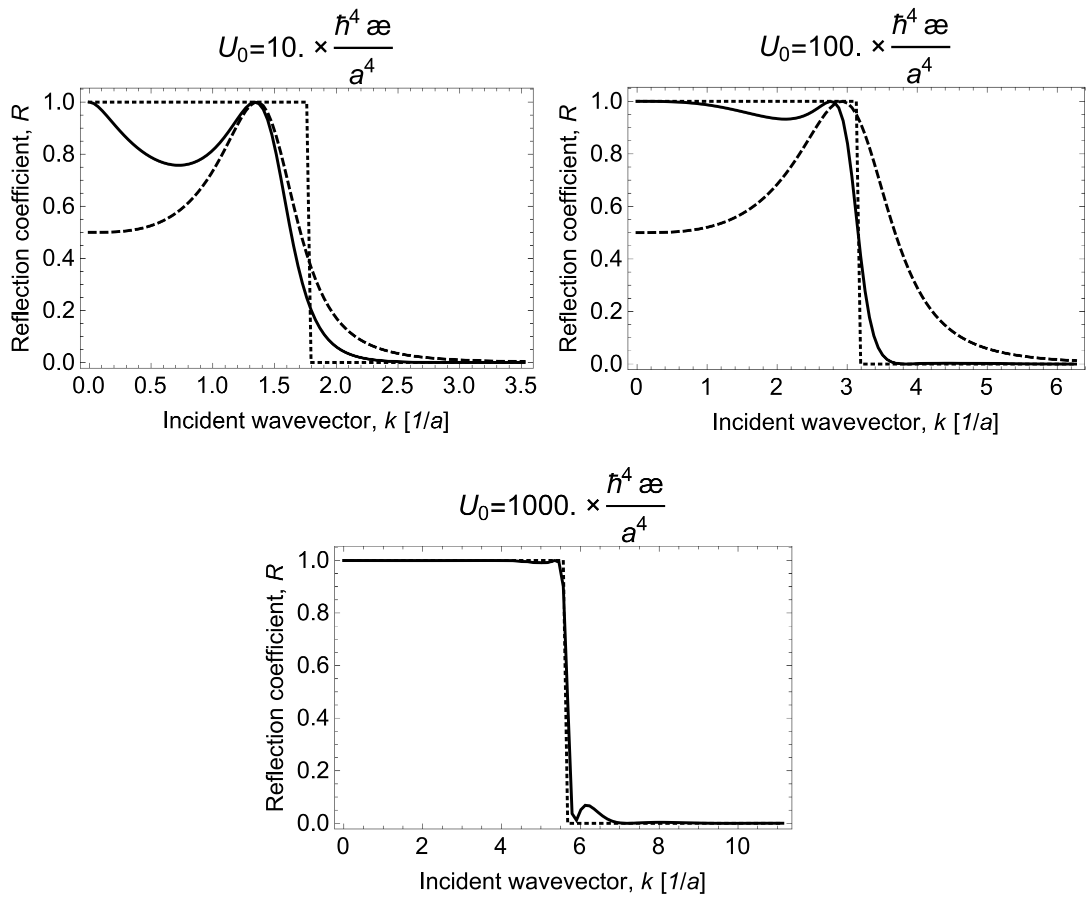


Figure 4.7: Scattering off a rectangular barrier, “classical” regime: *ab initio* calculation (solid line), δ-potential model (dashed line), classical model (dotted line).

and total transmission (zero reflection) if the incoming wavevector is above the barrier. As Figure 4.7 shows, the classical result is the better approximation when U_0 is large.

CHAPTER 5

BOUND VALUE PROBLEMS

The previous chapter focused on scattering problems, which deal with unbound solutions which can have continuous energy spectra. Bound value problems, in contrast, have the quantized energy levels, which are a hallmark of quantum systems. In this chapter, the boundary conditions for the infinite well problem will be determined, then applied to find the discrete energy spectrum of the bound states.

5.1 Derivation of Boundary Conditions

For an infinite well with hard walls, the boundary conditions can be determined from the results of the scattering off the step potential with incoming energy below the barrier discussed in Section 4.2.2. A hard wall requires that the probability current of the wavefunction outside the well must be zero. Examining the terms in (3.6) shows that for this to be the case

$$\begin{gathered} \frac{\partial^3}{\partial x^3}\Psi = 0 \quad \text{or} \quad \Psi = 0 \\ \text{and} \\ \frac{\partial}{\partial x}\Psi = 0 \quad \text{or} \quad \frac{\partial^2}{\partial x^2}\Psi = 0 \end{gathered} \tag{5.1}$$

when evaluated at the wall.

The hard wall condition is equivalent to an infinitely high potential barrier. The wavefunction will be defined as

$$\Psi(x) = \alpha e^{ikx} + \beta e^{-ikx} + \zeta e^{kx} \tag{5.2}$$

where $\alpha = 1$, and β and ζ are as defined in (4.10) and (4.11) respectively. It can then be shown that in the limit as $U_0 \to \infty$ only $\Psi \to 0$ and $\frac{\partial}{\partial x}\Psi \to 0$ when evaluated at the wall. The second and third derivatives have non-zero values when evaluated at the boundary. This means, then, that for bound states in the infinite well, boundary conditions require that the wavefunction and its first derivative be zero at the boundary.

5.2 Quantization

Knowing the boundary conditions, it is now possible to find bound state solutions for the infinite well potential, and determine the quantized energy spectrum. To make use of symmetry in the problem, consider a potential which has been re-centered, such that

$$V(x) = \begin{cases} 0 & \frac{-a}{2} < x < \frac{+a}{2} \\ +\infty & \text{otherwise} \end{cases} \tag{5.3}$$

As in conventional quantum mechanics, solutions separate into even- and odd-symmetry eigenstates. Inside the well, the wavefunction of energy $E = \hbar^4 \varkappa k^4$ that falls to zero ($\Psi = 0$) at the walls is

$$\begin{aligned} &\text{even:} \quad \psi_{even}(x,k) = \cos(kx) - \operatorname{sech}(\tfrac{ka}{2})\cos(\tfrac{ka}{2})\cosh(kx) \\ &\text{odd:} \quad \psi_{odd}(x,k) = \sin(kx) - \operatorname{csch}(\tfrac{ka}{2})\sin(\tfrac{ka}{2})\sinh(kx)\,. \end{aligned} \tag{5.4}$$

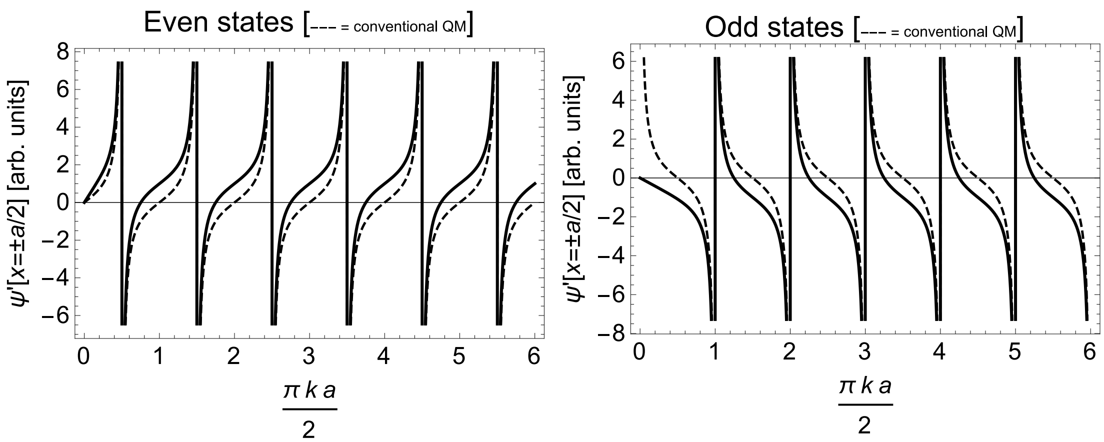


Figure 5.1: Left-hand side of the implicit equations determining the bound state k-vectors, within the right hand side set to zero: quartic dispersion (solid line), conventional quantum mechanics (dashed line).

When the second boundary condition from the previous section, $\frac{\partial}{\partial x}\Psi = 0$ is applied, this yields the following constraint on k:

$$\begin{aligned} &\text{even:} \quad \tan(\tfrac{ak}{2}) + \tanh(\tfrac{ak}{2}) = 0 \\ &\text{odd:} \quad \cot(\tfrac{ak}{2}) - \coth(\tfrac{ak}{2}) = 0 \end{aligned} \tag{5.5}$$

which is transcendental, and can not be solved analytically. Figure 5.1 plots a range of possible even and odd solutions, and compares them to the results gained in conventional quantum mechanics,

$$\begin{aligned} &\text{even:} \quad \tan(\tfrac{ak}{2}) = 0 \\ &\text{odd:} \quad \cot(\tfrac{ak}{2}) = 0\ . \end{aligned} \tag{5.6}$$

By finding numerical solutions to the roots of (5.5), it is possible to construct the groundstate, first, and second excited state wavefunction in the well (n = 1, 2, and 3, respectively). These are plotted in Figure 5.2.

To gain some insight as to the spacing of the energy levels under the quartic dispersion law, it would be useful to find a good approximation so that finding exact numerical

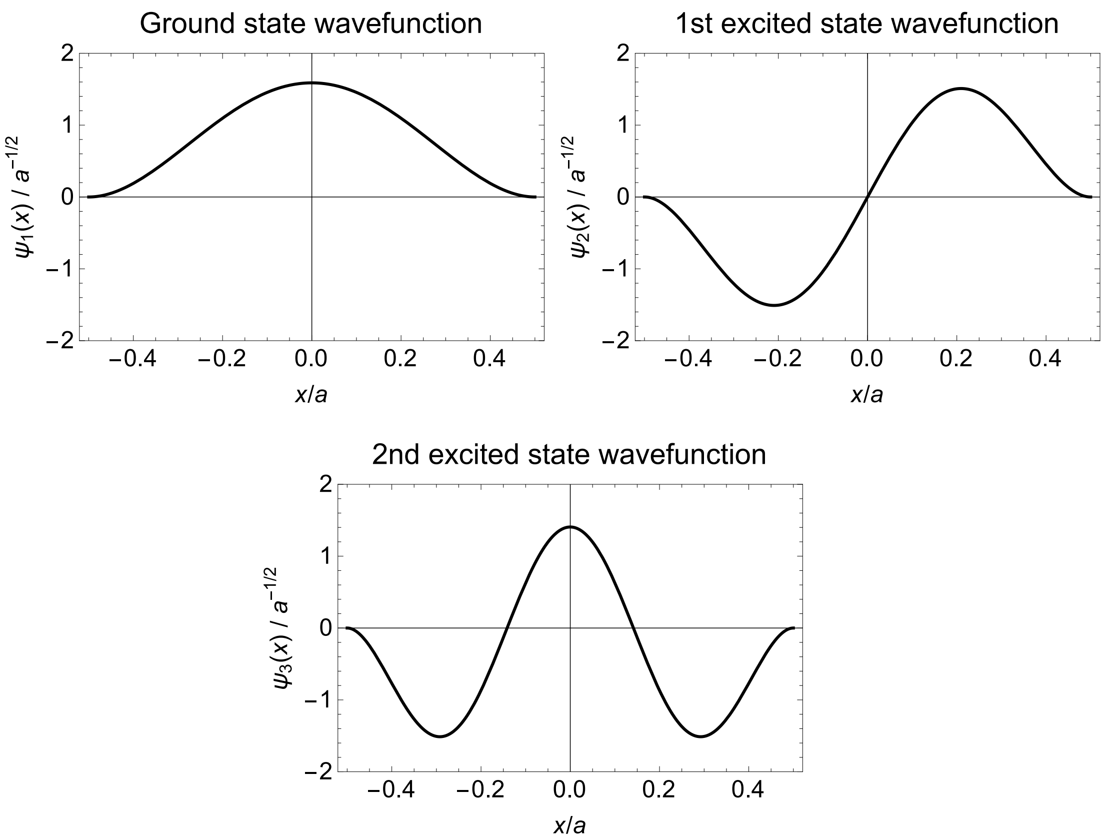


Figure 5.2: Ground state and excited state wavefunctions in the infinite well with quartic dispersion.

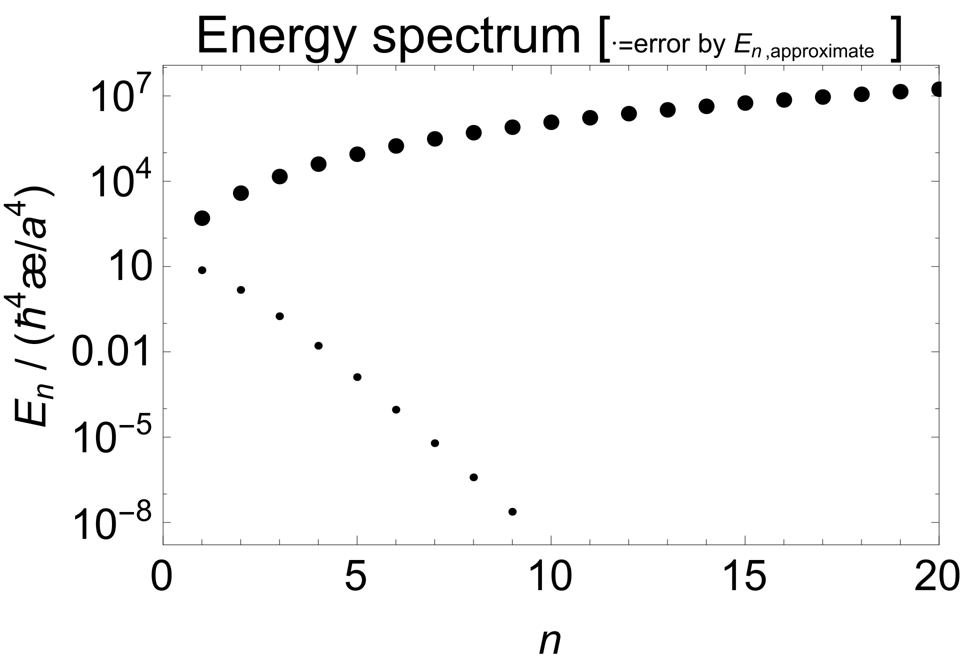


Figure 5.3: Energy spectrum of all eigenvalues (large dots) and the approximation error (small dots).

roots is not always necessary. A good approximation of the energy levels can be made, assuming that $\tanh(\frac{\pi a}{2}k)$ and $\coth(\frac{\pi a}{2}k) \approx 1$. When this is true, the approximation is

$$E_{n,approximate} = \frac{\varkappa(\frac{1}{2}+n)^4\pi^4\hbar^4}{a^4} \,. \tag{5.7}$$

Figure 5.3 plots the energy spectrum of all eigenvalues, and the corresponding error between the exact values and the approximate values obtained by (5.7), which can be observed to drop rapidly with increasing n.

This approximation can be further tested using Weyl's law, which is exact in the high energy limit, for the number of states with energies below a given energy E:

$$\mathcal{N}(E) = \frac{\mathcal{W}(E)}{(2\pi\hbar)^D} \,, \tag{5.8}$$

where $\mathcal{W}(E)$ is the classical phase-space volume occupied by points with energies below E, and D is number of spatial dimensions. For our system, the phase space volume $W(E)$ is $2ap(E)$, with the momentum p being $p(E) = (\frac{E}{\varkappa})^{\frac{1}{4}}$, and $D = 1$. Weyl's law then gives

$$E_{n,\text{Weyl}} = \frac{\varkappa n^4 \pi^4 \hbar^4}{a^4} \tag{5.9}$$

which, indeed, agrees with (5.7) for large values of n.

CHAPTER 6

FUTURE WORK

The work undertaken for this thesis has laid the groundwork for understanding quantum mechanics with a quartic dispersion law by solving one-dimensional scattering problems with the conventional barriers found in most introductory quantum mechanics text books, the bound value problem of an infinite well with hard walls showing quantization of available energy states, and by constructing the probability current functional that allows these results to be tested through conservation laws.

It should be noted that conservation of probability current allows for several different possible jump conditions at a discontinuity in potential. This work has chosen the most natural of these possible jump conditions, but ultimately they should be proven by using a limiting procedure on a continuous potential, making it progressively steeper.

Other work to be undertaken at this level will need to determine the phase difference between incident and reflected waves on a wall. Determining this phase difference is important because it can be used to calculate resonances and densities of state, and also will be important in predicting the $+\frac{1}{2}$ correction in the approximation of energy levels shown in (5.7). Furthermore, the energy dependence of the phase of the reflected wave reflected from an infinitely high wall is a property of quartic quantum mechanics that is not present in the conventional case. This requires further investigation.

Finally, to help realize the ultimate goal of experimentally realizing a three-dimensional matter wave, it will first be necessary to add attractive interactions of the form $-G|\psi|^2\psi$ to the time-dependent Schrödinger equation with quartic dispersion, and study both the static properties and the elementary excitations of the resulting solitary wave.

CHAPTER 7

CONCLUSION

In summary, this thesis has explored the basis for quantum mechanics with a quartic dispersion law. Conservation of probability was employed to construct the probability current functional, and this result used to link the behavior of the wavefunction on one side of the potential discontinuity to the one on the other side. The former was used to (a) solve a variety of the scattering problems and (b) to derive the boundary conditions on the surface of an infinitely high wall. Transmission and reflection amplitudes were determined for potentials commonly used to investigate behaviors in conventional quantum mechanics, and the scattering behavior was found to be well modeled by δ-potential scattering theory for narrow barriers, while classic behavior was recovered for broad barriers. Finally, the result (b) above was used quantize an infinitely deep potential well. A simple analytic approximation for the spectrum has been obtained. This expression was in turn compared with the predictions of Weyl's law.

The groundwork for understanding quantum mechanics with quartic dispersion is therefore laid. It remains to prove the jump conditions used are correct by beginning with a continuous potential and using a limiting procedure, and to determine the phase shift between an incident wave, and its reflected wave when incident on a wall, which will enable a more complete understanding of quantum systems with quartic dispersion. Finally, understanding how attractive interactions affect the static properties and the elementary excitations of solitary waves in systems with quartic dispersion should aid in experimental realization of such a system in a shaken optical lattice, and will provide a mechanism for producing stable, mobile three-dimensional matter waves.

CITATIONS

[1] K. E. Strecker, G. B. Partridge, A. G. Truscott, and R. G. Hulet, " Formation and propagation of matter wave soliton trains," *Nature* **417**, 150 (2002).

[2] L. Khaykovich, F. Schreck, G. Ferrari, T. Bourdel, J. Cubizolles, L. D. Carr, Y. Castin, and C. Salomon, "Formation of a matter-wave bright soliton," *Science* **296**, 1290 (2002).

[3] M. Olshanii, S. Choi, V. Dunjko, A. E. Feiguin, H. Perrin, J. Ruhl, and D. Aveline, "Three-dimensional Gross-Pitaevskii solitary waves in optical lattices: stabilization using the artificial quartic kinetic energy induced by lattice shaking," Submitted to *Phys. Rev. Lett.*

[4] V. Ahufinger, A. Sanpera, P. Pedri, L. Santos, and M. Lewenstein, "Creation and mobility of discrete solitons in Bose-Einstein condensates," *Phys. Rev. A* **69**, 053604 (2004).

[5] T. J. Alexander, E. A. Ostrovskaya, and Y. S. Kivshar, "Self-trapped nonlinear matter waves in periodic potentials," *Phys. Rev. Lett.* **96**, 040401 (2006).

[6] D. Mihalache, D. Mazilu, F. Lederer, B. A. Malomed, L.-C. Crasovan, Y. V. Kartashov, and L. Torner, "Stable three-dimensional solitons in attractive Bose-Einstein condensates loaded in an optical lattice," *Phys. Rev. A* **72**, 021601 (2005).

[7] H. Saito and M. Ueda, "Bose-Einstein droplet in free space," *Phys. Rev. A* **70**, 053610 (2004).

[8] O. V. Borovkova, Y. V. Kartashov, L. Torner, and B. A. Malomed, "Bright solitons from defocusing nonlinearities," *Phys. Rev. E* **84**, 035602 (2011).

[9] C. V. Parker, L.-C. Ha, and C. Chin, "Direct observation of effective ferromagnetic domains of cold atoms in a shaken optical lattice," *Nat. Phys.* **9**, 769 (2013).

[10] B. Eiermann, T. Anker, M. Albiez, M. Taglieber, P. Treutlein, K.-P. Marzlin, and M. K. Oberthaler, "Bright Bose-Einstein gap solitons of atoms with repulsive interaction," *Phys. Rev. Lett.* **92**, 230401 (2004).

[11] N. Gemelke, E. Sarajlic, Y. Bidel, S. Hong, and S. Chu, "Parametric amplification of matter waves in periodically translated optical lattices," *Phys. Rev. Lett.* **95**, 170404 (2005).

[12] H. Lignier, C. Sias, D. Ciampini, Y. Singh, A. Zenesini, O. Morsch, and E. Arimondo, “Dynamical control of matter-wave tunneling in periodic potentials,” *Phys. Rev. Lett.* **99**, 220403 (2007).

[13] S. Flügge, *Practical Quantum Mechanics*. Berlin: Springer (1994), Problem “Law of probability conservation”.

[14] ibid., Problem “Potential step”.

[15] ibid.,Problem “Reflection at a rectangular barrier”.

[16] ibid., Problem “Standing wave”.

[17] ibid., Problem “Rectangular potential hole”

LIST OF REFERENCES

V. Ahufinger, A. Sanpera, P. Pedri, L. Santos, and M. Lewenstein, "Creation and mobility of discrete solitons in Bose-Einstein condensates," *Phys. Rev. A* **69**, 053604 (2004).

T. J. Alexander, E. A. Ostrovskaya, and Y. S. Kivshar, "Self-trapped nonlinear matter waves in periodic potentials," *Phys. Rev. Lett.* **96**, 040401 (2006).

O. V. Borovkova, Y. V. Kartashov, L. Torner, and B. A. Malomed, "Bright solitons from defocusing nonlinearities," *Phys. Rev. E* **84**, 035602 (2011).

B. Eiermann, T. Anker, M. Albiez, M. Taglieber, P. Treutlein, K.-P. Marzlin, and M. K. Oberthaler, "Bright Bose-Einstein gap solitons of atoms with repulsive interaction," *Phys. Rev. Lett.* **92**, 230401 (2004).

S. Flügge, "Law of probability conservation," *Practical Quantum Mechanics*. Berlin: Springer (1994).

S. Flügge, "Potential step," *Practical Quantum Mechanics*. Berlin: Springer (1994).

S. Flügge, "Rectangular potential hole," *Practical Quantum Mechanics*. Berlin: Springer (1994).

S. Flügge, "Reflection at a rectangular barrier," *Practical Quantum Mechanics*. Berlin: Springer (1994).

S. Flügge, "Standing wave," *Practical Quantum Mechanics*. Berlin: Springer (1994).

N. Gemelke, E. Sarajlic, Y. Bidel, S. Hong, and S. Chu, "Parametric amplification of matter waves in periodically translated optical lattices," *Phys. Rev. Lett.* **95**, 170404 (2005).

L. Khaykovich, F. Schreck, G. Ferrari, T. Bourdel, J. Cubizolles, L. D. Carr, Y. Castin, and C. Salomon, "Formation of a matter-wave bright soliton," *Science* **296**, 1290 (2002).

H. Lignier, C. Sias, D. Ciampini, Y. Singh, A. Zenesini, O. Morsch, and E. Arimondo, "Dynamical control of matter-wave tunneling in periodic potentials," *Phys. Rev. Lett.* **99**, 220403 (2007).

D. Mihalache, D. Mazilu, F. Lederer, B. A. Malomed, L.-C. Crasovan, Y. V. Kartashov, and L. Torner, "Stable three-dimensional solitons in attractive Bose-Einstein condensates loaded in an optical lattice," *Phys. Rev. A* **72**, 021601 (2005)

M. Olshanii, S. Choi, V. Dunjko, A. E. Feiguin, H. Perrin, J. Ruhl, and D. Aveline, "Three-dimensional Gross-Pitaevskii solitary waves in optical lattices: stabilization using the artificial quartic kinetic energy induced by lattice shaking," Submitted to *Phys. Rev. Lett.*

C. V. Parker, L.-C. Ha, and C. Chin, "Direct observation of effective ferromagnetic domains of cold atoms in a shaken optical lattice," *Nat. Phys.* **9**, 769 (2013).

H. Saito and M. Ueda, "Bose-Einstein droplet in free space," *Phys. Rev. A* **70**, 053610 (2004).

K. E. Strecker, G. B. Partridge, A. G. Truscott, and R. G. Hulet, " Formation and propagation of matter wave soliton trains," *Nature* **417**, 150 (2002).