Wave Propagation in Systems with Alternating Linear and Nonlinear Layers

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IMM-THESIS-2003-51

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Preface

This Master Thesis was written at the Department of Informatics and Mathematical Modelling at the Technical University of Denmark during September 2002 - August 2003 with Professor, Dr. Techn. Peter Leth Christiansen as supervisor.

I would like to thank Guest Professors Yuri B. Gaididei and Alexander Zolotaryuk from the Bogolyubov Institute for Theoretical Physics, Kiev Ukraine, for mathematical assistance during the project. I also would like to thank Mark Wrobel and Toke Koldborg Jensen for the joyful beginning at the "project room 129" and Jens Arnbak for suggestions and corrections during the writing of the thesis.

And last but not least, I wish to express my gratitude to my wife and my daughter who have showed considerable patience during the last months of my project.

Kgs. Lyngby, September the 1st, 2003

Harald Arnbak

Abstract

The goal of this thesis, is to find the transmission for a delta prime shaped potential with Kerr nonlinearity. First, where necessary, Dirac's delta function and its derivatives are regularized with rectangular approximations, and the linear Schrödinger equation is solved. Then the corresponding Schrödinger equation with Kerr nonlinearity is introduced and investigated.

Keywords: *Dirac's Delta Function and its Derivatives, Linear Approximations, Nonlinear Schrödinger Equation*

Resumé på dansk

Målet er at finde transmissionen for en delta mærke formet potentiale med Kerr ikke–lineæritet. Først er Dirac's delta funktion og dens afledede om nødvendigt regulariseret ved hjælp af rektangulære approksimationer og Schrödinger ligningen er løst. Så bliver den korresponderende Schrödinger ligning med Kerr ulineæritet introduceret og undersøgt.

Contents

Chapter 1

Introduction

This thesis combines two different fields of study in modern mathematical physics, namely

- the use of the Schrödinger equation from quantum mechanics to determine the probability density function for the location of a particle moving in a potential field and
- adequate modelling of nonlinear potentials.

The combination in a useful model for propagation through a nonlinear potential of a quantum–mechanical system is difficult, but important. In general, the superposition principle does not apply with nonlinear potentials. This means that a combination of any two solutions to the relevant differential equation (here the nonlinear Schrödinger equation) is not necessarily itself a new solution. This study is focused on developing local analytical descriptions of nonlinear potentials by Dirac's delta function and/or its derivatives. Approximate numerical or symbolic computer methods can then be applied.

Microscopic potentials may be used as control elements for flows of particles on a similar scale. Examples are photons in low–loss optical waveguides and fibre bends [THLA02], electrons in nonlinear "nanotubes" [Dek99] and photons in a phase gate [GLT00] of a quantum computer, which requires the manipulation of quantum information at a very high rate.

The latter is similar to the nonlinear Kerr effect [ST91], discovered by the Scottish physicist John Kerr in the nineteenth century. The Kerr effect is in practical use in the photography of highly transient phenomena, as it can interrupt a light beam up to 10^{10} times per second, simply by raising or lowering the potential barrier for transmission of photons through an optical shutter of a camera.

The following sections of this chapter give a short introduction to quantum mechanics and its basic equations of importance.

1.1 Tunnelling

When a free–wheeling car approaches a small hill with sufficient speed, it will easily pass the hill top. See figure 1.1. But when the car does not have enough speed or the hill is too high, the car will stop at some point and start rolling backwards. To go beyond that specific point, the engine must be used. In physical terms: because the total energy of the car is exceeded by the barrier's potential, the car will turn in the so–called "turning point".

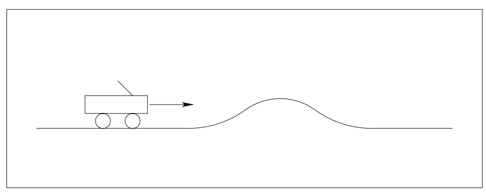


Figure 1.1: *Free–wheeling car approaching small hill.*

This scenario is as predicted by classical mechanics. In quantum mechanics however, although the particle's total energy is lower than the potential, there is a finite probability for the mass to actually pass that barrier! This phenomenon is called tunnelling [Gri95] page 52.

1.2 Quantum Mechanics

Consider a point particle with mass m, moving in one dimension, say along the x–axis, under the influence of a specified force F. See figure 1.2. Together with the appropriate initial conditions, it is now possible to determine the position $x(t)$ of the particle, using Newton's second law $F = ma$, where a is the acceleration of the particle. From this equation, any other dynamical variable of interest can be found. [Gri95] page 1 calls this the approach of classical mechanics.

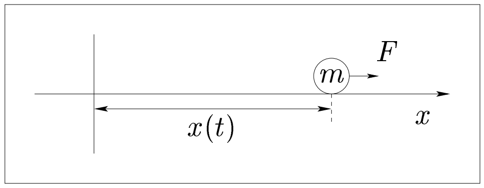


Figure 1.2: *Point particle with mass m and position $x(t)$, moving along the x–axis under influence of force F.*

1.2.1 Schrödinger Equation and Wavefunction

Quantum mechanics deals with the same problem quite differently. Now the approach is to find the wavefunction $\Psi(x,t)$, by solving the one–dimensional Schrödinger equation as seen in [ER85] page 150,

$$-\frac{\hbar^2}{2m}\frac{\partial^2\Psi(x,t)}{\partial x^2}+V(x,t)\Psi(x,t)=i\hbar\frac{\partial\Psi(x,t)}{\partial t}, \tag{1.1}$$

where $\hbar$ is Planck's constant and t is the time. $V(x,t)$ represents the potential energy function, that properly describes the force F acting on the particle.

The wavefunction contains all the mechanical properties of the particle and defines the probability density $P(x,t)$ of its instantaneous location. According to [Gri95] page 2, the probability of finding the particle between x and $x+dx$ at time t, is defined in the following manner

$$P(x,t)dx = |\Psi(x,t)|^2\,dx. \tag{1.2}$$

Because the particle exists, it must be located somewhere. Mathematically this is formulated as in [Gri95] page 11: the integral of the probability $P(x,t)$ over all space, in this case the whole x–axis, needs to be equal 1 at all time

$$\int_{-\infty}^{\infty} P(x,t)dx = \int_{-\infty}^{\infty} |\Psi(x,t)|^2 dx = 1. \tag{1.3}$$

This procedure is called normalization and is used to specify the amplitude of the wavefunction.

1.2.2 Time–Independence

In this thesis, all potentials are independent of time: $V(x,t)=V(x)$. Therefore, as suggested in [Gri95] page 20, we solve eq. (1.1) by the method of separation of variables, where the wavefunction is expressed as a product of an amplitude function and a time–dependent function

$$\Psi(x,t) = \psi(x)f(t).$$

Inserting this product in eq. (1.1) gives two ordinary differential equations, which are easily solved. Accordingly to [ER85] page 151, the problem is now transformed to

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} + V(x)\psi(x) = E\psi(x), \tag{1.4}$$

with the new wavefunction becoming

$$\Psi(x,t) = \psi(x)e^{-\frac{iEt}{\hbar}}. \tag{1.5}$$

The amplitude function $\psi(x)$ is a function of x alone, and E is the total energy of the particle in the system.

Eq. (1.4) is called the time–independent Schödinger equation, because the time does not enter in the equation. See [Gri95] page 22. [ER85] page 154 points out that its time–independent solutions $\psi(x)$ are eigenfunctions, which need to be finite, single–valued and continuous. This is needed to maintain mathematically "well–behaved" functions with physical relevance. They describe through eq. (1.5) the space–dependence of the wavefunction.

Although the wavefunction, as appearing in eq. (1.5), does depend on the time, the probability $P(x,t)dx$ is now time–independent. This is clearly seen when inserted in eq. (1.2)

$$\begin{aligned} P(x,t)dx &= \left|\Psi(x,t)\right|^2 dx \\ &= \Psi^*(x,t)\Psi(x,t)dx \\ &= \psi^*(x)e^{\frac{iEt}{\hbar}}\psi(x)e^{-\frac{iEt}{\hbar}}dx \\ &= \left|\psi(x)\right|^2 dx. \end{aligned}$$

(For normalizable solutions, the energy E must be real.) Because the probability, and in fact the expectation value of any dynamical variable, is time–independent, all solutions as appearing in eq. (1.5), are called the stationary states. See [Gri95] page 22.

1.2.3 Short–Range Potentials

All potentials treated in this thesis are not only time–independent, they are also so–called “short–range potentials”. This means that they are localized, implying $V(x) \to 0$ for $x \to \pm\infty$. When additionally the energy E is negative, eq. (1.5) represents a local bound state. However, the focus in this thesis is on the transmission through the potential, which is obtained by investigating the scattering states ($E \geq 0$). By introducing $E = k^2 \geq 0$ and using units as done in [CAZ+03], $\hbar^2/2m = 1$ and eq. (1.4) is further simplified to

$$-\psi''(x) + U(x)\psi(x) = k^2\psi(x), \tag{1.6}$$

where the prime denotes differentiation with respect to the spatial coordinate x. $U(x)$ is the new potential and is of dimension $[\text{length}]^{-2}$, while k from now on is of dimension $[\text{length}]^{-1}$.

The procedure is to find the general solutions to the Schrödinger equation and connect them with the help of the boundary conditions. This results in an equation in which the intensity of the incident wave is expressed as a function of the intensity of the transmitted wave. This is done, because the classical transmission defined as the fraction of the intensities of the transmitted wave and the incident wave, can not be determined for the nonlinear Schrödinger equation.

1.3 Outline of Thesis

The potentials appear as characteristic $U(x)$ in eq. (1.6) and are basically of the same geometrical shape. They can be divided into two classes: the linear and nonlinear potential classes.

1.3.1 Linear Potentials

In chapter 2, three potentials of the linear class are presented. These potentials illustrate the general procedure for all further calculations and underline the increasing complexity as the potential becomes more extended. Furthermore, these linear potentials are used for calibration, in the limit of vanishing nonlinearity, of the corresponding geometrical nonlinear potentials. The potentials of this class contain a linear term only

$$U(x) = u(x), \tag{1.7}$$

where the real valued function $u(x)$ depends on the spatial variable x. If $u(x) > 0$, the potential repels the particle while passing and is called a barrier. Similarly if $u(x) < 0$, the potential attracts and is called a well.

A well–known elementary example in quantum mechanics, Dirac's delta function barrier, is treated in section 2.1. This gives much insight into the type of potentials of the thesis, because the example is basic and easy to follow, which is helpful for understanding the more complicated potentials presented later. Furthermore, it is a simple example to illustrate tunnelling.

In section 2.2, the transmission for the first derivative of the delta function with respect to its spatial variable, the delta prime function, is investigated. In order to do so, the function is regularized by an approximation and the transmission for the approximation is obtained. Then this result is investigated in the limit, where the approximation tends towards the actual delta prime function. Some rather intuitively unexpected solutions occur!

The same method is applied to investigate the transmission for the second derivative of the delta function, the delta double–prime function. The approximation is a further increase in size and complexity and some lengthy calculations come across. This is done in section 2.3.

1.3.2 Nonlinear Potentials

Chapter 3 contains two potentials of the nonlinear class, which have Kerr nonlinearity incorporated in $U(x)$

$$U(x) = U\left(x, |\psi(x)|^2\right) = u(x) + v(x)|\psi(x)|^2, \tag{1.8}$$

where u is the same function as for the linear class (see eq. (1.7)) and $v(x)$ is a new real valued scaling function, which depends on x only. Clearly, the wavefunction now controls the strength of the potential, since its amplitude function $\psi(x)$ occurs in the right part of eq. (1.8). This means that the wavefunction itself determines the actual wave transmission for the potential.

In section 3.1 the simplest nonlinear case is presented: the delta function with nonlinearity. This potential is incorporated as a simple example. The effect of the nonlinearity is clearly seen in the figures. Finally in section 3.2, the regularizing approximation for the nonlinear delta prime potential is investigated and the transmission is found.

In chapter 4 the results are discussed and some suggestions for future work are made.

Chapter 2

Transmission for Dirac's Delta Function and its derivatives

In this chapter the transmissions for Dirac's delta function and its first and second derivative are investigated.

2.1 Delta Function

Dirac's delta function is a widely used theoretical potential, because it is perhaps the simplest example with both bound and scattering states. Furthermore, the tunnelling effect is easily demonstrated.

2.1.1 Dirac's Delta Function

Dirac's delta function, from now on referred to as the delta function $\delta(x)$, is an infinitely high, infinitesimally narrow spike at the origin, whose area is 1. See figure 2.1. Technically, it is not a function as it is not finite in the origin (mathematicians call it a generalized function). [Gri95] page 52 informally defines the delta function as follows

$$\delta(x) = \left\{ \begin{array}{ll} 0, & \text{if} \quad x \neq 0 \\ \infty, & \text{if} \quad x = 0 \end{array} \right\}, \text{ with } \int_{-\infty}^{\infty} \delta(x) dx = 1. \tag{2.1}$$

When the delta function is horizontally displaced to $x = x_1$, the function can be written as $\delta(x - x_1)$. Now, $f(x)\delta(x - x_1) = f(x_1)\delta(x - x_1)$, because

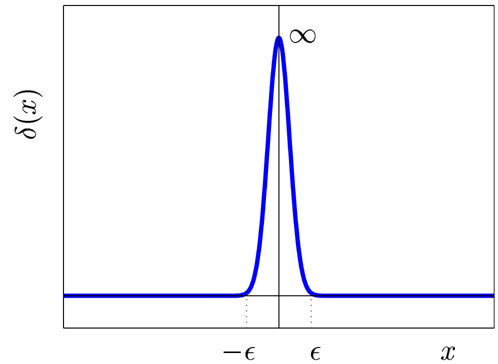


Figure 2.1: *Dirac's delta function. (ϵ is infinitesimally small)*

the product $f(x)\delta(x-x_1)$ is nonzero only at $x = x_1$ as stated in eq. (2.1). By integrating this product, the value $f(x_1)$ is isolated

$$\begin{aligned}\int_{-\infty}^{\infty} f(x)\delta(x-x_1)dx &= f(x_1)\int_{-\infty}^{\infty} \delta(x-x_1)dx \\ &= f(x_1). \end{aligned} \tag{2.2}$$

This is called the sifting property and illustrates the complexity of the delta function.

2.1.2 Transmission

The calculation of the transmission through the delta function barrier is straightforward and thus a widely used example in quantum mechanics. It can be found in for instance [Sco99] pages 44–46. Here, the approach of [Gri95] section 2.5 is followed. It begins with the insertion of the delta function multiplied with a real scaling parameter with dimension $[\text{length}]^{-1}$, α. Eq. (1.6) becomes

$$-\psi''(x) + \alpha\delta(x)\psi(x) = k^2\psi(x). \tag{2.3}$$

For practical reasons, the potential is now divided into two intervals, which need to be treated separately. Interval 1 corresponds to $x < 0$ and interval 2 to $x > 0$. In interval 1, the potential $\alpha\delta(x) = 0$, so eq. (2.3) simplifies to

$$-\psi''(x) = k^2\psi(x),$$

where only $k > 0$ is investigated, since the scattering states alone determine the transmission (see subsection 1.2.3). The general solution is found in eq. (A.2) and becomes for interval 1

$$\psi_1(x) = I(k)e^{ikx} + R(k)e^{-ikx}, \tag{2.4}$$

where $I(k)$ and $R(k)$ are the amplitude coefficient of the incident and reflected wave respectively. These coefficients are functions of k.

In interval 2 the potential $\alpha\delta(x) = 0$ again, but since we assume an incident wave from the left only, the solution for interval 2 looks like

$$\psi_2(x) = T(k)e^{ikx}, \tag{2.5}$$

where $T(k)$ is the amplitude coefficient of the transmitted wave. Again the coefficient is a function of k.

Now the two functions $\psi_1(x)$ and $\psi_2(x)$ need to be connected at $x = 0$. This is done with the help of the general boundary conditions as formulated in [Gri95] page 54. These are

$$\begin{array}{ll} 1. & \psi \text{ is always continuous, and} \\ 2. & \frac{d\psi}{dx} \text{ is continuous except at points} \\ & \text{where the potential is infinite.} \end{array} \tag{2.6}$$

The first general condition is easily fulfilled by equalizing the functions $\psi_1(x)$ and $\psi_2(x)$ at $x = 0$. Substitution of eq. (2.4) and eq. (2.5) leads to

$$\begin{aligned} &\psi_1(0) = \psi_2(0) \\ &\quad \Rightarrow \quad I(k) + R(k) = T(k). \end{aligned} \tag{2.7}$$

The second general boundary condition is of no help in this particular case, because the delta function is infinite at $x = 0$. This means that the delta function introduces a discontinuity in $\frac{d\psi}{dx}$ at $x = 0$. In order to determine this discontinuity, [Gri95] page 54 suggests to integrate eq. (2.3) from $+\epsilon$ to $-\epsilon$ and then let $\epsilon \to 0$. Integrating gives

$$-\int_{-\epsilon}^{+\epsilon} \psi''(x)dx + \int_{-\epsilon}^{+\epsilon} \alpha\delta(x)\psi(x)dx = \int_{-\epsilon}^{+\epsilon} k^2\psi(x)dx. \tag{2.8}$$

Now the limit $\epsilon \to 0$ is applied. Noticing that in this limit, the integral on the right is equal to zero and evaluating and rearranging the remaining terms, the equation simplifies to

$$\lim_{\epsilon \to 0} (\frac{d\psi}{dx}\Big|_{x=-\epsilon}^{\epsilon}) = \lim_{\epsilon \to 0} \int_{-\epsilon}^{+\epsilon} \alpha\delta(x)\psi(x)dx. \tag{2.9}$$

If the potential $\alpha\delta(x)$ would have been finite at $x = 0$, the integral on the right would be equal to zero again, implying that $\frac{d\psi}{dx}$ is continuous as stated in the second general boundary condition in (2.6). But $\alpha\delta(x)$ is not finite and the integral on the right can be found to be equal to $\alpha\psi(0)$. This is done with the help of eq. (2.2) and yields

$$\frac{d}{dx}\psi_2(x)\bigg|_{x=0} - \frac{d}{dx}\psi_1(x)\bigg|_{x=0} = \alpha\phi(0) = \alpha\phi_2(0),$$

where $\psi(0) = \psi_2(0)$, because $\psi(x)$ is always continuous according to the first general boundary condition in (2.6). Insertion of eq. (2.4) and eq. (2.5) leads to

$$ikT(k) - (ikI(k) - ikR(k)) = \alpha T(k).$$

Combining this equation with eq. (2.7), the transmission and reflection coefficients are found to be

$$I(k) = \frac{i2k - \alpha}{i2k} I(k),$$
$$R(k) = \frac{\alpha}{i2k} T(k).$$

Now the intensity of the incident wave can be expressed as function of the transmitted wave as follows

$$|I(k)|^2 = \frac{4k^2 + \alpha^2}{4k^2} |T(k)|^2. \tag{2.10}$$

2.1.3 Results

In figure 2.2 all the solutions are straight lines. This means that any combination of two solutions is again a solution and the barrier is linear. It can also be seen that the greater the energy of the particle (compared to the potential of the barrier), the higher the intensity of the transmitted wave. In the limit where the potential vanishes ($k \gg \alpha$), the intensities of the incident and transmitted wave correspond (this is most easily seen with eq. (2.10) if $k \to \infty$).

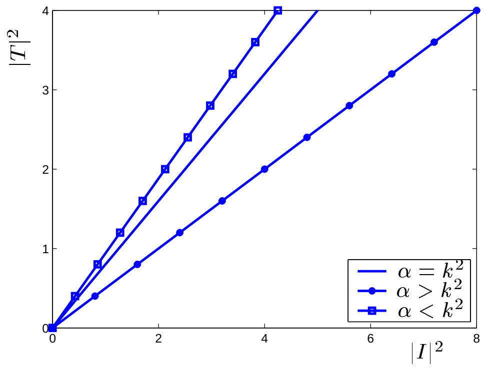


Figure 2.2: *Transmission for the linear delta potential for different combinations of α and k respectively; $\alpha = k^2 = 1$, $\alpha = 2 \wedge k^2 = 1$ and $\alpha = 1 \wedge k^2 = 4$.*

Furthermore, the tunnelling effect is apparent as the transmission does not drop to zero, when the potential becomes higher than the energy of the particle ($\alpha > k^2$). This is opposite to the classical equivalent, where the mass will "turn around". Only in the limit of infinite potential ($\alpha \to \infty$), the transmission will be zero (see again eq. (2.10)).

2.2 Delta Prime Function

The first derivative of the delta function with respect to its spatial variable, $\delta'(x)$, is depicted in figure 2.3. The potential, which is investigated in this section, is of the form $U(x) = \beta\delta'(x)$, where β is a dimensionless real constant.

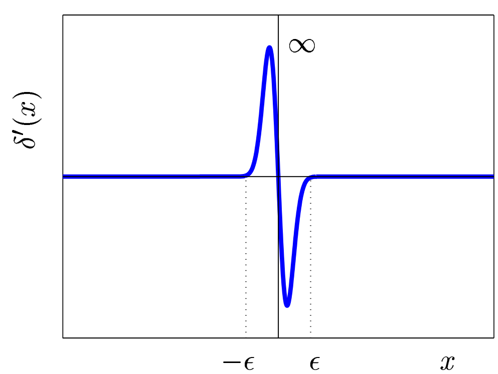


Figure 2.3: *The first derivative of the delta function (ϵ is infinitesimally small)*

If the same straightforward approach to find the transmission is followed as in subsection 2.1.2, the following integral would determine the discontinuity in $\frac{d\psi}{dx}$ (notice the correspondence with eq. (2.8))

$$-\int_{-\epsilon}^{+\epsilon} \psi''(x)dx + \int_{-\epsilon}^{+\epsilon} \beta\delta'(x)\psi(x)dx = \int_{-\epsilon}^{+\epsilon} k^2\psi(x)dx.$$

With the help of eq. (B.2), the second integral can be found to be equal to $-\beta\psi'(0)$. However, because the potential $\delta'(x)$ is infinite in the origin, the second general boundary condition in (2.6) implies that $\psi'(x)$ is not continuous at $x = 0$. Thus, $\psi'(0)$ is not defined and the second integral can not be solved! This problem can be avoided by regularizing the delta prime potential.

2.2.1 Regularization

In literature, the delta prime function has been regularized in many ways. We choose to use the rectangular–like approximation $\Delta'_{u,a}(x)$ as proposed by [CAZ$^+$03]: a sequence of two step–functions with width $a > 0$ and alternating height $u > 0$

$$\Delta'_{u,a}(x) = \begin{cases} 0, & \text{if } -\infty < x < -a, \\ u, & \text{if } -a < x < 0, \\ -u, & \text{if } 0 < x < a, \\ 0, & \text{if } a < x < \infty. \end{cases} \tag{2.11}$$

where a has the dimension [length]. u must have the same dimension as $\delta'(x)$, i.e. [length]$^{-2}$. The potential is depicted in figure 2.4.

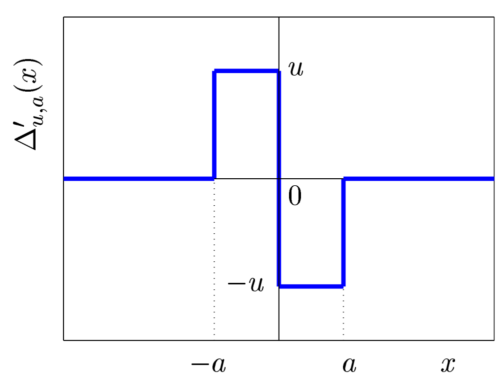


Figure 2.4: *The rectangular regularization of $\delta'(x)$ by two step–functions with width a and alternating height u.*

It can be seen with the help of eq. (B.3) that in the limit of $a \to 0$ the integral of the approximation $\Delta'_{u,a}(x)$ multiplied with an arbitrary "smooth" function $f(x)$ approaches $-f'(0)$ if $u = 1/a^2$. Mathematically stated,

$$\begin{aligned} \int_{-\infty}^{\infty} f(x)\Delta'_{u,a}(x)dx &= -ua^2 f'(0) + O(a^4) \\ &\to -f'(0) \text{ if } u = \frac{1}{a^2} \text{ and } a \to 0. \end{aligned}$$

This is equal to the solution of the integral of $\delta'(x)$ multiplied with that same "smooth" function $f(x)$, see eq. (B.2). Hence,

$$\Delta'_{u,a}(x) \to \delta'(x) \text{ if } u = \frac{1}{a^2} \text{ and } a \to 0.$$

2.2.2 Transmission

One advantage of the regularizing potential $\Delta'_{u,a}(x)$ is that it is nowhere infinite. Hence, both the amplitude function $\psi(x)$ and its first derivative $\psi'(x)$ are always continuous according to the general boundary conditions in (2.6). So now the transmission can be obtained in the same straightforward manner as applied in subsection 2.1.2. The Schrödinger equation, eq. (1.6), becomes

$$-\psi''(x) + \Delta'_{u,a}(x)\psi(x) = k^2\psi(x). \tag{2.12}$$

It is important to be sure that the dimension of the equation is always correct. Because the amplitude function $\psi(x)$ is present in all terms of eq. (2.12), its dimension can be divided out. In subsection 1.2.3 it was explained that k is of dimension $[\text{length}]^{-1}$ and the approximation is only nonzero when $\Delta'_{u,a}(x) = \pm u$. Thus, the dimension of u must be $[\text{length}]^{-2}$, which is also the case. See section 2.2.1.

On the left and the right of the potential, $\Delta'_{u,a}(x) = 0$ Because we consider an incident wave from the left only, eq. (2.4) and eq. (2.5) can be adopted, for $x < -a$ and $x > a$. The general solution for $x < -a$, which we call interval 1, is

$$\psi_1(x) = Ie^{ikx} + Re^{-ikx}, \tag{2.13}$$

and for $x > a$, interval 4,

$$\psi_4(x) = Te^{ikx}. \tag{2.14}$$

I, R and T are the amplitude coefficient belonging to the incident, reflected and transmitted wave respectively. These coefficients are functions of k, but are not written as functions for simplicity matters. Again only the scattering states are investigated, which implies $E > 0 \Rightarrow k > 0$ (see subsection 1.2.3).

In interval 2 the potential $\Delta'_{u,a}(x) = u$ is always positive, so it is a barrier. The Schödinger equation eq. (2.12) for the barrier becomes

$$-\psi''(x) + u\psi(x) = k^2\psi(x).$$

Eq. (A.1) can be used as the general solution for the Scrhödinger equation in interval 2, because $S = u - k^2 > 0$ as only the tunnelling effect is investigated. See section 1.1 and 1.2 for more details. This gives

$$\psi_2(x) = B_1 \cosh(qx) + B_2 \sinh(qx), \tag{2.15}$$

where the amplitude functions B_1 and B_2 vary with k. Once more this dependence is not denoted for simplicity matters. The coefficient $q = \sqrt{u - k^2}$ is larger than zero.

In interval 3 the potential $\Delta'_{u,a}(x) = -u < 0$ and the Schödinger equation (2.12) is now

$$-\psi''(x) - u\psi(x) = k^2\psi(x).$$

Eq. (A.2), where $S = -(u + k^2) < 0$ in particular, gives the general solution

$$\psi_3(x) = A_1 \cos(\kappa x) + A_2 \sin(\kappa x), \tag{2.16}$$

with the amplitude functions A_1 and A_2, which depend on k. Again these amplitudes are not denoted as functions for simplicity matters. The coefficient $\kappa = \sqrt{u + k^2}$ is larger than zero.

Now that the general solution in all four intervals are known, they can be connected at the three intersection points $x = a, 0, -a$. As mentioned before, both the amplitude function and its first derivative are continuous at these points (because the potential $\Delta'_{u,a}(x)$ is always finite), yielding at $x = a$

$$\begin{cases} \psi_3(a) &= \psi_4(a) \\ \psi_3'(a) &= \psi_4'(a) \end{cases}$$

Inserting eq. (2.14) and eq. (2.16) and rearranging, gives

$$\begin{cases} A_1 &= Te^{ika}\{\cos(\kappa a) - \frac{ik}{\kappa}\sin(\kappa a)\}, \\ A_2 &= Te^{ika}\{\sin(\kappa a) + \frac{ik}{\kappa}\cos(\kappa a)\}. \end{cases} \tag{2.17}$$

The amplitude function in the barrier is specified, so the intensity of the wave in the barrier, $|\psi_3(x)|^2$, can be obtained. Inserting the amplitudes A_1 and A_2 in eq. (2.16) and calculating the modulus squared value of $\psi_3(x)$ gives

$$|\psi_3(x)|^2 = \frac{|T|^2}{2\kappa^2}\{u + 2k^2 + u\cos\Big(2\kappa(x-a)\Big)\}. \tag{2.18}$$

Connecting the general solutions for the amplitude function and its first derivative at $x = 0$ yields

$$\begin{cases} B_1 &= A_1, \\ B_2 &= \frac{\kappa}{q}A_2. \end{cases} \tag{2.19}$$

By inserting these values and followingly eqs (2.17) in the expression for $\psi_2(x)$ in eq. (2.15) and then considering the modulus squared with a lot of trigonometric adjustments, specifies the intensity of the wave in the well, $|\psi_2(x)|^2$. The result is

$$\begin{aligned} |\psi_2(x)|^2 &= \frac{|T|^2}{2\kappa^2 q^2}\Big\{[u(u+2k^2) - uk^2\cos(2\kappa a)]\cosh(2qx) \\ &\quad + u\kappa q\sin(2\kappa a)\sinh(2qx) + u^2\cos(2\kappa a) - (u+2k^2)k^2\Big\}. \end{aligned} \tag{2.20}$$

The calculations for the boundary conditions at $x = -a$ are slightly more complicated. The equation, which belongs to the continuity of the amplitude function, is multiplied with ik and added to the other equation. A second expression in which the amplitude coefficient of the reflected wave appears can be obtained with subtraction. But it has been omitted as it has no influence on the propagation. The equation with I becomes

$$2Ie^{-ika} = B_1\{\cosh(qa) + \frac{iq}{k}\sinh(qa)\} - B_2\{\sinh(qa) + \frac{iq}{k}\cosh(qa)\}. \quad (2.21)$$

Multiplying eq. (2.21) with its complex conjugate and inserting eq. (2.17) and eq. (2.19) gives the intensity of the incident wave $|I|^2$ as a function of the power of the transmitted wave $|T|^2$. Rearranging yields

$$|T|^2 = \frac{4}{|D|^2}|I|^2, \quad (2.22)$$

with

$$\begin{aligned} D &= 2\cos(\kappa a)\cosh(qa) + (\frac{q}{\kappa} - \frac{\kappa}{q})\sin(\kappa a)\sinh(qa) \\ &\quad +i(\frac{q}{k} - \frac{k}{q})\cos(\kappa a)\sinh(qa) - i(\frac{k}{\kappa} + \frac{\kappa}{k})\sin(\kappa a)\cosh(qa), \quad (2.23) \end{aligned}$$

with the abbreviations $\kappa = \sqrt{u + k^2}$ and $q = \sqrt{u - k^2}$.

The same transmission is found as in the article [CAZ+03], but in this thesis the calculations are carried out with different notations to match the nonlinear equivalent presented in section 3.2. For a detailed description of the result, please refer to the article.

2.3 Delta Double–Prime Function

With the unexpected transmission for the delta prime function in mind, the second derivative of the delta function with respect to its spatial variable, the delta double–prime function, could have a special transmission too. This function can be seen in figure 2.5.

Now the potential becomes $U(x) = \gamma\delta''(x)$, where γ represents a real scaling parameter with dimension [length]. Noticing that this potential is infinite at the origin, the calculation of the discontinuity of $\psi'(x)$ at $x = 0$ again gives rise to problems if the same straightforward approach as in subsection 2.1.2 is followed. This time the equation

$$-\int_{-\epsilon}^{+\epsilon}\psi''(x)dx + \int_{-\epsilon}^{+\epsilon}\gamma\delta''(x)\psi(x)dx = \int_{-\epsilon}^{+\epsilon}k^2\psi(x)dx$$

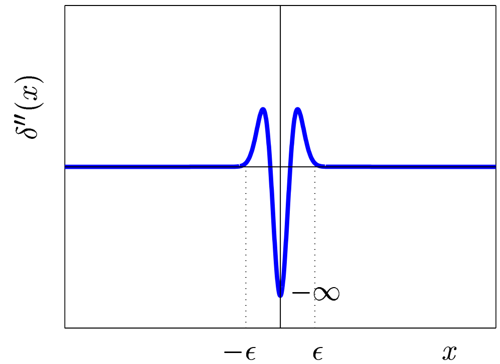


Figure 2.5: *The second derivative of the delta function. (ϵ is infinitesimally small)*

can not be solved. According to eq. (B.4), the second integral appearing in the equation is equal to $\gamma\psi''(0)$. But $\psi''(0)$ is not defined as $\psi'(x)$ is not continuous at $x = 0$ (as pointed out by the second general boundary condition in (2.6)). Hence, the second integral can not be solved. Again a regularization is needed.

2.3.1 Regularization

$\delta''(x)$ can be regularized in many ways, but we have chosen a variable rectangular approximation that is governed by four regularizing parameters. These parameters will give more control of the limit in which the approximation tends to $\delta''(x)$, as earlier private studies of fixed approximations did not predict any transmission. The approximation reads mathematically (the intervals will be used in the next section)

$$\Delta''_{\bar{u},r,d,\bar{a}}(x) = \begin{cases} 0, & \text{if } -\infty < x < -r-d-\bar{a}, & \text{interval } 1, \\ \bar{u}, & \text{if } \mp(r+d)-\bar{a} < x < \mp(r+d)+\bar{a}, & \text{interval } {}^{2}_{8}, \\ 0, & \text{if } \mp r - d + \bar{a} < x < \mp r + d - \bar{a}, & \text{interval } {}^{3}_{7}, \\ -\bar{u}, & \text{if } \mp(r-d)-\bar{a} < x < \mp(r-d)+\bar{a}, & \text{interval } {}^{4}_{6}, \\ 0, & \text{if } -r+d+\bar{a} < x < r-d-\bar{a}, & \text{interval } 5, \\ 0, & \text{if } r+d+\bar{a} < x < \infty, & \text{interval } 9, \end{cases} \tag{2.24}$$

where r, d, and $\bar{a}$ have the dimension [length] and $\bar{u}$ must have the same dimension as $\delta''(x)$, which is [length].

The approximation looks like two staggered versions of the approximation $\Delta'_{u,a}(x)$ used in subsection 2.2.1, with a space between every stepfunction. See figure 2.6. r is the horizontal length from the origin to the equivalent of the center of mass for the two left or right stepfunctions. d is the horizontal distance from r to the center of the two nearest stepfunctions and $\bar{a}$ is the half–width length from the center to the border of the stepfunctions.

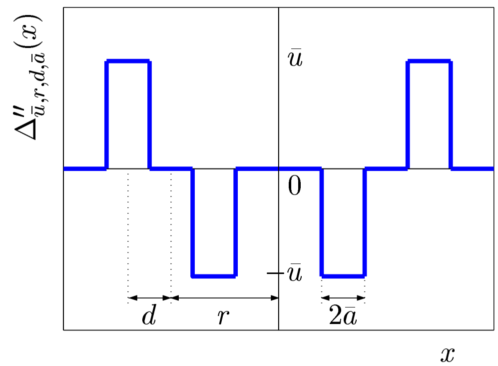


Figure 2.6: *The rectangular regularization of $\delta''(x)$.*

$\bar{u}$ is the height of the stepfunctions. If $\bar{u} = 1/8rd\bar{a}$ in particular, then the integral of the $\Delta''_{\bar{u},r,d,\bar{a}}(x)$ multiplied with an arbitrary "smooth" function $f(x)$ tends to $f''(0)$ in the limit of for instance $r \to 2\bar{a}$, $d \to \bar{a}$ and $\bar{a} \to 0$. This can be seen with the help of eq. (B.5)

$$\begin{aligned}\int_{-\infty}^{\infty} f(x)\Delta''_{\bar{u},r,d,\bar{a}}(x)dx &= 8rd\bar{u}\bar{a}f''(r) + O(d^3)\\ &\to f''(0) \text{ if } \bar{u} = \frac{1}{8rd\bar{a}} \text{ and } (r,d,\bar{a}) \to 0.\end{aligned}$$

Because the result of this limit is equal to the solution of the integral of $\delta''(x)$ multiplied with that same "smooth" function $f(x)$, see eq. (B.4),

$$\Delta''_{\bar{u},r,d,\bar{a}}(x) \to \delta''(x) \text{ if } \bar{u} = \frac{1}{8rd\bar{a}} \text{ and } (r,d,\bar{a}) \to 0. \tag{2.25}$$

Note that if the transmission is found to be nonzero in the next section, close attention has to be paid in which manner the limits $(r,d,\bar{a}) \to 0$ to reassure that the approximation tends to the second derivative of the delta function.

2.3.2 Transmission

Obtaining the transmission for the regularizing potential $\Delta''_{\bar{u},r,d,\bar{a}}(x)$ is a tedious matter, as this potential has 9 different intervals. See figure 2.6 and eq. (2.24). For each interval, the general solution must be found and connected to its nearest solutions. The general boundary conditions in (2.6) state that the general solutions and their first derivatives will always be continuous, because the regularizing potential is never infinite. This simplifies the extensive calculations considerably.

Procedure

As a start, the regularizing potential function $\Delta''_{\bar{u},r,d,\bar{a}}(x)$ must be substituted for $U(x)$ in eq. (1.6). Here a dimension conflict arises. In subsection 1.2.3 the dimension of $U(x)$ is shown to be $[\text{length}]^{-2}$, but the approximation is of dimension $[\text{length}]^{-3}$! This conflict is solved by introducing a real scaling variable $\sigma > 0$. The Schrödinger equation becomes

$$-\psi''(x) + \sigma^2 \Delta''_{\bar{u},r,d,\bar{a}}(x)\psi(x) = k^2\psi(x), \tag{2.26}$$

where the square in σ^2 is used to simplify calculations. The dimensions agree if σ is of dimension $[\text{length}]^{\frac{1}{2}}$.

The general solutions for $\Delta''_{\bar{u},r,d,\bar{a}}(x)$ in the different intervals can be found with the help of eq. (A.1) and eq. (A.2). They have the following form

$$\begin{aligned}
\psi_r(x) &= A_r \exp(ikx) + B_r \exp(-ikx) \text{ with } r = (1,3,5,7,9),\\
\psi_s(x) &= A_s \exp(-\frac{\eta x}{2\bar{a}}) + B_s \exp(\frac{\eta x}{2\bar{a}}) \text{ with } s = (2,8),\\
\psi_t(x) &= A_t \exp(\frac{i\vartheta x}{2\bar{a}}) + B_t \exp(-\frac{i\vartheta x}{2\bar{a}}) \text{ with } t = (4,6),
\end{aligned}$$

where the indices r, s, t refer to the intervals defined in eq. (2.24) and A_j and B_j with $j = (1, 2, \ldots, 9)$ are the corresponding amplitude coefficients. All the coefficients are functions of k, but this is not denoted for the sake of simplicity. The dimensionless coefficients have the form $\eta = 2\bar{a}\sqrt{\sigma^2\bar{u} - k^2}$ and $\vartheta = 2\bar{a}\sqrt{\sigma^2\bar{u} + k^2}$.

The general solutions of the neighboring intervals can be coupled by using the general boundary conditions in (2.6), resulting in the following sets

$$\mathcal{A}_i = \begin{cases} \psi_i(x_i) &= \psi_{i+1}(x_i),\\ \psi'_i(x_i) &= \psi'_{i+1}(x_i), \end{cases}$$

where $i = (1, 2, \ldots, 8)$ and the x_i's are the intersection points for all neighboring intervals, being $x_1 = -r - d - \bar{a}$, $x_2 = -r - d + \bar{a}$, $x_3 = -r + d - \bar{a}$, $x_4 = -r + d + \bar{a}$, $x_5 = r - d - \bar{a}$, $x_6 = r - d + \bar{a}$, $x_7 = r + d - \bar{a}$ and $x_8 = r + d + \bar{a}$.

From the $\mathcal{A}_i$'s an equation for A_i and B_i can be obtained, in which each coefficient is expressed as a function of A_{i+1} and B_{i+1}. This gives a new set of equations

$$\mathcal{B}_i = \begin{cases} A_i &= \text{function}(A_{i+1}, B_{i+i}), \\ B_i &= \text{function}(A_{i+1}, B_{i+i}). \end{cases}$$

Because we are interested in the transmission, an incident wave from the left only is applied. As B_9 represents an incoming wave from the right; $B_9 = 0$. Looking at the set $\mathcal{B}_8$ it is easily seen, that A_8 and B_8 are functions of A_9 only. By substituting $\mathcal{B}_8$ into $\mathcal{B}_7$ and so forth recursively, A_1 and B_1 can be expressed as functions of A_9! The transmission for the approximation $\Delta''_{\bar{u},r,d,\bar{a}}(x)$ is now defined as

$$\frac{|A_9|^2}{|A_1|^2} = |T_{\Delta''}|^2, \tag{2.27}$$

where $T_{\Delta''} = A_9/A_1$ is the transmission coefficient for the total potential.

Doing these calculations is a very tedious job and mistakes are easily made, so we turn to a symbolic computer program called Maple7. The Maple Work Sheets are found in appendix C.

Algebraic Expression

With the help of the Maple Work Sheet `Transmission.mws`, listed in appendix C.1, an enormous expression with 684 terms is found for $T^{-1}_{\Delta''}$. This fraction equation can be reduced to 54 terms, by collecting the terms containing the same exponents. An investigation of these different exponents learns that e^{η}, $e^{i\vartheta}$, e^{ikr}, e^{ikd} and $e^{ik\bar{a}}$ appear as products with various orders, for example $e^{i(4k(r+d-\bar{a})+2\vartheta)}$ and $e^{i(8kd-2\vartheta)-2\eta}$. Most of the order ranges are shifted, to be more precise: by multiplying the fraction $T^{-1}_{\Delta''}$ with $e^{-2ik(r+d+\bar{a})}$ all order ranges are centered around zero.

The fraction equation can be further simplified with the aid of two definitions found in [AS66] 4.5, which help to write two specific combinations of exponential functions as hyperbolic functions, in detail

$$\begin{aligned} e^{x} + e^{-x} &= 2\cosh(x), \\ e^{x} - e^{-x} &= 2\sinh(x). \end{aligned}$$

The following conversions to trigonometric functions, as stated in [AS66] 4.3, are also frequently applied

$$\begin{aligned} \cosh(ix) &= \cos(ix), \\ \sinh(ix) &= i\sin(x). \end{aligned}$$

These simplifications concern only exponentials with multiples of η and $i\vartheta$ in the argument.

The fraction equation $T_{\Delta''}^{-1}$ is now reduced to only 10 terms before the following Maple Work Sheet `Transmission trigonometric.mws` takes over. This sheet is listed in appendix C.2 and starts with gathering the terms with the same exponential arguments. Now only 6 terms are left and the expression is of the form

$$\begin{aligned} T_{\Delta''}^{-1} &= e^{i2k(r+d+\bar{a})}/256 \\ &\quad \times\{Ae^{ik(2r+2d-6\bar{a})} + Be^{ik(2r-6d+2\bar{a})} + C1e^{ik(2r-2d-2\bar{a})} \\ &\quad +C2e^{ik(-2r+2d+2\bar{a})} + Ee^{ik(-2r-2d+6\bar{a})} + Fe^{ik(-2r+6d-2\bar{a})}\}. \end{aligned}$$

With the help of eq. (B.6) this can be rewritten as

$$\begin{aligned} T_{\Delta''}^{-1} &= e^{i2k(r+d+\bar{a})}/256 \\ &\quad \times\{[K\cos(4k(d-\bar{a})) + L\sin(4k(d-\bar{a})) + M]\cos(2k(r-d-\bar{a})) \\ &\quad +[N\cos(4k(d-\bar{a})) + O\sin(4k(d-\bar{a})) + P]\sin(2k(r-d-\bar{a}))\}, \end{aligned} \tag{2.28}$$

with the coefficient K shown in eq. (B.7) in the appendix. The coefficients L, M, N, O and P are of the same form, but may have two more or less terms. The orders of the coefficients are always within the range of powers between $(k\bar{a})^{-4}$ and $(k\bar{a})^{4}$.

2.3.3 Results

We are interested in the transition where the approximating function tends to $\delta''(x)$. The regularizing parameters r and d are each set equal to $\bar{a}$ multiplied with a real constant and then the limit $\bar{a} \to 0$ is applied. This is done in `Transmission investigated.mws` found in appendix C.3.

Inspection of eq. (2.28) learns that $d = \bar{a}$ and $r = 2\bar{a}$ is an obvious choice (it can easily be verified, that in this case the limit in eq. (2.25) still holds). Noticing that for these values $u = \frac{1}{16\bar{a}^3}$ and

$$\left.\begin{array}{l} \eta = 2\bar{a}\sqrt{\sigma^2 u - k^2} \to \frac{\sigma}{2\sqrt{\bar{a}}} = \frac{\tau}{2} \\ \theta = 2a\sqrt{\sigma^2 u - k^2} \to \frac{\sigma}{2\sqrt{\bar{a}}} = \frac{\tau}{2} \end{array}\right. \text{ if } \bar{a} \to 0.$$

Inserting these values in eq. (2.28) yields

$$\begin{aligned} T_{\Delta''}^{-1} &= K + M \\ &\to \cosh(\tau)\cos(\tau) - \frac{2i\sin(\tau)\,k\sigma^2}{\tau^3} - \frac{i\sin(\tau)\,\tau^3}{8k\sigma^2} \\ &\quad + \frac{i\sinh(\tau)\cos(\tau)\,\tau^3}{8k\sigma^2} - \frac{2i\sinh(\tau)\cos(\tau)\,k\sigma^2}{\tau^3}. \end{aligned}$$

Finally applying $\tau = \frac{\sigma}{\sqrt{\bar{a}}} \to \infty$ if $a \to 0$, the fraction equation results in

$$T_{\Delta''}^{-1} \to \frac{e^\tau}{2}\cos(\tau) - \frac{i\sin(\tau)\tau^3}{8k\sigma^2} + \frac{ie^\tau\cos(\tau)\tau^3}{16k\sigma^2} - \frac{ie^\tau\cos(\tau)\,k\sigma^2}{\tau^3}.$$

$T_{\Delta''}^{-1}$ becomes a heavily oscillating function with growing amplitude, when $\bar{a}$ is sufficiently small. In the limit of $\bar{a} \to 0$, $T_{\Delta''}$ is not well–defined and this can only mean that the transmission $|T|^2$ and thus the transmission for the $\delta''(x)$ potential does not exist.

This result in a slightly different form is published in [CAZ$^+$03].

Chapter 3

Nonlinear Potentials

In this chapter the transmissions for Dirac's delta function and the regularizing approximation for its first derivative are calculated. Now a nonlinear term is added to the potential.

3.1 Nonlinear Delta Function

To illustrate the effect of a nonlinear term, first a simple nonlinear potential barrier is demonstrated in this section. The barrier has the physical shape of the Dirac's delta function, which is discussed in section 2.1.

3.1.1 Transmission

The total potential is written as $U(x) = \{\alpha + \nu|\psi(x)|^2\}\delta(x)$, where α is the same scaling parameter as appearing with the linear delta barrier in section 2.1. Insertion in the Schrödinger equation, eq. (1.6), gives

$$-\psi''(x) + \{\alpha + \nu|\psi(x)|^2\}\delta(x)\psi(x) = k^2\psi(x). \qquad (3.1)$$

The new term is $\nu|\psi(x)|^2$, where ν is a constant coefficient. $|\psi(x)|^2$ is the intensity of the wavefunction and with the help of eq. (1.3) its dimension can be determined to be $[\text{length}]^{-1}$. Because the dimensions of α and $\nu|\psi(x)|^2$ must agree and the dimension of α is $[\text{length}]^{-1}$, ν must be a dimensionless constant.

The x-axis is divided into interval 1 and 2 as in section 2.1: interval 1 corresponds to $x < 0$ and interval 2 to $x > 0$. Because the potential $\{\alpha + \nu|\psi(x)|^2\}\delta(x)$ is zero in both intervals and we assume an incoming wave from the left only, the general solutions in the intervals have exactly the same form as eq. (2.4) and eq. (2.5), yielding

$$\psi_1(x) = I(k)e^{ikx} + R(k)e^{-ikx} \tag{3.2}$$
$$\psi_2(x) = T(k)e^{ikx}, \tag{3.3}$$

where $I(k)$, $R(k)$ and $T(k)$ are the amplitude coefficients of the incoming, reflected and transmitted wave respectively. The coefficients are functions of k. Recall that k is a measure for the energy of the particle, which is in this case positive. This is because the tunnelling effect is considered, where $E = k^2$ is always positive, see section 1.1.

Now the two general solutions are connected together. The first general boundary condition in (2.6) states that the amplitude function $\psi(x)$ is always continuous. The general solutions must be equal in the origin and eq. (2.7) is adopted, hence

$$\begin{aligned} &\psi_1(0) = \psi_2(0) \\ &\quad\Rightarrow\quad I(k) + R(k) = T(k). \end{aligned} \tag{3.4}$$

Because the nonlinear potential is infinite in the origin, the first derivatives of the general solutions at $x = 0$ are not equal. See the second general boundary condition. The discontinuity of $\psi'(x)$ can now be computed by integrating eq. (3.1) from ϵ and $-\epsilon$ and letting $\epsilon \to 0$. The calculation reduces to an equivalent of eq. (2.9)

$$\lim_{\epsilon\to 0}\left(\frac{d\psi}{dx}\Big|_{x=-\epsilon}^{\epsilon}\right) = \lim_{\epsilon\to 0}\int_{-\epsilon}^{+\epsilon}\{\alpha + \nu|\psi(x)|^2\}\delta(x)\psi(x)dx.$$

The integral on the right can be determined with the sifting property in eq. (2.2) and is found to be equal to $\{\alpha + \nu|\psi(0)|^2\}\psi(0)$. Because $\psi(x)$ is always continuous, we can choose $\psi(0) = \psi_2(0)$ and the integral equation changes to

$$\frac{d}{dx}\psi_2(x)\bigg|_{x=0} - \frac{d}{dx}\psi_1(x)\bigg|_{x=0} = \{\alpha + \nu|\psi(0)|^2\}\psi(0).$$

What remains is the insertion of the general solutions eq. (3.2) and eq. (3.3), and thereafter an equation for the transmission can be found. Insertion gives

$$ikT(k) - \{ikI(k) - ikR(k)\} = \{\alpha + \nu|T(k)|^2\}T(k).$$

Together with eq. (3.4) an equation in which the intensity of the incident wave is expressed as a function of the intensity of the transmitted wave, can be stated

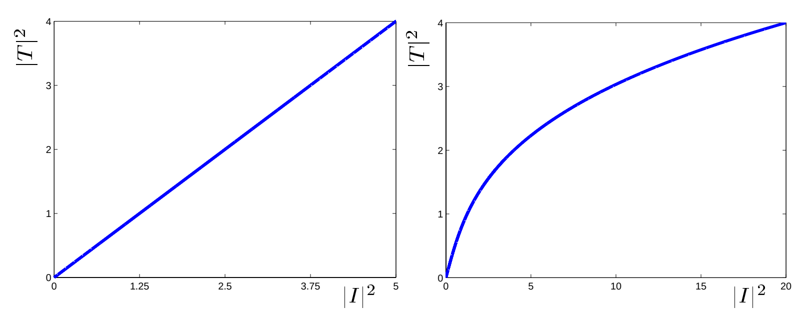
$$|I(k)|^2 = (1 + \frac{\{\alpha + \nu|T(k)|^2\}^2}{4k^2})|T(k)|^2. \tag{3.5}$$

3.1.2 Results

An important check is to see whether the transmission for $\{\alpha + \nu|\psi|^2\}\delta(x)$ tends to the transmission equation for the linear equivalent if the nonlinearity vanishes. This is obviously the case, as

$$|I(k)|^2 \to \frac{4k^2 + \alpha^2}{4k^2}|T(k)|^2 \text{ if } \nu \to 0,$$

is equal to eq. (2.10). The linear behaviour is also clearly seen in figure 3.1(a), where the nonlinear parameter ν is equal to zero and the figure becomes a straight line. In figure 3.2(b) $\alpha = 0$ and $\nu \neq 0$; so the line curves. Now the superposition principle obviously does not hold as a combination of two solutions is not necessarily a new solution.



(a) $\alpha = 1$, $\nu = 0$ and $k = 1$. (b) $\alpha = 0$, $\nu = 1$ and $k = 1$.

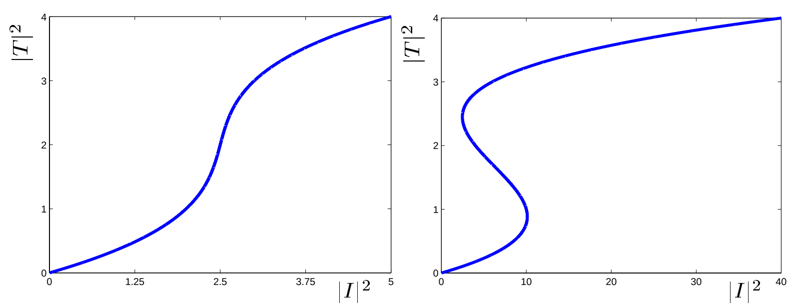
Figure 3.1: *Effect of linearity and nonlinearity of the delta prime potential.*

For greater insight in the possible combinations of α and ν, the left hand side of eq. (3.5) is considered as a function $f(z)$ with $z = |T|^2 > 0$. The function and its first derivative with respect to z look like

$$\begin{cases} f(z) = (1 + \frac{\{\alpha+\nu z\}^2}{4k^2})z, \\ f'(z) = 1 + \frac{\alpha^2+4\alpha\nu z+3\nu^2 z^2}{4k^2}, \end{cases}$$

where the prime denotes differentiation with respect to z.

The first derivative determines the curvature of the function; where it is equal to zero a stationary point exists. Because $f(z)$ is a third order polynomial, it can have at most two of these stationary points, one being a local maximum and the other a local minimum. If they coexist, some function values occur for a triplet of different z-values. In order for the triplets to contain only positive real values of z (only these are of interest as they represents a wave intensity), α and ν must have different signs and $\alpha > \sqrt{12}k$. This can be seen in figure 3.2(a), where α is too small for triplets of $|T|^2$ to occur.



(a) $\alpha = 3$, $\nu = -1$ and $k = 1$.

(b) $\alpha = 10$, $\nu = -4$ and $k = 1$.

Figure 3.2: *Effect of the magnitude of α with opposite signs of α and ν in the nonlinear delta potential.*

The phenomenon hysteresis van be seen if If $\alpha > \sqrt{12}k$. This phenomenon is depicted in figure 3.2(b), where the line is curved in an s-form with a lower, middle and upper branch. When a solution on the lower branch is perturbed in the positive $|I|^2$-direction, it suddenly jumps upwards without reaching the middle branch. The middle branch is also avoided when a solution on the upper branch is perturbed in the other direction. This is a typical band structure, where the allowed positive intensities are interrupted by gaps [Gri95] page 205.

This example demonstrates the complex behaviour of nonlinearity.

3.2 Nonlinear Delta Prime Regularization

In section 2.2 a rectangular approximation of $\delta'(x)$ was investigated. Here a nonlinear term $v|\psi(x)|^2$ is added to the regularizing potential $\Delta'_{u,a}(x)$, as follows

$$\widetilde{\Delta}'_{u,v,a}(x) = \begin{cases} 0, & \text{if } -\infty < x < -a, \\ u + v|\psi(x)|^2, & \text{if } -a < x < 0, \\ -u - v|\psi(x)|^2, & \text{if } 0 < x < a, \\ 0, & \text{if } a < x < \infty. \end{cases} \tag{3.6}$$

where u is the same scaling parameter with dimension $[\text{length}]^{-2}$ as presented with the linear approximation and v is a new nonlinear coefficient. Dimension analysis shows that the dimension of v is $[\text{length}]^{-1}$.

The potential in interval $-a < x < 0$ is a barrier, because $u, v, |\psi(x)|^2$ are all positive and thus the potential itself is always positive. With the same reasoning it can be concluded, that potential in $0 < x < a$ is always negative and it is a well.

3.2.1 Transmission

Introducing the nonlinear potential $\widetilde{\Delta}'_{u,v,a}(x)$ in eq. (1.6) gives the proper Schrödinger equation. Solving this equation for the four different values of $\widetilde{\Delta}'_{u,v,a}(x)$ provides four different general solutions, which after being coupled, result in an equation for the transmission. The Schrödinger equation reads

$$-\psi''(x) + \widetilde{\Delta}'_{u,v,a}(x)\psi(x) = k^2\psi(x). \tag{3.7}$$

General Solutions

We assume again an incident wave from the left only. Therefore, the same general solutions as for the linear case are obtained in the regions where the nonlinear potential is zero, i.d. $x < -a$ and $x > a$. See eq. (2.13) and eq. (2.14). In the regions where the potential is nonzero, the Schrödinger equation eq. (3.7) is nonlinear. There a solution is applied, which describe scattering states, as the scattering determines the transmission. The amplitude function can be expressed as

$$\psi(x) = \begin{cases} I(k)e^{ikx} + R(k)e^{-ikx}, & \text{if} \quad -\infty < x < -a, \\ A_b(x)e^{i\theta_b(x)}, & \text{if} \quad -a < x < 0, \\ A_w(x)e^{i\theta_w(x)}, & \text{if} \quad 0 < x < a, \\ T(k)e^{ikx}, & \text{if} \quad a < x < \infty, \end{cases} \tag{3.8}$$

where $I(k)$, $R(k)$ and $T(k)$ are the amplitude coefficients of the incident, reflected and transmitted wave. $A_b(x)$ and $\theta_b(x)$ are the real amplitude and real phase of the wave in the barrier and $A_w(x)$ and $\theta_w(x)$ the real amplitude and real phase of the wave in the well. All of these are functions of k or x, but in the following calculations this dependence is not always denoted. The function values in specific points will always be explicitly stated.

The general solution for the amplitude function in the barrier can be specified by substitution in eq. (3.7). The resulting equation is then split into a real and an imaginary part, respectively

$$-A_b'' + A_b(\theta_b')^2 + (u + vA_b^2)A_b = k^2 A_b, \tag{3.9}$$

and

$$2A_b'\theta_b' + A_b\theta_b'' = 0.$$

The latter equation, which belongs to the imaginary part, can be rewritten as an ordinary differential equation and hereafter solved by integration. The integration constant L_b is introduced and the solution is

$$\frac{1}{A_b}\frac{d}{dx}(A_b^2\theta_b') = 0 \Rightarrow \theta_b' = \frac{L_b}{A_b^2}. \tag{3.10}$$

Inserting this integration solution in eq. (3.9) and multiplying with dA_b, gives a new equation. When this equation is rearranged and integrated, another integration constant E_b is developed. At this point, a new notation for the intensity of the wave $N_b = A_b^2$ is introduced and substituted, which finally results in a differential equation for the intensity of the wave in the barrier. The calculations are done in appendix D and yield eq. (D.1),

$$\frac{1}{2}N_b' = \sqrt{2E_bN_b - L_b^2 + (u - k^2)N_b^2 + \frac{v}{2}N_b^3}, \tag{3.11}$$

with

$$N_b = A_b^2. \tag{3.12}$$

Similarly, a differential equation for the intensity of the wave in the well can be obtained. Now L_w and E_w are created and $N_w = A_w^2$ is the intensity of the wave in the well. The corresponding set of equations for the well looks like

$$\theta_w' = \frac{L_w}{A_w^2}, \tag{3.13}$$

$$\frac{1}{2}N_w' = \sqrt{2E_wN_w - L_w^2 - (u+k^2)N_w^2 - \frac{v}{2}N_w^3}, \tag{3.14}$$

$$N_w = A_w^2. \tag{3.15}$$

Wave Intensity in Well

Now that the general solutions for the scattering states have been specified, all the general solutions are connected at the intersection points $x = -a, 0, a$. Because the potential $\widetilde{\Delta}'_{u,v,a}$ is never infinite, both the function value and its first derivative of the amplitude function are always continuous. See the general boundary conditions in eq. (2.6). This gives for the continuity of the amplitude function and its first derivative at $x = a$ respectively

$$A_w(a)e^{i\theta_w(a)} = Te^{ika}, \tag{3.16}$$

$$\{A_w'(a) + i\theta_w'(a)A_w(a)\}e^{i\theta_w(a)} = ikTe^{ika}. \tag{3.17}$$

A value for $A_w(a)$ is found by applying the modulus to eq. (3.16),

$$|A_w(a)e^{i\theta_w(a)}| = |Te^{ika}| \Rightarrow A_w(a) = |T|. \tag{3.18}$$

Additionally, if eq. (3.16) is substituted in eq. (3.17) and the result is divided with $A_w(a)$, a real and a imaginary equation are obtained. Noticing that $N_w = A_w^2$ in eq. (3.15), the real equation determines $N_w'(a)$. The value for L_w is found by evaluating the imaginary equation and substituting eq. (3.13) and eq (3.18), yielding

$$\text{Re:} \qquad A_w'(a) = 0 \Rightarrow N_w'(a) = 0, \tag{3.19}$$

$$\text{Im:} \qquad \theta_w'(a) = k \Rightarrow L_w = k|T|^2. \tag{3.20}$$

The constant E_w is now obtained by evaluation of eq. (3.14) at $x = a$ and insertion of eq. (3.18), eq. (3.19) and eq. (3.20). This yields

$$0 = \sqrt{2E_w N_w(a) - L_w^2 - (u+k^2)N_w^2(a) - \frac{v}{2}N_w^3(a)}$$
$$\Rightarrow \quad E_w = k^2|T|^2 + \frac{u}{2}|T|^2 + \frac{v}{4}|T|^4. \tag{3.21}$$

Substitution in eq. (3.14) and reformulation gives

$$\frac{dN_w}{\sqrt{(|T|^2 - N_w)(N_w - N_+)(N_w - N_-)}} = \sqrt{2v}dx, \tag{3.22}$$

with

$$N_\pm = \Big\{ -(u + k^2 + \frac{v}{2}|T|^2) \pm \sqrt{(u + k^2 + \frac{v}{2}|T|^2)^2 + 2vk^2|T|^2} \Big\}/v. \tag{3.23}$$

From the form of eq. (3.22), it can be seen that $|T|^2 > N_w$, $N_w > N_+$ and $N_w > N_-$. Because all the terms appearing in N_+ and N_- in eq. (3.23) are positive, $N_+ > N_-$. Hence, $|T|^2 > N_w > N_+ > N_-$. Now eq. (3.22) is integrated with the help of [BF71] 236.00 and the intensity of the wave in the well is expressed as a function of $|T|$

$$N_w(x) = |T|^2 - (|T|^2 - N_+)\mathrm{sn}^2(\bar{\kappa}(x-a)|\mu), \tag{3.24}$$

where sn is the so–called "sine amplitudine" function of the Jacobian elliptic functions with the modulus μ. $\bar{\kappa}$ is an abbreviation. Specifically,

$$\mu = \frac{|T|^2 - N_+}{|T|^2 - N_-}, \tag{3.25}$$

$$\bar{\kappa} = \sqrt{\frac{v}{2}(|T|^2 - N_-)}. \tag{3.26}$$

Wave Intensity in Barrier

The wave functions for the well and the barrier and their first derivatives must be equal at $x = 0$, because the potential is never infinite. Splitting both resulting equations in a real and an imaginary part and rewriting the whole set of equations gives us four specific boundary conditions

$$\begin{aligned}A_b(0) &= A_w(0),\\ A_b'(0) &= A_w'(0),\\ \theta_b(0) &= \theta_w(0),\\ \theta_b'(0) &= \theta_w'(0).\end{aligned} \tag{3.27}$$

The first condition in eqs. (3.27) states that the amplitudes of the waves in the barrier and the well are equal in that point. This must also hold for their intensities, which substitution with the expressions of eq. (3.12) and eq. (3.15) confirms. By finally specifying the value of $N_w(0)$ with eq. (3.24) and introducing an abbreviation N_0, the following expression is obtained

$$N_b(0) = N_w(0) = N_0 = |T|^2 - (|T|^2 - N_+)\mathrm{sn}^2(\bar{\kappa}a|\mu). \tag{3.28}$$

The integration constant E_b in eq. (3.11) is found easily. The first derivatives of the amplitudes of the waves in the well and the barrier are equal and so are the first derivatives of the intensities. This is seen by substituting eq. (3.12) and eq. (3.15) in the second equation of eqs. (3.27). Now the expressions for these intensities eq. (3.11) and eq. (3.14), are introduced and evaluated at $x = 0$. The expressions become

$$\begin{aligned}N_b'(0) &= 2E_bN_0 - L_b^2 + (u - k^2)N_0^2 + \frac{v}{2}N_0^3\\ N_w'(0) &= 2E_wN_0 - L_w^2 - (u + k^2)N_0^2 - \frac{v}{2}N_0^3\\ N_b'(0) = N_w'(0) &\Rightarrow E_b = E_w - uN_0 - \frac{v}{2}N_0.\end{aligned} \tag{3.29}$$

According to the conditions in eqs. (3.27) the amplitudes and the phases of the waves in the barrier and the well must be equal at $x = 0$. Hence eq. (3.10) and eq. (3.13), which express the phases by their corresponding constants respectively L_b and L_w, are also equal. Dividing with the equal amplitudes at $x = 0$, the constant L_b must be equal to the constant L_w. In eq. (3.20) the constant L_w is specified. This gives

$$\theta_b'(0) = \theta_w'(0) \Rightarrow \frac{L_b}{A_b(0)^2} = \frac{L_w}{A_w(0)^2} \Rightarrow L_b = L_w = k|T|^2. \tag{3.30}$$

Inserting eq. (3.30) in the differential equation for $N_b(x)$, eq. (3.11), and reformulating yields

$$\frac{dN_b}{\sqrt{\frac{4}{v}E_bN_b - \frac{2}{v}k^2|T|^4 + \frac{2}{v}(u - k^2)N_b^2 + N_b^3}} = \sqrt{2v}dx. \tag{3.31}$$

In order to solve this integral with Jacobian elliptic functions, the cubic polynomial in the denominator must be written as a polynomial with three factors: $(N_b - N_1)(N_b - N_2)(N_b - N_3)$. Doing this, three very lengthy expressions for the roots emerge. The limits of these roots for vanishing nonlinearity are (see section D.2)

$$N_{1,2} = \Big\{ -E_b \pm \sqrt{E_b^2 + (u-k^2)k^2|T|^4} \Big\} / (u - k^2), \tag{3.32}$$

$$N_3 = -\frac{2(u-k^2)}{v}. \tag{3.33}$$

The terms in the square roots in N_1 and N_2 are all positive. Hence the square root is also positive and $N_1 > N_2$. For vanishing nonlinearity N_3 has the largest negative value and $N_1 > N_2 > N_3$ is valid. The polynomial with the factors is only positive, when N_b is greater than all three roots.

Eq. (3.31) is now integrated with the help of [BF71] 237.00. We assume that the intensity of the wave in the barrier N_b is bounded and never grows to infinity. As an upper bound for the integral, we choose $N_b(0) = N_0$. So for the result to be valid $N_0 > N_b > N_1 > N_2 > N_3$ must hold. The intensity of the wave in the barrier becomes

$$N_b(x) = N_2 + (N_1 - N_2)/\mathrm{cn}^2(\bar{q}x + \chi|m), \tag{3.34}$$

where cn is the "cosine amplitudine" function of the Jacobian elliptic functions, with the modulus m. $\bar{q}$ is an abbreviation and the phase χ is determined by evaluating eq. (3.34) at $x = 0$, where it must be equal N_0. This gives

$$m = \frac{N_2 - N_3}{N_1 - N_3}, \tag{3.35}$$

$$\bar{q} = \sqrt{\frac{v}{2}(N_1 - N_3)}, \tag{3.36}$$

$$\mathrm{sn}(\chi|m) = \sqrt{\frac{N_0 - N_1}{N_0 - N_2}}. \tag{3.37}$$

Wave Intensity of Incoming Wave

Because the problem is solved backwards by expressing the wave intensity in the well as a function of the intensity of the transmitted wave and so forth recursively, finally the intensity of the incident wave is found as an function of the transmitted wave (and some other parameters). The calculations are completed by coupling the general solutions in eq. (3.8) at $x = a$. The boundary conditions become

$$\begin{aligned} Ie^{-ika} + Re^{ika} &= A_b(-a)e^{i\theta_b(-a)}, \\ ikIe^{-ika} - ikRe^{ika} &= \{A_b'(-a) + i\theta_b'(-a)A_b(-a)\}e^{i\theta_b(-a)}. \end{aligned}$$

If the first equation is multiplied with ik and added to the second, the amplitude coefficient of the reflected wave disappears. Because we are interested in the wave propagation of the system, only the amplitude of the incoming wave will be used. Expressing this amplitude in terms of its intensity by substituting eq. (3.12) and rewriting the first derivative of the phase with eq. (3.10) and eq. (3.30), the following equation is obtained

$$i4kI\sqrt{N_b(-a)}e^{-ika} = [N_b'(-a) + i2k\{N_b(-a) + |T|^2\}]e^{\theta_b(-a)}. \tag{3.38}$$

Multiplying with its complex conjugate, inserting the specific values for the intensity of the wave in the barrier and its first derivative at $x = -a$ (this is done with the help of eq. (3.34)) and rearranging results in an equation in which the intensity of the incoming wave $|I|^2$ is expressed as a function of the intensity of the transmitted wave $|T|^2$, i.d.

$$\begin{aligned} &4k^2|I|^2\{N_1 - N_2\mathrm{sn}^2(\bar{q}a - \chi|m)\}\mathrm{cn}^2(\bar{q}a - \chi|m) \\ &= \bar{q}^2(N_1 - N_2)^2\mathrm{sn}^2(\bar{q}a - \chi|m)\mathrm{cn}^{-2}(\bar{q}a - \chi|m)dn^2(\bar{q}a - \chi|m) \\ &\quad +k^2\{N_1 - N_2 + (N_2 + |T|^2)\mathrm{cn}^2(\bar{q}a - \chi|m)\}^2. \end{aligned} \tag{3.39}$$

These calculations were done parallel with [Gai02].

3.2.2 Comparison with Linear Case

The nonlinear delta prime potential can be interpreted as a perturbation of the linear potential presented in section 2.2. Thus, by creating the power series expansion for small v of the nonlinear equations obtained in the previous section and letting $v \to 0$ the linear results should be obtained.

In section 2.2 the wave intensities in the barrier and the well for the linear equivalent are obtained. The intensity in the nonlinear well $N_w(x)$ is determined with eq. (3.24). The modulus μ tends to zero for vanishing nonlinearity. But when the modulus of a "sine amplitudine" function is zero, the function can be replaced with an ordinary trigonometric sinus function according to [BF71] 122.08. $\bar{\kappa}$ approaches the κ in the linear case and using the limit for N_+ it is found that

$$\begin{aligned} N_w(x) &\rightarrow |T|^2 - (|T|^2 - \frac{k^2|T|^2}{\kappa^2}) sin^2(\kappa(x-a)) \\ &\rightarrow \frac{|T|^2}{2\kappa^2}\{u + 2k^2 + u\cos\Big(2\kappa(x-a)\Big)\}. \end{aligned}$$

This result is exactly the same as for the linear case, see eq. (2.18), and at $x = 0$ it is also equal to eq. (D.7). Thus, so far so good.

Now, the wave intensities in the barrier are compared for the linear and nonlinear case. First eq. (3.34) is rewritten with the help of the addition formula for the "cosine amplitudine" function in [BF71] 123.01. Furthermore it is noticed that the corresponding modulus m approaches one; in that case the elliptic functions change into hyperbolic functions as stated in [BF71] 122.09. Using eq. (3.37), applying $\bar{q} \rightarrow q$ if $v \rightarrow 0$ and collecting the different terms with the same hyperbolic functions, gives (see eq. (D.12))

$$\begin{aligned} N_b(x) &= \frac{2N_0 - N_1 - N_2}{2}\cosh(2qx) \\ &\quad + \sqrt{(N_0 - N_1)(N_0 - N_2)}\sinh(qx) + \frac{N_1 + N_2}{2}. \end{aligned}$$

Inserting the limiting values for N_0, N_1 and N_2 found in appendix D.3 and a lot of rearranging with trigonometric functions results in

$$\begin{aligned} N_b(x) &= \frac{|T|^2}{2\kappa^2 q^2}\Big\{[u(u+2k^2) - uk^2\cos(2\kappa a)]\cosh(2qx) \\ &\quad + u\kappa q\sqrt{\sin^2(2\kappa a)}\sinh(2qx) + u^2\cos(2\kappa a) - (u+2k^2)k^2\Big\}, \end{aligned} \tag{3.40}$$

but here a big problem arises. The square root does not appear in eq. (2.20) and the root of a square with a real argument will always be positive even though the argument is negative! This means that the two equations are not equivalent when $\sin(2\kappa a)$ is negative.

Unfortunately, no perturbed equivalent for χ in eq. (3.37) is found. A step in the right direction is set by observing that the modulus m is close to 1.

Then the “sine amplitudine” function in the left hand side of the equation can be transformed with [BF71] 127.02 to an expression containing χ, m and the hyperbolic functions. But the right hand side gets enormous when the perturbed equivalents for N_0, N_1 and N_2 are substituted. This means that eq. (3.39) is not perturbed and cannot be compared with the eq. (2.22).

Another check can be performed. Eq. (3.39) is created by evaluating the boundary conditions at $x = -a$. Instead of using the wave intensity for the nonlinear barrier as done in section 3.2.1, the linear equivalent eq. (2.20) is substituted in the boundary condition eq. (3.38) and it is checked whether the equality still holds. Doing this in a computer program called Mathematica4.2 shows that eq. (3.39) is valid.

Sign–Function

Further research on the inequality of the intensities in the nonlinear and linear barriers is done by returning to the perturbed equations in section D.3. The square root in front of the $\sinh(qx)$-term in eq. (3.40) originates from $\sqrt{(N_0 - N_1)(N_0 - N_2)}$ (see eq. (D.12)). In fact any other occurrence of this square root is squared. Therefore I expect that multiplying this root by $\mathrm{sign}[\sin(sin(2\kappa a))]$ will solve the inequality of the intensities in the nonlinear and linear barriers for vanishing nonlinearity.

The numerical results of eq. (3.39) and eq. (2.22) differ only when the sign–function is negative. This is clearly seen in figure 3.3, where the dashdotted line represents the sign–function: everywhere the sign–function is negative (under the straight line in the figure) the equations differ. Furthermore, it can be shown that after correction of eq. (3.37) with the sign–function the difference disappears when $\nu \to 0$!

With eq. (3.37) substituted by

$$\mathrm{sn}(\chi|m) = \mathrm{sign}[\sin(2a\kappa)]\sqrt{\frac{N_0 - N_1}{N_0 - N_2}}, \tag{3.41}$$

some numerical results were obtained with the help of Mathematica4.2, but a new problem surfaced. This is clearly seen in figure 3.4, where the solutions are an a curved line and a kink in the line exists. Removing the sign–function resulted in appearance of the same kinks, so another solution had to be found.

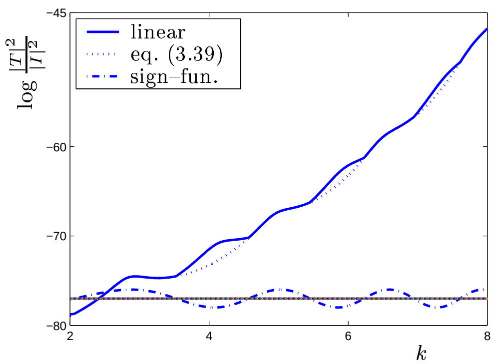


Figure 3.3: *Effect of the sign–function for the values* $a = 4$, $u = 2$ *and* $v = 10^{-20}$.

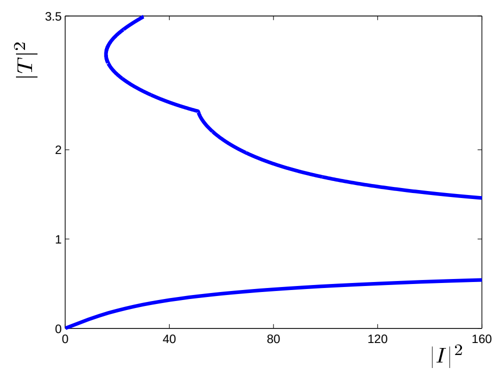


Figure 3.4: *Effect of the sign–function for the values* $a = 1$, $k = .1$, $u = 5.5$ *and* $v = 1$.

Reconsidering the introduced sign–function, a peculiarity was discovered. The right hand side of eq. (3.41) is a Jacobian elliptic function, while the left hand side contains an ordinary trigonometric function. This "unbalance" can be repaired with the introduction of a new argument in the sign–function. Addition to eq. (3.37) gives

$$\mathrm{sn}(\chi|m) = \mathrm{sign}[\mathrm{sn}(2a\bar{\kappa}|\mu)]\sqrt{\frac{N_0 - N_1}{N_0 - N_2}}. \tag{3.42}$$

Now the equation is in "balance" and furthermore it tends to eq. (3.41) if $\nu \to 0$; as $\bar{\kappa} \to \kappa$, $\mu \to 0$ and thus $\mathrm{sn}(2a\bar{\kappa}|\mu) \to \sin(2a\kappa)$. With this new argument the discontinuity disappears, as can be seen in figure 3.5.

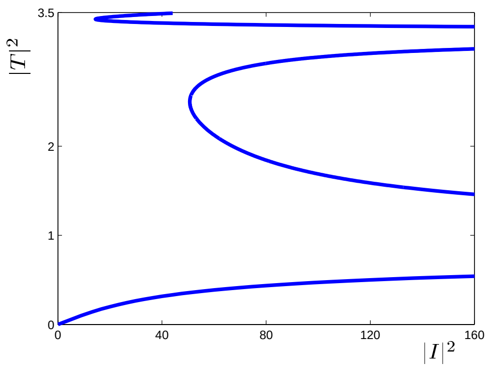


Figure 3.5: *Effect of the new sign–function for the values $a = 1$, $k = .1$, $u = 5.5$ and $v = 1$.*

3.2.3 Results

Pairs of solutions $(|I|^2, |T|^2)$ for eq. (3.39) with eq. 3.42 are found by substitution of $|T|^2$ and a set of parameters a, k, u and v; then the equation can be solved as it has only one unknown, $|I|^2$. So all transmission curves in figure 3.6 are found "backwards" and, if existing, are of the same fundamental form for different sets of parameters.

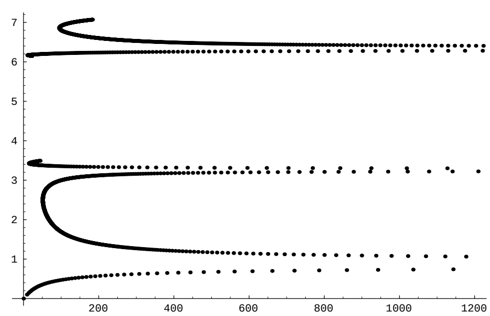


Figure 3.6: *Result for the nonlinear delta prime potential with $a = 1$, $k = .1$, $u = 5.5$ and $v = 1$. The vertical axis represents $|T|^2$ and the horizontal axis $|I|^2$.*

In general three types of curves exist. There is always the lowest curve, which starts in the origin. The second type curve seemingly arrives from infinity, curls up-/downwards and disappears again towards infinity. The third type exhibits the same behaviour but ends abruptly. This happens for the case, that $N_0 < N_1$; eq. (3.34) is not valid any more and the solution pairs becomes complex. The intervals in which this is the case two interpretations are possible: no physical solution exists or the assumption $N_0 > N_1$ is violated.

One approach is starting in the origin and "turning up" the intensity of the incident field. Now the solution moves along the lower line and the incident field of the transmitted wave stabilizes, if the solution is not suddenly "excited" to the second curve (which cannot be explained with the figure at hand).

Looking at the figure though, it must be remembered that for chosen output values of $|T|^2$ the corresponding value's of $|I|^2$ were found. In this sense it is possible to start on any curve and remain on that curve as there are no intersections. This phenomenon is called band–structure and might originate from resonances between the layers of the regularized nonlinear delta prime function, which lead to special trapped modes with only a very small percentage of the incident intensity being transmitted. This is typically the case for resonance in a cavity.

Chapter 4

Conclusion and Recommendation

Solution of a nonlinear differential equation is often very difficult, but not new in mathematical physics. The theoretical break–through and the practical use of differential calculus took place at the end of the seventeenth century, in competition between Isaac Newton in England and Gottfried Leibniz in Germany.

In this thesis the linear and Kerr–nonlinear Schrödinger equations were solved with the aim to find the transmission through Dirac's delta function and its derivatives. Only the scattering states were investigated, as they determine the transmission through a potential.

Dirac's delta function could fulfill the general boundary conditions; delta prime and the delta–double prime functions were regularized with rectangular approximations.

The tunnelling effect was demonstrated for the linear delta potential and it was seen that even low energy particles have a finite probability of passing the barrier. The superposition principle, which is valid for all linear differential equations in general, was emphasized.

The transmissions for the linear approximations of the delta prime and double–prime functions were calculated. The latter becomes a heavily oscillating function with growing amplitude in the zero–range limit, hence its transmission as an approximation for the delta double–prime function is not well–defined.

The behaviour of the linear and the nonlinear delta prime potential were compared and for vanishing nonlinearity the nonlinear potential was shown to tend to the linear potential. A phenomenon called hysteresis occurs for the nonlinear case; a band–structure arises.

Finally, the nonlinear delta prime potential was solved and perturbation analysis was implemented for the investigation of the limit of vanishing nonlinearity. In order for the limit to tend to the linear equivalence a sign–function was introduced and its effect was analyzed. The obtained transmission points to the existence of resonances and a band–structure; the assumption $N_0 > N_1$ and the bound states need further investigation.

The regularized one-dimensional versions of Dirac's delta function or its derivatives should also be investigated for physical use. The approximations, as discussed in this thesis, could be used for realistic modelling of the novel microscopic structures known as "nanotubes" or "nanowires" discussed in [Dek99]. These are cylindrical shaped, artificial molecules with a length of several microns, but a diameter of only one nanometer. Such tubes are for mathematical intents and are often considered one-dimensional.

Appendix A

General Solutions of the Linear Schrödinger Equation

In this appendix the general solutions of the time–independent Schrödinger equation as appearing in eq. (1.6) are obtained. First the equation is restated in a slightly different form

$$\psi''(x) = S\psi(x).$$

with $S = U(x) - k^2$.

This can be rewritten as the first derivative of a vector

$$\begin{pmatrix} \psi(x) \\ \psi'(x) \end{pmatrix}' = \begin{pmatrix} 0 & 1 \\ S & 0 \end{pmatrix} \begin{pmatrix} \psi(x) \\ \psi'(x) \end{pmatrix}.$$

Solving gives

$$\begin{vmatrix} \lambda & -1 \\ -S & \lambda \end{vmatrix} = \lambda^2 - S = 0 \Rightarrow \lambda^2 = S.$$

Now introduce $s > 0$. If $S = s^2 > 0$

$$\psi(x) = A(k)e^{-sx} + B(k)e^{sx} = C(k)\cosh(sx) + D(k)\sinh(sx), \qquad \text{(A.1)}$$

with $C(k) = A(k) + B(k)$ and $D(k) = -A(k) + B(k)$. The general solution is the solution for a bound state, since $S = U(x) - k^2 > 0 \Rightarrow U(x) > k^2 = E$.

A scattering state is found when $S = -s^2 < 0 \Rightarrow E > U(k)$ is considered

$$\psi(x) = E(k)e^{isx} + F(k)e^{-isx} = G(k)\cos(sx) + H(k)\sin(sx), \qquad \text{(A.2)}$$

with $G(k) = E(k) + F(k)$ and $H(k) = i(E(k) - F(k))$. Here the general solution represents a travelling wave, which is connected with scattering states.

Appendix B

Dirac's Delta Function and its derivatives

Here various lengthy calculations for chapter 2 are shown.

B.1 Dirac's Delta Function

$$\begin{aligned}
\int_{-\infty}^{\infty} xg(x)\delta'(x)dx &= \int_{-\infty}^{\infty} xg(x)d\Big(\delta(x)\Big) \\
&= xg(x)\delta(x)\Big|_{-\infty}^{\infty} - \int_{-\infty}^{\infty} \delta(x)d\Big(xg(x)\Big) \\
&= -\int_{-\infty}^{\infty} \delta(x)\Big[g(x) + xg'(x)\Big]dx \\
&= -\int_{-\infty}^{\infty} \delta(x)g(x)dx
\end{aligned}$$

$$\Rightarrow \delta'(x) = -\frac{\delta(x)}{x} \tag{B.1}$$

B.2 Delta Prime Function

$$\begin{aligned}
\int_{-\infty}^{\infty} f(x)\delta'(x)dx &= \int_{-\infty}^{\infty} f(x)d\Big(\delta(x)\Big) \\
&= \int_{-\infty}^{\infty} d\Big(f(x)\delta(x)\Big) - \int_{-\infty}^{\infty} \delta(x)d\Big(f(x)\Big) \\
&= f(x)\delta(x)\Big|_{-\infty}^{\infty} - \int_{-\infty}^{\infty} \delta(x)f'(x)dx \\
&= 0 - f'(0) = -f'(0)
\end{aligned} \tag{B.2}$$

$$\begin{aligned}
\int_{-\infty}^{\infty} f(x)\Delta'_{u,a}(x)dx &= -\int_{0}^{a} f(x)udx + \int_{-a}^{0} f(x)udx \\
&= -f(\frac{a}{2})ua + f(-\frac{a}{2})ua \\
&= -\Big[f(0) + f'(0)(\frac{a}{2}) + \frac{f''(0)}{2}(\frac{a}{2})^2 + O(a^3)\Big]ua \\
&\quad +\Big[f(0) + f'(0)(-\frac{a}{2}) + \frac{f''(0)}{2}(-\frac{a}{2})^2 + O(a^3)\Big]ua \\
&= \Big[-f'(0)a + O(a^3)\Big]ua \\
&= -ua^2 f'(0) + O(a^4) \qquad \text{(B.3)}
\end{aligned}$$

B.3 Delta Double–Prime Function

$$\begin{aligned}
\int_{-\infty}^{\infty} f(x)\delta''(x)dx &= \int_{-\infty}^{\infty} f(x)d\Big(\delta'(x)\Big) \\
&= \int_{-\infty}^{\infty} d\Big(f(x)\delta'(x)\Big) - \int_{-\infty}^{\infty} \delta'(x)d\Big(f(x)\Big) \\
&= f(x)\delta'(x)\Big|_{-\infty}^{\infty} - \int_{-\infty}^{\infty} \delta'(x)f'(x)dx \\
&= -f(x)\frac{\delta(x)}{x}\Big|_{-\infty}^{\infty} - \int_{-\infty}^{\infty} f'(x)d\Big(\delta(x)\Big) \\
&= 0 - \Big[\int_{-\infty}^{\infty} d\Big(f'(x)\delta(x)\Big) - \int_{-\infty}^{\infty} \delta(x)d\Big(f'(x)\Big)\Big] \\
&= -f'(x)\delta(x)\Big|_{-\infty}^{\infty} + \int_{-\infty}^{\infty} \delta(x)f''(x)dx \\
&= 0 + f''(0) = f''(0) \qquad \text{(B.4)}
\end{aligned}$$

$$\begin{aligned}
\int_{-\infty}^{\infty} f(x)\Delta''_{\bar{u},r,d,\bar{a}}(x)dx &= \int_{-r-d-\bar{a}}^{-r-d+\bar{a}} f(x)\bar{u}dx - \int_{-r+d-\bar{a}}^{-r+d+\bar{a}} f(x)\bar{u}dx \\
&\quad - \int_{r-d-\bar{a}}^{r-d+\bar{a}} f(x)\bar{u}dx + \int_{r+d-\bar{a}}^{r+d+\bar{a}} f(x)\bar{u}dx \\
&= f(-r-d)\bar{u}2\bar{a} - f(-r+d)\bar{u}2\bar{a} \\
&\quad -f(r-d)\bar{u}2\bar{a} + f(r+d)\bar{u}2\bar{a} \\
&= \Big[[f(-r) + f'(-r)(-d) + \frac{f''(-r)}{2}(-d)^2 + O(d^3)] \\
&\quad -[f(-r) + f'(-r)d + \frac{f''(-r)}{2}d^2 + O(d^3)]
\end{aligned}$$

$$
\begin{aligned}
&-[f(r)+f'(r)(-d)+\frac{f''(r)}{2}(-d)^2+O(d^3)] \\
&+[f(r)+f'(r)d+\frac{f''(r)}{2}d^2+O(d^3)]\Big]\bar{u}2\bar{a} \\
=\;& \Big[-f'(-r)2d+f'(r)2d+O(d^3)\Big]\bar{u}2\bar{a} \\
=\;& 2r\Big[\frac{f'(r)-f'(-r)}{2r}\Big]4d\bar{u}\bar{a}+O(d^3) \\
=\;& 8rd\bar{u}\bar{a}f''(r)+O(d^3)
\end{aligned}
\tag{B.5}
$$

$$
\begin{aligned}
& Ae^{ik(2r+2d-6\bar{a})}+Be^{ik(2r-6d+2\bar{a})}+C1e^{ik(2r-2d-2\bar{a})}+ \\
& C2e^{ik(-2r+2d+2\bar{a})}+Ee^{ik(-2r-2d+6\bar{a})}+Fe^{ik(-2r+6d-2\bar{a})} \\
=\;& [Ae^{ik(2r-2d-2\bar{a})}+Fe^{-ik(2r-2d-2\bar{a})}]e^{i4(d-\bar{a})}+ \\
& [Be^{ik(2r-2d-2\bar{a})}+Ee^{-ik(2r-2d-2\bar{a})}]e^{-i4(d-\bar{a})}+ \\
& C1e^{ik(2r-2d-2\bar{a})}+C2e^{-ik(2r-2d-2\bar{a})} \\
=\;& [(A+F)\cosh(i2k(r-d-\bar{a}))+ \\
& (A-F)\sinh(i2k(r-d-\bar{a}))]e^{i4k(d-\bar{a})}+ \\
& [(B+E)\cosh(i2k(r-d-\bar{a}))+ \\
& (B-E)\sinh(i2k(r-d-\bar{a}))]e^{-i4k(d-\bar{a})}+ \\
& [(C1+C2)\cosh(i2k(r-d-\bar{a}))+ \\
& (C1-C2)\sinh(i2k(r-d-\bar{a}))] \\
=\;& \{[(A+F)+(B+E)]\cos(2k(r-d-\bar{a}))+ \\
& i[(A-F)+(B-E)]\sin(2k(r-d-\bar{a}))\}\cosh(i4k(d-\bar{a}))+ \\
& \{[(A+F)-(B+E)]\cos(2k(r-d-\bar{a}))+ \\
& i[(A-F)-(B-E)]\sin(2k(r-d-\bar{a}))\}\sinh(i4k(d-\bar{a}))+ \\
& (C1+C2)\cos(2k(r-d-\bar{a}))+i(C1-C2)\sin(2k(r-d-\bar{a})) \\
=\;& \{[A+B+E+F]\cos(2k(r-d-\bar{a}))+ \\
& i[A+B-E-F]\sin(2k(r-d-\bar{a}))\}\cos(4k(d-\bar{a}))+ \\
& \{i[A-B-E+F]\cos(2k(r-d-\bar{a}))+ \\
& [-A+B-E+F]\sin(2k(r-d-\bar{a}))\}\sin(4k(d-\bar{a}))+ \\
& (C1+C2)\cos(2k(r-d-\bar{a}))+i(C1-C2)\sin(2k(r-d-\bar{a})) \\
=\;& \{[A+B+E+F]\cos(4k(d-\bar{a})) \\
& +i[A-B-E+F]\sin(4k(d-\bar{a}))+ \\
& (C1+C2)\}\cos(2k(r-d-\bar{a}))+ \\
& \{i[A+B-E-F]\cos(4k(d-\bar{a}))+ \\
& [-A+B-E+F]\sin(4k(d-\bar{a}))+ \\
& i(C1-C2)\}\sin(2k(r-d-\bar{a})) \\
=\;& \{K\cos(4k(d-\bar{a}))+L\sin(4k(d-\bar{a}))+M\}\cos(2k(r-d-\bar{a}))+ \\
& \{N\cos(4k(d-\bar{a}))+O\sin(4k(d-\bar{a}))+P\}\sin(2k(r-d-\bar{a}))
\end{aligned}
\tag{B.6}
$$

with

$$\begin{aligned}
K &= [A + B + E + F] \\
L &= i[A - B - E + F] \\
M &= (C1 + C2) \\
N &= i[A + B - E - F] \\
O &= [-A + B - E + F] \\
P &= i(C1 - C2)
\end{aligned}$$

$$\begin{aligned}
K = \; & [4i\eta^2\vartheta(\cosh 2\eta - 1)\sin 2\vartheta](k\bar{a})^{-3} + \\
& [16\eta\vartheta \sinh 2\eta \sin 2\vartheta](k\bar{a})^{-2} + \\
& \Big[64i\eta \sinh 2\eta \cos 2\vartheta + \\
& \frac{16i}{\vartheta}((\eta^2 - 2\vartheta^2)\cosh 2\eta - (\eta^2 + 2\vartheta^2))\sin 2\vartheta\Big](k\bar{a})^{-1} + \\
& 256 \cosh 2\eta \cos 2\vartheta + \frac{64(\eta^2 - \vartheta^2)}{\eta\vartheta} \sinh 2\eta \sin 2\vartheta - \\
& \Big[\frac{64i}{\eta^2\vartheta}((2\eta^2 - \vartheta^2)\cosh 2\eta + (2\eta^2 + \vartheta^2))\sin 2\vartheta + \\
& \frac{256i}{\eta} \sinh 2\eta \cos 2\vartheta\Big](k\bar{a}) - \\
& [\frac{256}{\eta\vartheta} \sinh 2\eta \sin 2\vartheta](k\bar{a})^2 + \\
& [\frac{256i}{\eta^2\vartheta}(\cosh 2\eta - 1)\sin 2\vartheta](k\bar{a})^3
\end{aligned} \tag{B.7}$$

Appendix C

Maple

The symbolic computer language Maple is used to calculate the transmission in subsection 2.3.2.

C.1 Transmission.mws

```
Transmission.mws, Aug the 23rd 2003
An expression for the transmission is calculated.
> restart;

solution asumptions
> zero:=(i,x)->A[i]*exp(I*k*x)+B[i]*exp(-I*k*x);
> pos:=(i,x)->A[i]*exp(-eta/(2*a)*x)+B[i]*exp(eta/(2*a)*x);
> neg:=(i,x)->A[i]*exp(I*theta/(2*a)*x)+B[i]*exp(-I*theta/(2*a)*x);
> psi[1]:=(x)->zero(1,x);
> psi[2]:=(x)->pos(2,x);
> psi[3]:=(x)->zero(3,x);
> psi[4]:=(x)->neg(4,x);
> psi[5]:=(x)->zero(5,x);
> psi[6]:=(x)->neg(6,x);
> psi[7]:=(x)->zero(7,x);
> psi[8]:=(x)->pos(8,x);
> psi[9]:=(x)->A[9]*exp(I*k*x);

boundary conditions
> bound[1]:=-r-d-a;
> bound[2]:=-r-d+a;
> bound[3]:=-r+d-a;
> bound[4]:=-r+d+a;
> bound[5]:=+r-d-a;
> bound[6]:=+r-d+a;
> bound[7]:=+r+d-a;
> bound[8]:=+r+d+a;
> for i from 1 to 8 do
    eq[i]:=psi[i](bound[i])=psi[i+1](bound[i]);
```

```
    diff_eq[i]:=subs(x=bound[i],diff(psi[i](x),x)=diff(psi[i+1](x),x));
  od;
```

solutions to boundary conditions

```
  for i from 1 to 8 do
    sols[i]:=solve({eq[i],diff_eq[i]},{A[i],B[i]}); od;
  for i from 1 to 8 do
    j:=9-i; assign(sols[j]); od;
```

code

```
> rank:=[cosh,sinh,cos,sin,exp];
> expand(expandoff());
> expandoff(cos,sin,cosh,sinh);
> check := proc(input)
    global rank;
    local  values;

    values := {a=l/2,d=l/2,r=l,k=eta/l};
    collect(combine(expand(subs(values,input)),exp),rank);
  end:
> lhdeg := proc(input,par)
    local temp,l,h;

    temp := collect(expand(input),exp(par));
    l    := ldegree(temp,exp(par));
    h    := degree(temp,exp(par));

    [l, h];
  end:
> opset := proc(input)
    local output;

    if (op(0,input)=`*`)
      then output := {input};
      else output := {op(input)}; fi;

    output
  end:
> cons := proc(eq,par)
    local temp,deg,i,co,j,l,pos,neg;

    temp := collect(expand(eq),exp(par));
    deg  := max(-ldegree(temp,exp(par)),degree(temp,exp(par)));

    for i from -deg to deg do
      if (i<>0) then co[i] := coeff(temp,exp(par)^i);
                else co[i] := 0 fi; od;
    co[0] := temp - sum('co[j]*exp(par)^j',j=-deg..deg);

    temp := co[0];
    for l from 1 to deg do
      if (co[-l]<>0 and co[l]<>0) then
        pos    := opset(co[l]) intersect opset(co[-l]);
        neg    := opset(co[l]) intersect opset(-co[-l]);
```

```
        pos    := convert(pos,`+`);
        neg    := convert(neg,`+`);

        co[l]  := co[l]-pos-neg;
        co[-l] := co[-l]-pos+neg;

        temp   := neg*2*sinh(l*par) + pos*2*cosh(l*par) + temp; fi;
      temp := co[l]*exp(par)^l + co[-l]*exp(par)^(-l) + temp; od;

    if (eq=0) then temp:=0 fi;
    collect(combine(expand(temp),exp),rank);
  end:

> T:=A1/A9=collect(combine(expand(A[1]/A[9]),exp),exp);
> T:=T*2^8*exp(-2*I*k*(r+d+a)):
> temp:=cons(rhs(T),eta);
> temp:=cons(temp,I*theta);
> T := lhs(T) = temp;
> check(temp/16);
```

C.2 Transmission trigonometric.mws

```
Transmission trigonometric.mws, Aug the 25th of 2003
The found transmission is rewritten in a trigonometric form.
> restart;
> expand(expandoff());
> expandoff(cos,sin,cosh,sinh);
> check := proc(input)
    local  values;

    values := {a=l/2, d=l/2, r=l, k=eta/l};
    collect(combine(expand(subs(values,input)),exp),
                           [cosh,sinh,cos,sin,exp]);
  end:

T, transmission imported from Transmission.mws

T_trig, transmission T rewritten in terms of trigonometric functions and
                                             comparison of T_trig with T

> temp := collect(combine(expand(rhs(T)),exp),exp);
> term1 := expand(2*k*(  r +  d -3*a)):
> term2 := expand(2*k*(  r -3*d +  a)):
> term3 := expand(2*k*(  r -  d -  a)):
> term4 := -term3:
> term5 := -term1:
> term6 := -term2:
> term1 := combine(expand(exp(I*term1)),exp);
> term2 := combine(expand(exp(I*term2)),exp);
> term3 := combine(expand(exp(I*term3)),exp);
> term4 := combine(expand(exp(I*term4)),exp);
```

```
> term5 := combine(expand(exp(I*term5)),exp);
> term6 := combine(expand(exp(I*term6)),exp);
> A  := coeff(temp,term1):
> B  := coeff(temp,term2):
> C1 := coeff(temp,term3):
> C2 := coeff(temp,term4):
> E  := coeff(temp,term5):
> F  := coeff(temp,term6):
> temp := A*term1 +B*term2 +C1*term3 +C2*term4 +E*term5 +F*term6:
> check(temp/16);

> arg[1] := expand(op(1,term3)/I);
> arg[2] := expand(4*k*(d-a));
> AA := (A+F)*cos(arg[1])+I*(A-F)*sin(arg[1]);
> BB := (B+E)*cos(arg[1])+I*(B-E)*sin(arg[1]);
> CC := (C1+C2)*cos(arg[1])+I*(C1-C2)*sin(arg[1]);
> T_trig := lhs(T) = (AA+BB)*cos(arg[2])+I*(AA-BB)*sin(arg[2])+CC:
> check(T_trig/16);
> check1 := convert(expand(rhs(T)),exp):
> check2 := convert(expand(rhs(T_trig)),exp):
> expand(check2-check1);

T_trig, transmission T_trig rewritten in orderly fashion and
                            comparison of new T_trig with T
> arg[1] := 2*k*r-2*k*d-2*k*a;
> arg[2] := 4*k*d-4*k*a;
> temp := subs({arg[1]=arg1, arg[2]=arg2}, rhs(T_trig)):

> co_cos := coeff(expand(temp),cos(arg1));
> K := coeff(co_cos,cos(arg2));
> L := coeff(co_cos,sin(arg2));
> M := expand(co_cos -K*cos(arg2) -L*sin(arg2));
> expand(co_cos -(K*cos(arg2) +L*sin(arg2)+M));

> co_sin := coeff(expand(temp),sin(arg1));
> N := coeff(co_sin,cos(arg2));
> Oo := coeff(co_sin,sin(arg2));
> P := expand(co_sin -N*cos(arg2) -Oo*sin(arg2));
> expand(co_sin -(N*cos(arg2) +Oo*sin(arg2) +P));

> if(K=0 or L=0 or M=0 or N=0 or Oo=0 or P=0) then
                    print("Something is wrong!!");
  else print("check OK!!"); fi;
> T_trig := lhs(T) = (K*cos(arg[2]) +L*sin(arg[2]) +M)*cos(arg[1]) +
                    (N*cos(arg[2]) +Oo*sin(arg[2]) +P)*sin(arg[1]);
> check(T_trig/16);
> check1 := convert(expand(rhs(T)),exp):
> check2 := convert(expand(rhs(T_trig)),exp):
> expand(check2-check1);
```

C.3 Transmission investigated.mws

```
Transmission investigated.mws, Aug the 25th of 2003
The trigonometric form of the transmission is investigated.
> restart;
> expand(expandoff());
> expandoff(cos,sin,cosh,sinh);

> arg[1] := 2*k*r-2*k*d-2*k*a;
> arg[2] := 4*k*d-4*k*a;
> T_trig := 256*exp(-2*I*k*(r+d+a))*A1/A9 =
            (K*cos(arg[2]) +L*sin(arg[2]) +M)*cos(arg[1]) +
            (N*cos(arg[2]) +Oo*sin(arg[2]) +P)*sin(arg[1]);
> d := a;
> r := 2*a;
> T_trig;

Coeffs A, B, C, K, L & M

> T_trig;
> eta := 2*a*sqrt(sigma^2*u-k^2);
> theta := 2*a*sqrt(sigma^2*u+k^2);
> u := 1/8/r/d/a;

> eta :=sigma/2/sqrt(a);
> theta :=sigma/2/sqrt(a);
> eq := subs(sigma=tau*sqrt(a),T_trig);
```

Appendix D

Nonlinear Delta Prime

D.1 Differential Equation

Substitution of $\theta_b' = \frac{L_b}{A_b^2}$ into eq. (3.9) and multiplication with dA_b yields

$$-A_b'' dA_b + A_b(\frac{L_b}{A_b^2})^2 dA_b + (u + vA_b^2)A_b dA_b = k^2 A_b dA_b.$$

Rearranging gives

$$-\frac{1}{2}d((A_b')^2) - \frac{L_b^2}{2}d(\frac{1}{A_b^2}) + \frac{u}{2}d(A_b^2) + \frac{v}{4}d(A_b^4) = \frac{k^2}{2}d(A_b^2).$$

Integrating with the integrating constant L_b gives

$$-\frac{k^2}{2}A_b^2 - \frac{L_b^2}{2}\frac{1}{A_b^2} + \frac{u}{2}A_b^2 + \frac{v}{4}A_b^4 + E_b = \frac{1}{2}(A_b')^2.$$

Here the intensity $N_b = A_b^2$ is introduced. Substitution gives

$$-\frac{k^2}{2}N_b - \frac{L_b^2}{2}\frac{1}{N_b} + \frac{u}{2}N_b + \frac{v}{4}N_b^2 + E_b = \frac{1}{8}\frac{(N_b')^2}{N_b}.$$

Now the equation is rearranged and the derivative N_b' is isolated,

$$\frac{1}{2}N_b' = \sqrt{2E_b N_b - L_b^2 + (u - k^2)N_b^2 + \frac{v}{2}N_b^3}. \tag{D.1}$$

D.2 Factorization

The approximation is estimated in two phases. First it is noticed, that the cubic polynomial behaves like a square polynomial for very small nonlinearity. This square polynomial has two roots N_1 and N_2. Mathematically,

$$\begin{aligned}
&\frac{4}{v}E_bN_b - \frac{2}{v}k^2|T|^4 + \frac{2}{v}(u-k^2)N_b^2 + N_b^3 \\
&\quad\to \{4E_bN_b - 2k^2|T|^4 + 2(u-k^2)N_b^2\}/v \text{ if } v \to 0 \\
&\quad\to \{(N_b - N_1)(N_b - N_2)\}/v \text{ if } v \to 0,
\end{aligned}$$

with the two roots

$$N_{1,2} = \Big\{ -E_b \pm \sqrt{E_b^2 + (u-k^2)k^2|T|^4}\Big\}/(u-k^2). \tag{D.2}$$

Expanding

$$\begin{aligned}
&(N_b - N_1)(N_b - N_2)(N_b - N_3) \\
&\quad = \frac{4}{v}E_bN_b - \frac{2}{v}k^2|T|^4 + \frac{2}{v}(u-k^2)N_b^2. + N_b^3
\end{aligned}$$

$$\begin{aligned}
\Rightarrow N_3 &= -\frac{2(u-k^2)}{v} - \frac{N_b(k^2|T|^4 - 2E_bN_b)}{2E_bN_b - k^2|T|^4 + (u-k^2)N_b^2} \\
&\to -\frac{2(u-k^2)}{v} \text{ if } v \to 0.
\end{aligned}$$

D.3 Perturbation

Start with rewriting eq. (3.23)

$$\begin{aligned}
N_\pm &= \Big\{ -(u+k^2+\frac{v}{2}|T|^2) \pm \sqrt{(u+k^2)^2 + (3k^2+u)|T|^2v + O(v^2)}\Big\}/v \\
&= \Big\{ -(u+k^2+\frac{v}{2}|T|^2 \pm (u+k^2)\{1 + \frac{(3k^2+u)|T|^2)}{2(u+k^2)^2}v + O(v^2)\}\Big\}/v
\end{aligned}$$

$$N_+ = -\frac{|T|^2}{2} + \frac{(3k^2+u)|T|^2}{2(u+k^2)} + O(v) = \frac{k^2}{u+k^2}|T|^2 + O(v), \quad \text{(D.3)}$$

$$N_- = -\frac{2(u+k^2)}{v} - \frac{(2k^2+u)}{k^2+u}|T^2| + O(v). \quad \text{(D.4)}$$

Inserting these values in eq.3.25 and eq.3.26 yields

$$\mu = \frac{v|T|^2 - v(\frac{k^2}{u+k^2}|T|^2 + O(v))}{2(u+k^2) + O(v)} = 0 + O(v), \quad \text{(D.5)}$$

$$\begin{aligned} \bar{\kappa} &= \sqrt{\frac{v}{2}|T|^2 + (u+k^2) + O(v)} \\ &= \sqrt{u+k^2} + O(v) = \kappa + O(v). \end{aligned} \quad \text{(D.6)}$$

The "sine amplitudine" with vanishing modulus approaches the trigonometric sinus. This is found in [BF71] 122.08. With the help of eq. (D.3)

$$\begin{aligned} N_0 &= |T|^2 - (|T|^2 - \{\frac{k^2}{\kappa^2}|T|^2 + O(v)\}) sin^2(\kappa - a) \\ &= \frac{|T|^2}{2\kappa^2}\{u + 2k^2 + u\cos(2\kappa a)\} + O(v). \end{aligned} \quad \text{(D.7)}$$

Inserting this equation in eq. (3.29) and with the help of eq. (3.21)

$$\begin{aligned} Eb &= k^2|T|^2 + \frac{u}{2}|T|^2 - u\frac{|T|^2}{2\kappa^2}\{u + 2k^2 + u\cos(2\kappa a)\} + O(v) \\ &= \frac{|T|^2}{2\kappa^2}\{2k^4 + k^2 u - u^2\cos(2\kappa a)\} + O(v). \end{aligned} \quad \text{(D.8)}$$

Inserting eq. (D.8) in eq. (3.35)

$$\begin{aligned} m &= \frac{v(-E_b + \sqrt{E_b^2 + (u-k^2)k^2|T|^4}) + 2(u-k^2)}{v(-E_b - \sqrt{E_b^2 + (u-k^2)k^2|T|^4}) + 2(u-k^2)} \\ &= \frac{O(v) + 2(u-k^2)}{O(v) + 2(u-k^2)} = 1 + O(v). \end{aligned} \quad \text{(D.9)}$$

Inserting eq. (3.32) and eq. (3.33) in eq. (3.36) and using eq. (D.8)

$$
\begin{aligned}
\bar{q} &= \sqrt{\frac{v\{E_b + \sqrt{E_b^2 + (u-k^2)k^2|T|^4}\}}{2(u-k^2)} + u - k^2} \\
&= \sqrt{u-k^2} + O[v] = q + O[v]
\end{aligned}
$$

Introducing [BF71] 123.01

$$
\mathrm{cn}^{-1}(\bar{q}x + \chi|m) = \frac{1 - m\mathrm{sn}^2(\bar{q}x|m)\mathrm{sn}^2(\chi|m)}{\mathrm{cn}(\bar{q}x|m)\mathrm{cn}(\chi|m) - \mathrm{sn}(\bar{q}x|m)\mathrm{sn}(\chi|m)\mathrm{dn}(\bar{q}x|m)\mathrm{dn}(\chi|m)}
$$

For $m = 1$ and $\bar{q} = q$ [BF71] 122.09

$$
\left\{
\begin{array}{lcl}
\mathrm{sn}(\bar{q}x|m) &=& \tanh(qx) \\
\mathrm{cn}(\bar{q}x|m) &=& \mathrm{sech}(qx) \\
\mathrm{dn}(\bar{q}x|m) &=& \mathrm{sech}(qx)
\end{array}
\right.
$$

and

$$
\mathrm{dn}(\chi|m) = \mathrm{cn}(\chi|1)
$$

$$
\begin{aligned}
\mathrm{cn}^{-2}(qx + \chi|1) &= \Big(\frac{1 - \tanh^2(qx)\mathrm{sn}^2(\chi|1)}{1 - \tanh(qx)\mathrm{sn}(\chi|1)} \frac{\cosh(qx)}{\mathrm{cn}(\chi|1)}\Big)^2 \\
&= \Big(\cosh(qx) + \sinh(qx)\mathrm{sn}(\chi|1)\Big)^2 \frac{1}{\mathrm{cn}^2(\chi|1)}
\end{aligned}
$$

Intorducing

$$
\left\{
\begin{array}{l}
\cosh^2(qx) = \frac{1}{2}(\cosh(2qx) + 1) \\
\sinh^2(qx) = \frac{1}{2}(\cosh(2qx) - 1) \\
\sinh(qx)\cosh(qx) = \frac{1}{2}\sinh(2qx)
\end{array}
\right.
$$

gives

$$
\begin{aligned}
\mathrm{cn}^{-2}(qx + \chi|1) &= \frac{1}{2}\Big(\{1 + \mathrm{sn}^2(\chi|1)\}\cosh(2qx) + 2\mathrm{sn}(\chi|1)\sinh(2qx) \\
&\quad +1 - \mathrm{sn}^2(\chi|1)\Big)^2 \frac{1}{\mathrm{cn}^2(\chi|1)}. \qquad \text{(D.10)}
\end{aligned}
$$

With eq. (3.37) and [BF71] 121.00

$$\mathrm{cn}^2(\chi|m) = 1 - \mathrm{sn}^2(\chi|m) = 1 - \frac{N_0 - N_1}{N_0 - N_2} = \frac{N_1 - N_2}{N_0 - N_2}$$

$$\begin{aligned} \mathrm{cn}^{-2}(qx + \chi|m) &= \frac{1}{2}\Big(\{\frac{(N_0 - N_2) + (N_0 - N_1)}{N_0 - N_2}\}\cosh(2qx) \\ &\quad + 2\sqrt{\frac{N_0 - N_1}{N_0 - N_2}}\sinh(2qx) + \frac{N_1 - N_2}{N_0 - N_2}\Big)\frac{1}{\mathrm{cn}^2(\chi|m)} \end{aligned} \tag{D.11}$$

$$\begin{aligned} N_b(x) &= N_2 + (N_1 - N_2)/\mathrm{cn}^2(\bar{q}x + \chi|m) \\ &= \frac{2N_0 - N_1 - N_2}{2}\cosh(2qx) \\ &\quad + \sqrt{(N_0 - N_1)(N_0 - N_2)}\sinh(qx) + \frac{N_1 + N_2}{2}. \end{aligned} \tag{D.12}$$

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