Nonlinear Scattering of Bose-Einstein Condensates on a Finite Barrier

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Abstract

We seek stationary state solutions to the nonlinear Schrödinger equation (NLS) for piecewise-constant potentials V(x). In this case, we are able to find complete stationary solutions, i.e. exact solutions which are separable in time and space, in terms of Jacobi elliptic functions. These special functions can be defined as an inverse integral and are an interpolation between the circular and hyperbolic trigonometric functions.

As an important mathematical application of our exact solutions, we will seek a nonlinear generalization of the transfer matrix. When this matrix, which is commonly used in electromagnetic transmission problems, is applied to the coefficient vector characterizing the solution in the region to the left of the first boundary, it yields the coefficient vector for any region to the right. To solve this general problem, we begin with the nontrivial case of two boundaries, which corresponds to a potential step or barrier. This has a direct physical application to an atom laser incident on such a potential, as occurs in Bose-Einstein condensates on a chip. Our work provides the first step towards formulating a completely general nonlinear scattering theory.

Executive Summary

We seek plots of the transmission coefficient, described in Section 3.1, for the stationary state solutions of the nonlinear Schrödinger equation. These plots will provide a great aid to our understanding of nonlinear scattering phenomena.

The main goal for the 2007 field term was to write *Mathematica* code that is capable of generating these transmission plots. This goal has been achieved, and we can now plot the transmission coefficient as a function of the eigenvalue μ for given values of input parameters. In the case of negligible nonlinearity, our results converge to the results for the linear case.

Some work still remains to be done on the transmission project. The code is extremely sensitive to the numerical input parameters, and this issue should be explored to see whether the code can be made more stable. In addition, the plots must be analyzed in order to gain an understanding of the physical and theoretical causes of unusual features in the transmission plots. This is the first step toward a general theory of nonlinear scattering.

Contents

1 Introduction

This project included several goals. The first goal was to check the *Mathematica* code which was written last semester for generality and robustness. This code was written to plot solutions to the nonlinear Schrödinger equation (NLS) for arbitrary input parameters. The code was checked to ensure that no algebraic or syntax errors existed and that all possible solutions were found. Furthermore, the code must be able to work correctly for arbitrary values of the input parameters. The code was modified to remove all unnecessary mathematical assumptions which restricted the region of validity.

The final goal was to generate transmission plots for the NLS solutions. These are described in detail in Section 3.1 below.

2 Background Physics

2.1 Bose-Einstein Condensates

Every particle in the known universe is either a boson or a fermion. Fermions (e.g. electrons, protons) are characterized by their "exclusivity": one will *never* find two fermions in *exactly* the same quantum-mechanical state. (This is the basis of the Pauli Exclusion Principle seen in chemistry.) In contrast, bosons (e.g. photons, the particles of light) are often found in the same state. A Bose-Einstein condensate (BEC) refers to a large number of ultra-cold bosons which "condense" into the same state, as shown in Figure 1. The existence of BECs was predicted in 1924, but they were not discovered until 1995 [1].

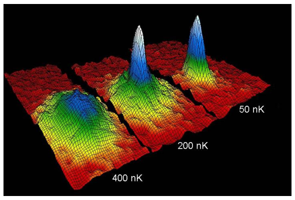


Figure 1: BECs from the original JILA experiment in 1995 [2].

2.2 Scattering

Scattering theory is very important in physics. Scattering is used to study particles that are too small to observe directly. Scattering is also used to study the behavior of particles in the presence of an external potential.

Scattering occurs when a particle is incident on a potential barrier. Classically, the process can be visualized as throwing a ball at a wall [3]. If the ball has sufficient energy, it will pass over the wall; otherwise it will "scatter" from it. These cases are illustrated in Fig. 2.

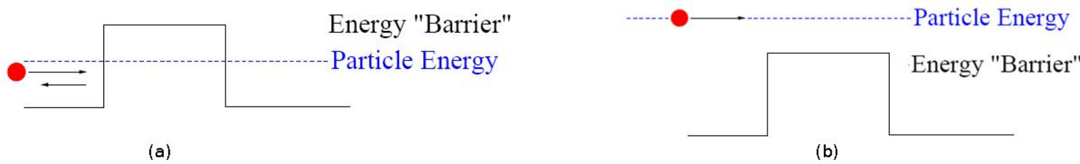


Figure 2: Classical scattering for (a) $E_{particle} > E_{barrier}$ and (b) $E_{particle} < E_{barrier}$.

Quantum mechanically, the particle is represented by its wave function $\Psi(x,t)$. The square modulus of $\Psi(x,t)$ gives the probability per unit length of finding the particle at a given position, so that $|\Psi(x,t)|^2dx$ is the probability of finding the particle in a width dx about position x at time t [4]. In linear quantum mechanical scattering, part of the wave reflects from the barrier and part of it is transmitted, regardless of the magnitude of the particle energy relative to the barrier energy (Fig. 3). Therefore, the probability of finding the particle on either side of the barrier, or inside of it, is in general nonzero. In the classical scenario, this means that the ball could pass through the wall, or bounce back from some point above the wall. This is very counterintuitive based on everyday experiences; however, it is a common occurrence in quantum mechanics.

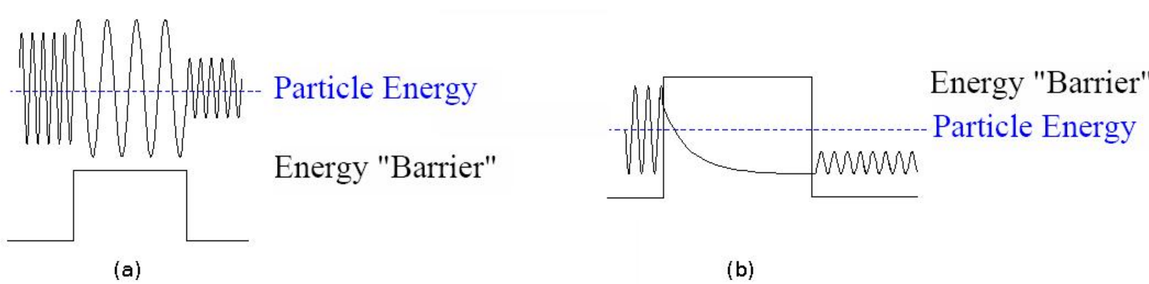


Figure 3: Quantum mechanical scattering for (a) $E_{particle} > E_{barrier}$ and (b) $E_{particle} < E_{barrier}$.

Nonlinear scattering is conceptually similar. However, the mathematics are quite different due to the nonlinear term in the differential equation for $\Psi(x,t)$. In the linear case, the superposition principle is applicable. The superposition principle states that any linear combination of solutions of the differential equation will also satisfy the equation. For the nonlinear equation, the superposition principle fails. Thus it is difficult to distinguish the incident and scattered portions of the wave.

3 Nonlinear Schrödinger Equation

The differential equation for the wave function $\Psi(x,t)$ in nonlinear quantum mechanics is the nonlinear Schrödinger equation (NLS),

$$i\partial_t\Psi(x,t) = -\frac{1}{2}\partial_{xx}\Psi(x,t) + g|\Psi(x,t)|^2\Psi(x,t) + V(x)\Psi(x,t), \tag{1}$$

where g is the interaction strength or nonlinearity and $V(x)$ is the external potential. Carr, Clark, and Reinhardt have obtained analytical stationary-state solutions to Eq. (1) for piecewise constant potentials [5, 6]. A stationary state is one in which the probability density $|\Psi(x,t)|^2$ is independent of time [4]. The potential barrier illustrated in Fig. 3 is an example of a piecewise constant potential. Such solutions are obtained by a method similar to separation of variables. We begin with an initial ansatz of the form

$$\Psi(x,t) = \sqrt{\rho(x)}\; e^{i\phi(x)}\; e^{-i\mu t} \tag{2}$$

where $\rho(x)$ is the particle density, $\phi(x)$ is the phase, and μ is the eigenvalue. We take the potential $V(x)$ to be constant. Physically, the phase ϕ represents a velocity potential for vortices in a superfluid. This is mathematically described by

$$\vec{v} = \frac{\hbar}{m}\vec{\nabla}\phi. \tag{3}$$

By substituting Eq. (2) into the NLS, Eq. (1), separating the equation, and equating real and imaginary parts on either side, solutions for the density $\rho(x)$ and phase $\phi(x)$ can be found. The density has the form

$$\rho(x) = A\ \mathrm{sn}^2(bx + x_0, k) + B \tag{4}$$

where A is the amplitude of oscillations, B is the density offset, b is the wave number, and x_0 is the horizontal shift. The function sn is one of the 12 Jacobi elliptic functions. These functions interpolate between the circular and hyperbolic trigonometric functions [7]. The parameter k is called the elliptic modulus [9] and corresponds geometrically to the eccentricity e of an ellipse [10]. When $k = 0$, the Jacobi elliptic functions reduce to the circular functions; when $k = 1$, the Jacobi functions become the hyperbolic functions. Figure 4 shows plots of $\mathrm{sn}(x,k)$ for several values of k.

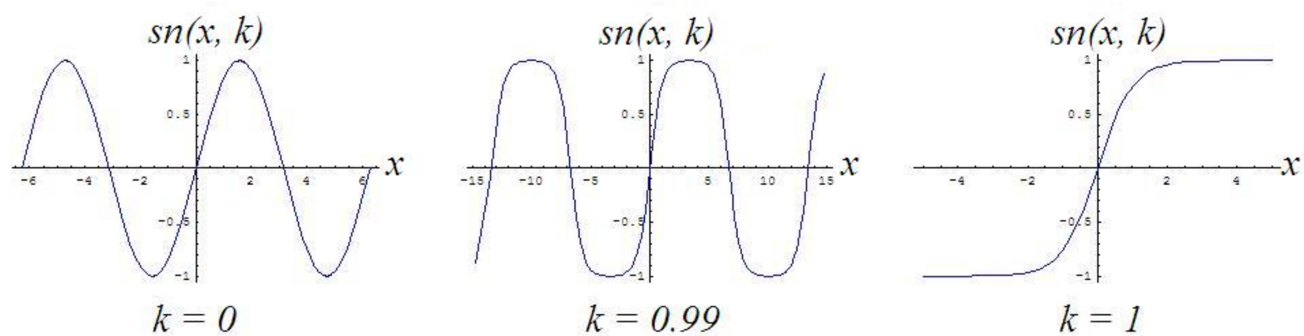


Figure 4: Jacobi sn function.

The phase is obtained from the equation

$$\partial_x\phi = \frac{\alpha}{\rho(x)} \tag{5}$$

where α is an integration constant resulting from the solution of the density equation.

When the potential $V(x)$ is piecewise constant, the density has the form given by Eq. (4) in each region of constant potential. At the boundaries (points of discontinuity in potential), we require that the wave function and its first spatial derivative be continuous. That is,

$$\Psi(x_i^+, t) = \psi(x_i^-, t); \tag{6}$$
$$\partial_x \Psi(x,t)|_{x=x_i^+} = \partial_x \Psi(x,t)|_{x=x_i^-} \tag{7}$$

where x_i is the location of the boundary, x_i^+ denotes evaluation of the function from the right side of the boundary, and x_i^- denotes evaluation from the left side of the boundary. From conditions (6) and (7), we obtain five boundary conditions [7]:

$$\rho(x_i^+) = \rho(x_i^-) \tag{8}$$
$$\partial_x \rho(x_i^+) = \partial_x \rho(x_i^-) \tag{9}$$
$$\phi(x_i^+) = \phi(x_i^-) + 2\pi n, \quad n \in \mathbb{Z} \tag{10}$$
$$\alpha(x_i^+) = \alpha(x_i^-) \tag{11}$$
$$\mu(x_i^+) = \mu(x_i^-) \tag{12}$$

Given the values of μ and g and the parameters $A,\ B,$ and x_0 on the left side of a boundary, conditions (8) through (12) and the general solution (4) can be used to obtain values of b and k on the left side and values for all of the parameters on the right side. This procedure can be applied repeatedly to obtain solutions for an arbitrary number of boundaries. A plot of the density for a two-boundary potential barrier is shown in Figure 5, where a subscript L refers to values for the left side of the leftmost boundary. The red curve denotes the potential barrier, for clarity.

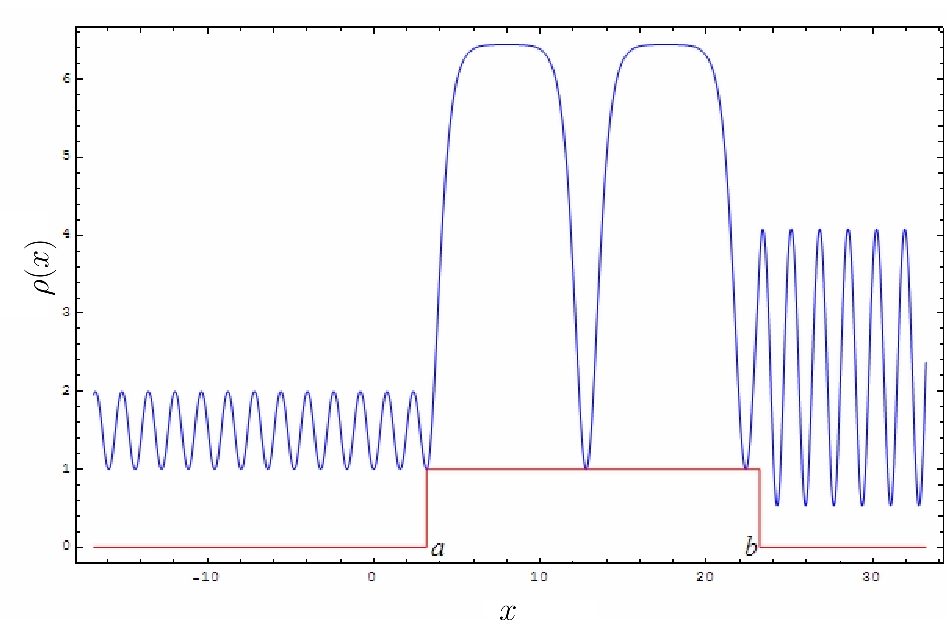


Figure 5: $\rho(x)$, with $g = 0.2,\ b_L = 2,\ A_L = 1,\ B_L = 1,\ x_{0L} = 0$. The boundaries are located at $a = 3.18$ and $b = 23.18$.

3.1 Transmission

Having obtained the density solutions, we can compute the transmission coefficient T. The transmission coefficient is defined in general as

$$T = \frac{|\Psi_{trans}(x,t)|^2}{|\Psi_{inc}(x,t)|^2} \tag{13}$$

where Ψ_{trans} is the transmitted wave function and Ψ_{inc} is the incident wave function. From Equation (2), we see that $|\Psi(x,t)|^2 = |\sqrt{\rho(x)}|^2$. Since $\rho(x)$ is the particle density, it must be real and nonnegative in order to be physically sensible. Therefore $|\Psi(x,t)|^2 = \rho(x)$. Since the density depends on x, we must take an average. Therefore,

$$T = \overline{\rho_3}/\overline{\rho_1} \tag{14}$$

where regions 1 and 3 are shown for a two-boundary barrier in Figure 6 and the average density in the ith region is given by

$$\overline{\rho_i} = \frac{1}{2K(k_i)/b_i} \int_{a_i}^{a_i+2K(k_i)/b_i} \rho_i(x)dx. \tag{15}$$

In Eq. (15), $K(k)$ is the complete elliptic integral of the first kind [11], $2K(k)/b$ is the period of the density given by Eq. (4), and a_i refers to a general lower limit which is different for each region. The important feature is that the density is averaged over a full period on each side of the boundary.

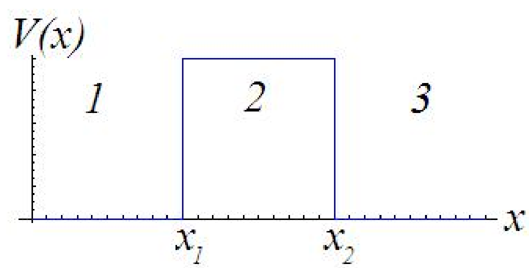


Figure 6: Notation for general two-boundary barrier.

Plots of the transmission coefficient were generated in *Mathematica* by fixing A, B, and x_0 in region 1, and allowing μ to vary. The T-values were computed numerically. A representative plot is shown in Figure 7.

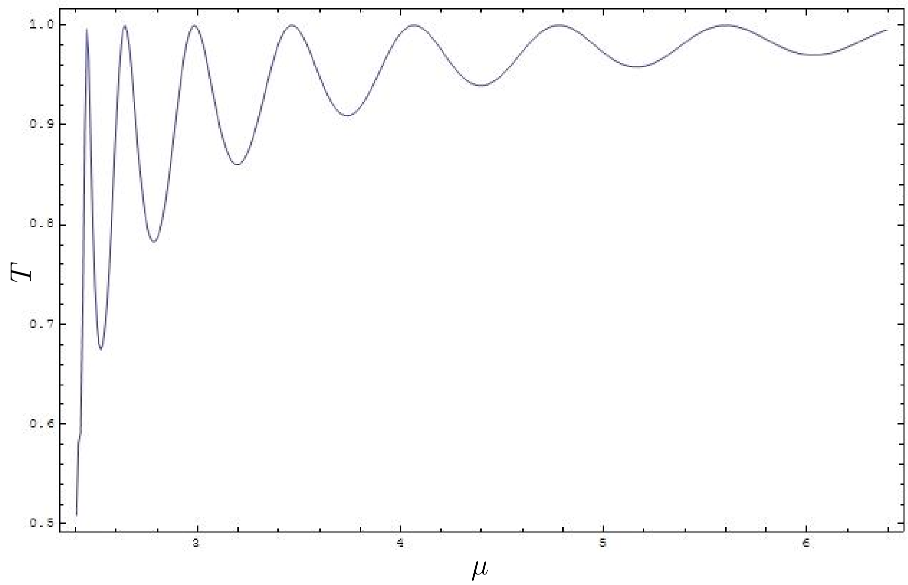
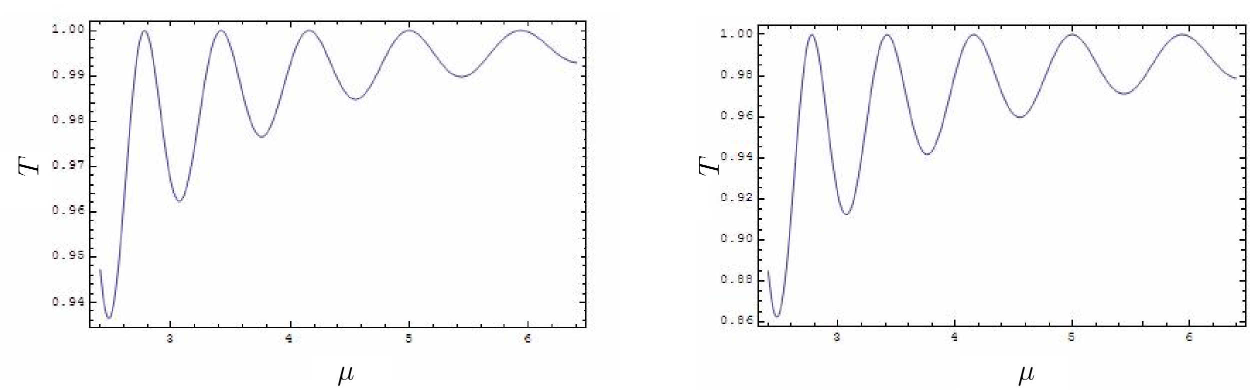


Figure 7: Transmission as a function of μ, with $A_1 = 0.16,\ B_1 = 1.7,\ x_{0,1} = 0, g = 0.2$.

To verify that the code is correct, it is straightforward to check the linear limit. When the nonlinearity g is zero, the NLS (1) reduces to the linear Schrödinger equation (LSE). The linear problem is well understood, and an analytical expression for the transmission coefficient can be found for the linear case. Figure 8 (a) shows a plot of the analytical linear transmission coefficient. Figure 8 (b) shows the numerical plot for a small value of g. It is clear from these plots that the nonlinear result is converging to the linear result, as we should expect.



(a)

(b)

Figure 8: Transmission coefficient for (a) LSE and (b) NLS, with $g = 2 \times 10^{-25}$.

4 Future Work

When the *Mathematica* code for plotting the density was checked for accuracy, it was discovered that some of the solutions did not satisfy the boundary condition (9). A review of the mathematics showed that the boundary conditions, as well as several expressions for parameters, were obtained by squaring both sides of an equation. This can lead to extraneous solutions: expressions that satisfy the squared equation, but do not satisfy the original equation. We have not yet determined a way to identify and eliminate these solutions in general. Currently, the code finds extraneous solutions by checking whether the boundary conditions are satisfied. This must be checked for each possible solution. We will seek a way to identify the extraneous solutions directly from the algebraic expressions. In this case, we can discard those solutions immediately, without a need to check the boundary conditions individually. This will likely speed up the execution of the code.

In addition, we will explore whether it is possible to obtain an analytic expression for the transmission coefficient T in the nonlinear case. It is possible that no such expression exists; however, we are not certain at this time.

Future researchers will seek a nonlinear generalization of the transfer matrix. This is a matrix which, when applied to the first region, yields the results in another region.
Also, an experiment is currently underway in Europe which will test our theoretical work. The experiment is being performed by Alain Aspect and Chris Westbrook. They are investigating the $m = 1$ limit in which the Jacobi sn function becomes the hyperbolic tangent.

If the Westbrook and Aspect experiment reveals new physical phenomena, it is quite likely that further theoretical investigation will be required for the ideas discussed in this report. The ultimate goal is to formulate a theory of nonlinear scattering in complete generality, and much research remains to be done in order to achieve this goal.

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