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**POPULATION OF QUANTUM STATES IN THE POTENTIAL
WELL DURING SCATTERING OF A MATTER WAVE
SOLITON**

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ABSTRACT

Scattering of a matter-wave soliton incident on the Gaussian potential well has been studied by means of a variational approach and numerical simulations of the Gross-Pitaevskii equation. As a result of scattering, some part of the wave packet is trapped in the potential well. We define this process as population of the quantum state in the potential well. Since the amplitude of the wave packet trapped in the potential well is small, compared to that of the incident wave packet, the role of nonlinearity is negligible. We consider the process long after the scattering event takes place.

The main goal of the present diploma work is the investigation of population dynamics of the ground state in the Gaussian potential well. With this objective in mind at first we determine the energy of the ground state by solving the stationary Schrödinger equation. As a trial function we consider the well known ground state function for the harmonic oscillator potential, namely a Gaussian function with parameters to be determined from the variational approach. The parameters are determined from the condition of minimal energy for the ground state. When these parameters are defined, we compare the shape of the localized wave packet, trapped in the potential well due to scattering of the matter wave soliton, with the Gaussian function predicted by our theoretical model.

Contents

Abstract	1
Introduction	2
1 Matter wave soliton and the Gross-Pitaevskii equation	4
1.1 The Gross-Pitaevskii equation	5
1.2 The initial condition for GPE	6
2 Bound states of a Gaussian potential well	8
2.1 Variational calculation of the ground state energy	9
2.2 First excited state of a Gaussian potential well	11
2.3 Algorithm for numerical simulations	12
2.4 Implementation of the algorithm in Mathematica software package	13
2.5 Numerical results for Gaussian potential well	15
3 Scattering on the Dirac delta function potential well	17
3.1 Calculaton of bound state energy	17
3.2 Numerical results for Dirac delta function well	19
Conclusions	20
References	22

Introduction

Manifestation of quantum effects in the dynamics of macroscopic objects always attracts great interest. One of the remarkable examples in this field was the recent discovery of the quantum reflection of matter-wave solitons from the attractive potentials [1, 2] and a negative potential steps [3]. Here the term quantum refers to the fact that reflection occurs without reaching a classical turning point, and to its relevance to the wave nature of the soliton. It has been shown that there exists a critical speed for the soliton, incident on the potential well, at which the reflection turns to passage through the potential well [4].

During the process of scattering some part of matter wave packet can be captured by the well, and this process is interpreted as the population of quantum states in the potential well. The main objective of this diploma work is to study the population dynamics of the ground state of a Gaussian potential well.

The problem will be addressed by analytical methods and numerical simulations of the Gross-Pitaevskii equation, which describes the dynamics of matter wave packets. At first we reduce the original three-dimensional Gross-Pitaevskii equation to one-dimensional form. Then apply variational approximation to the reduced equation and perform numerical simulations of the scattering process. At the time instance long after the scattering event, we extract the part of the wave packet, which is trapped in the potential well. Comparing the shape of the trapped wave packet with the ground state solution of the Schrödinger equation we conclude about population of this quantum state.

Chapter 1

Matter wave soliton and the Gross-Pitaevskii equation

Solitons are exceptionally stable localized waves that appear in a variety of physical systems. They have ability to propagate without spreading due to a fine balance between the dispersion and nonlinearity of the physical medium. As an example, both bright and dark optical solitons, which are intensity maxima and minima of the light field, respectively, have been observed in silica fibers. Optical solitons can be used in fiber optic communication systems for information transfer.

In this diploma work we consider solitons in Bose-Einstein condensates (BEC) of neutral atoms, which are known also as matter wave solitons [5]. Nonlinearity of BEC originates from interaction between atoms in the condensate. The character of interactions can be both attractive and repulsive. The dynamics of BEC is described by the Gross-Pitaevskii equation which is presented below

1.1 The Gross-Pitaevskii equation

The model is based on the Gross-Pitaevskii equation (GPE), which governs the mean-field dynamics of the condensate

$$i\hbar \frac{\partial \Psi}{\partial t} = \left[-\frac{\hbar^2}{2m} \nabla^2 + \frac{1}{2} m \omega_{\perp}^2 r^2 + V(x) + \frac{4\pi \hbar^2 a_s}{m} |\Psi|^2 \right] \Psi, \quad (1.1)$$

where Ψ is the macroscopic wave function of the condensate, normalized to the number of atoms $N = \int_{-\infty}^{\infty} |\Psi|^2 d\mathbf{r}$ with mass m and characterized by the s -wave scattering length a_s . Both signs of this parameter are physically relevant: positive sign ($a_s > 0$) corresponds to repulsive interatomic interactions in the condensate, while negative sign ($a_s < 0$) implies attractive interactions. To avoid collapse instability inherent to 3D BEC with focusing nonlinearity, the initial s -wave scattering length should be positive, but tuned to a negative value, employing the Feshbach resonance technique, at the stage of generation of solitons. Strong confinement in the radial direction ($r^2 = y^2 + z^2$) creates a quasi-1D waveguide for the condensate with trapping frequency ω_{\perp} . The condensate acquires a cigar shape when the longitudinal size of the condensate is much greater than both the healing length $\xi = (8\pi n_0 a_s)^{-1/2}$, where n_0 is the peak density of BEC, and the radial oscillator length. In addition, the chemical potential has to be much less than the radial harmonic oscillator ground state energy to suppress radial excitations of the condensate. When these conditions are met, the condensate displays a quasi-1D behavior. This setting, however, assumes some initial trapping potential in the axial direction as well. The scattering potential $V(x)$ can be created by a laser beam with the frequency red detuned from atomic transitions, so that the resulting force on condensate atoms points in the direction of increasing field intensity, as in optical traps.

As mentioned above, when the radial confinement is strong enough, the transverse dynamics of the condensate is suppressed, which means that one

can factorize the wave function as follows

$$\Psi(r, x, t) = \psi(x, t) \phi(r) \exp(-i\omega_{\perp}t), \quad (1.2)$$

where

$$\phi(r) = \frac{1}{\pi^{1/2}a_{\perp}} \exp\left(-\frac{r^2}{2a_{\perp}^2}\right)$$

is the ground state wave function of the radial harmonic trap, with $a_{\perp} = \sqrt{\hbar/m\omega_{\perp}}$ being its characteristic length. Substitution of Eq. (1.2) into Eq. (1.1) and integration over transverse variable r yields the 1D GPE for the longitudinal wave function $\psi(x, t)$

$$i\hbar\psi_t = -\frac{\hbar^2}{2m}\psi_{xx} + V(x)\psi + 2\hbar\omega_{\perp}a_s|\psi|^2\psi, \quad (1.3)$$

where indices in $\psi(x, t)$ denote the corresponding derivatives. Finally, by introducing dimensionless variables $t \rightarrow \omega_{\perp}t$, $x \rightarrow x/a_{\perp}$, $g = -2a_s/a_{\perp}$, $V(x) \rightarrow V(x)/\hbar\omega_{\perp}$, $\psi \rightarrow a_{\perp}^{1/2}\psi$, we obtain the main equation of our model

$$i\psi_t + \frac{1}{2}\psi_{xx} - V(x)\psi + g|\psi|^2\psi = 0. \quad (1.4)$$

We consider the BEC wave packet with attractive interaction between atoms ($a_s < 0$, therefore $g > 0$) confined in a quasi-1D atomic waveguide, so that the system supports bright matter-wave solitons [6]

1.2 The initial condition for GPE

We study the scattering of a matter wave soliton by the Gaussian potential well, therefore at the initial state the soliton and potential well should be far separated, as illustrated in Fig. 1.2. The initial state for the GPE (2.21) is the bright soliton of the GPE without potential and attractive nonlinearity $g = 1$. For simplicity we assume the fundamental soliton

$$\psi(x, 0) = \operatorname{sech}(x + x_0) \cdot e^{iv(x+x_0)}, \quad (1.5)$$

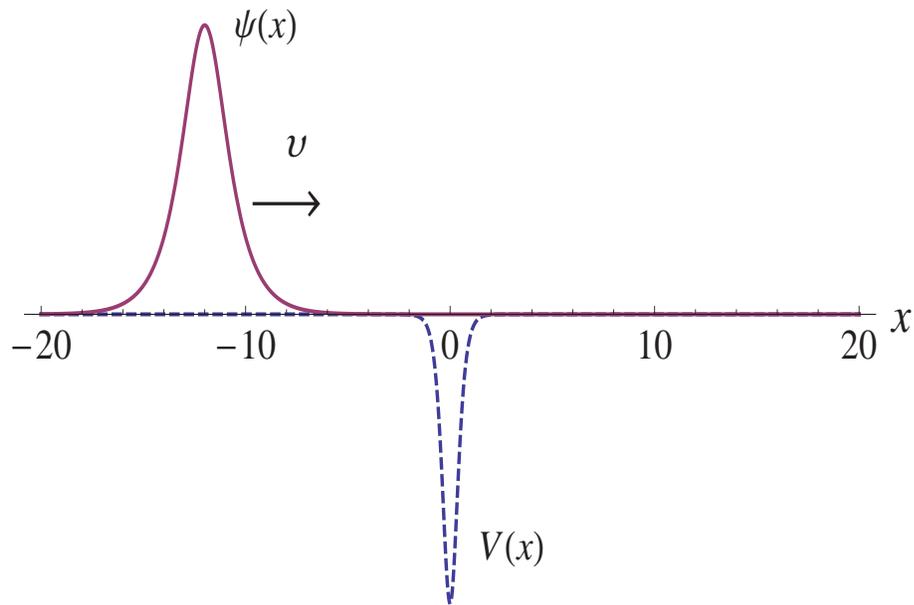


Figure 1.1: The initial configuration for matter wave soliton scattering on a potential well. At $t = 0$ soliton is far away ($x_0 = -12$) from the potential well $V(x)$, situated at the origin ($x = 0$), and therefore they do not interact.

where x_0 is the initial position of the soliton, v is the initial velocity of the soliton toward the Gaussian potential well. When the soliton is set in motion with some velocity v toward the potential well, the scattering event takes place. The outcome of scattering depends on the initial velocity and parameters of the potential well. If the velocity is below the critical value, it is reflected by the potential well. At greater velocity soliton traverses the potential well and some part of it becomes trapped.

Chapter 2

Bound states of a Gaussian potential well

First we define the energy of the ground state of a particle in a potential well by solving the stationary Schrödinger equation.

$$-\frac{\hbar^2}{2m}\psi_{xx} + V(x)\psi = E\psi \quad (2.1)$$

with a Gaussian potential well

$$V(x) = -V_0e^{-\alpha x^2}, \quad (2.2)$$

where $V_0 > 0$, α are the strength and inverse width of the potential well respectively, $\psi(x)$ is the wave function of the particle with mass m confined in the potential well.

For simplicity we adopt the units, where $\hbar = m = 1$ and rewrite the Eq. (2.1) as

$$H\psi = E\psi, \quad H = -\frac{1}{2}\frac{d^2}{dx^2} + V(x). \quad (2.3)$$

with the Hamiltonian H and energy E .

For the Hamiltonian (2.3) to have a bound state it is sufficient that its expectation value be negative for a *real* and normalized wave function

$$\langle H \rangle = \int_{-\infty}^{\infty} \psi H \psi dx < 0, \quad (2.4)$$

which means

$$\langle H \rangle = \int_{-\infty}^{\infty} \psi \left[-\frac{1}{2} \frac{d^2}{dx^2} + V(x) \right] \psi dx = \int_{-\infty}^{\infty} \left[\frac{1}{2} \psi_x^2 + V(x) \psi^2 \right] dx. \quad (2.5)$$

Here it was taken into regard that $\psi(x)$ is a localized wave packet, and performed integration by parts

$$-\frac{1}{2} \int_{-\infty}^{\infty} \psi \psi_{xx} dx = -\frac{1}{2} \psi \psi_x \Big|_{-\infty}^{\infty} + \frac{1}{2} \int_{-\infty}^{\infty} \psi_x^2 dx. \quad (2.6)$$

Now we introduce the quantity L , which is the length scale of the wave function, proportional to its width and define $\psi(x) = (1/\sqrt{L}) \phi(x/L)$. Substitution of this into Eq. (2.5) yields

$$\langle H \rangle = \frac{1}{2L^2} \cdot \int_{-\infty}^{\infty} \phi_x^2 dx + \frac{1}{L} \cdot \int_{-\infty}^{\infty} V(x) \phi^2 dx = \frac{a_1}{2L^2} + \frac{a_2}{L}. \quad (2.7)$$

At large L the second term in Eq. (2.7) dominates. In this case also one can write $[\phi(x/L)] \sim [\phi(0)]^2$, and take it out of the integral

$$a_2 = \int_{-\infty}^{\infty} V(x) \phi^2(x) dx \simeq \phi^2(0) \int_{-\infty}^{\infty} V(x) dx$$

It is clear that a_1 is a positive quantity, and the sign of a_2 depends on the sign of $\int_{-\infty}^{\infty} V(x) dx$. From this we conclude that there is at least one bound state in the potential well if the following integral is negative

$$\int_{-\infty}^{\infty} V(x) dx < 0 \quad (2.8)$$

It should be stressed that the above condition is sufficient, but not necessary. Recall, for example, the harmonic oscillator potential.

2.1 Variational calculation of the ground state energy

To calculate the ground state energy we select a Gaussian trial function which is normalized to one

$$\psi(x) = \left(\frac{2b}{\pi} \right)^{1/4} e^{-bx^2}, \quad (2.9)$$

where b is proportional to the inverse width of the wave function and is linked to above mentioned quantity L .

Next we estimate the expectation value of the Hamiltonian (2.5) using the trial function (2.9)

$$H_1 = \frac{1}{2} \int_{-\infty}^{\infty} \psi_x^2 dx = \frac{1}{2} \cdot \left(\frac{2b}{\pi}\right)^{1/2} \cdot 4b^2 \int_{-\infty}^{\infty} x^2 e^{-2bx^2} dx = \frac{b}{2}, \quad (2.10)$$

$$H_2 = \int_{-\infty}^{\infty} V(x)\psi^2(x)dx = -V_0 \left(\frac{2b}{\pi}\right)^{1/2} \cdot \int_{-\infty}^{\infty} e^{-(2b+\alpha)x^2} dx = -V_0 \cdot \sqrt{\frac{2b}{2b+\alpha}}. \quad (2.11)$$

Therefore, the ground state energy calculated for the Gaussian potential well (2.2) and trial function (2.9) is

$$\langle H \rangle = \frac{b}{2} - V_0 \cdot \sqrt{\frac{2b}{2b+\alpha}}. \quad (2.12)$$

The width of the ground state wave function can be found from the condition of minimum for energy

$$d \langle H \rangle / db = 0$$

$$\frac{d \langle H \rangle}{db} = 0, \quad \frac{1}{2} - \frac{\alpha V_0}{\sqrt{2b} \cdot (2b+\alpha)^{3/2}} = 0, \quad (2.13)$$

which can be reduced to following form

$$b \cdot (2b+\alpha)^3 = 2V_0^2 \alpha^2. \quad (2.14)$$

Solution of this equation with respect to b for given parameters of the potential well V_0 and α is sufficient to draw the ground state wave function and corresponding energy (2.12). Simple Mathematica code for solution of Eq. (2.14) is presented in Fig. 2.1. In particular, for parameters of the potential well $V_0 = 1$, $\alpha = 1$ we find $b = 0.3742$ and $\langle H \rangle = -0.4671$. In Fig. 2.6 we illustrate the ground state occupation due to scattering of the soliton.

```

(* This program finds the parameter "b" from numerical solution of Eq. (2.14)*)
V0 = 1.; a = 1.;
NSolve[b * (2 * b + a) ^ 3 - 2 * V0 ^ 2 * a ^ 2 == 0, b]

{{b -> -1.10867}, {b -> -0.382767 - 0.675348 i}, {b -> -0.382767 + 0.675348 i}, {b -> 0.374201}}

(* we should select the real and positive root *)
b0 = 0.3742;
(* then calculate corresponding ground state energy *)
En =  $\frac{b0}{2} - V0 * \text{Sqrt}\left[\frac{2 * b0}{2 * b0 + a}\right]$ 
-0.467154

```

Figure 2.1: Mathematica code for calculation of the parameter b in Eq. (2.14) and corresponding ground state energy (2.12).

2.2 First excited state of a Gaussian potential well

For convenience we again adopt the units $\hbar = m = 1$ and set the parameter value $\alpha = 1$. Then the potential in Eq. (2.3) will have the form $V(x) = -V_0 e^{-x^2}$

As a trial function for the first excited state of the Gaussian potential well we consider

$$\psi(x) = \left(\frac{2^5 b^3}{\pi}\right)^{1/4} x e^{-bx^2}, \quad (2.15)$$

where the amplitude is determined from normalization condition.

Variational calculations similar to the previous section lead to the following equation for parameter b

$$(2b + 1)(4b^2 + 4b + 1)^2 - 8V_0^2 b = 0. \quad (2.16)$$

Real positive root of this equation gives the possibility to calculate the energy of the first excited state

$$\langle H \rangle = -\frac{b(8b^2 + 2b - 1)}{2(2b + 1)} \quad (2.17)$$

The Mathematica program for finding the roots of the Eq. (2.16) and the energy of the first excited state Eq. (2.17) is shown in Fig. 2.2.

```

(* First excited state of the Gaussian potential well *)
v0 = 4;
v[x_] := -v0 * Exp[-x^2];
NSolve[(2 * b + 1) * (4 * b^2 + 4 * b + 1)^2 - 8 * b * v0^2 == 0, b]
{{b -> -2.01851}, {b -> -0.616792 - 1.43845 i},
 {b -> -0.616792 + 1.43845 i}, {b -> 0.00849948}, {b -> 0.743596}}

b0 = 0.7436;
amp = Sqrt[Sqrt[32 * b0^3 / Pi]];
f1[x_] := amp * x * Exp[-b0 * x^2];
evar = 
$$\frac{-b0 * (8 * b0^2 + 2 * b0 - 1)}{2 * (2 * b0 + 1)}$$

-0.734082

```

Figure 2.2: Mathematica code for calculation of the parameter b in Eq. (2.16) and corresponding ground state energy (2.17).

In Fig. 2.3 the ground state and first excited state of the Gaussian potential well are depicted

2.3 Algorithm for numerical simulations

Algorithm of our numerical simulations consists of the following steps.

- Second spatial derivative is approximated by the following expression $u_{xx} = (u_{n+1} + u_{n-1} - 2u_n)/h^2$, where h is the discrete step size $h = L/N$, $u_n = u(x_n)$, $x_n = n \cdot h$, $n = 0, 1, 2, \dots, N$, N – number of discrete intervals. Spatial domain is given by $x \in [-L, L]$. External potential also given in discrete representation as $V_n = V(x_n)$.
- Then the Gross-Pitaevskii equation acquires the form

$$i\dot{u}_n = -c(u_{n+1} + u_{n-1} - 2u_n) - V_n u_n - g|u_n|^2 u_n, \quad c = 1/(2 \cdot h^2). \quad (2.18)$$

- We express the complex discrete function via its real and imaginary parts $u_n = u_n + iv_n$, which leads to the following equation

$$i\dot{u}_n - \dot{v}_n = -c(u_{n+1} + u_{n-1} - 2u_n) - ic(v_{n+1} + v_{n-1} - 2v_n) - V_n u_n - iV_n v_n - g(u^2 + v^2)u_n - ig(u^2 + v^2)v_n.$$

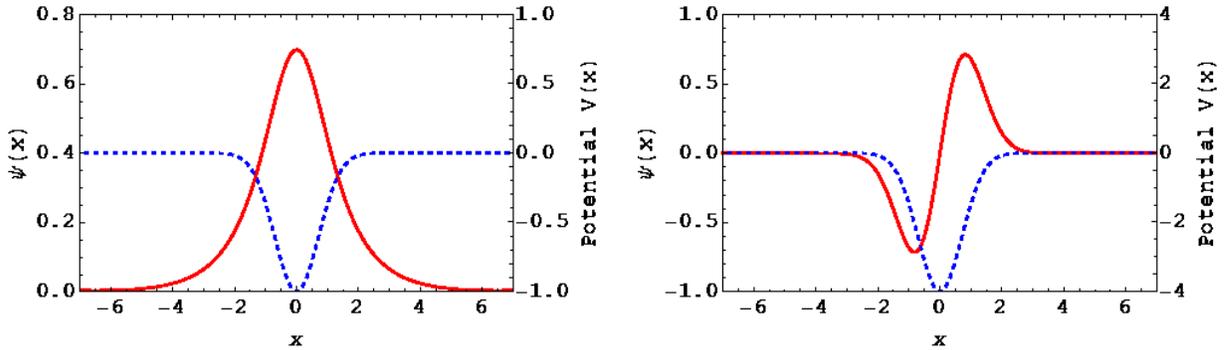


Figure 2.3: Ground state (left panel), and first excited state (right panel) of the Gaussian potential well, found from variational method, using Eq. (2.9) and Eq.(2.15). Blue dashed line depicts the Gaussian potential well $V(x)$. Parameters: $V_0 = 1$, $b = 0.3742$ for the ground state, and $V_0 = 4$, $b = 0.7436$ for the first excited state, respectively.

- The last equation can be written separately for real and imaginary parts

$$\dot{u}_n = -c(v_{n+1} + v_{n-1} - 2v_n) - g(u^2 + v^2)v_n + V_n v_n, \quad (2.19)$$

$$\dot{v}_n = c(u_{n+1} + u_{n-1} - 2u_n) - g(u^2 + v^2)u_n + V_n u_n. \quad (2.20)$$

The obtained system of first order differential equations allows to explore the time evolution of the wave packet. In order to start numerical simulations we need initial conditions, namely the form of the wave packet at the beginning $u_n(0) = u_n(0) + iv_n(0)$. This waveform is inserted in Eqs. (2.19) - (2.20). We employ the Runge-Kutta method [7] to solve the system.

2.4 Implementation of the algorithm in Mathematica software package

Nowadays several highly effective analytic and numerical calculation software packages are available, such as Mathematica, Matlab, Mathcad and Maple. In our work we employ Mathematica-7 package for numerical simulation of the Gross-Pitaevskii equation.

At the initial time we define the parameters of the wave packet and Gaussian potential. Then we insert the initial waveform as hyperbolic secant function, which corresponds to solitonic solution of the Gross-Pitaevskii equation without external potential. If we select in NDSolve procedure the command `Method` \rightarrow “MethodOfLines”, it will implement the above presented algorithm. Below in Fig. 2.4 the full text of the program is presented.

Scattering of a soliton by Gaussian potential well

```

In[16]= L = 60.; np = 2048; dx = L/np; (* space domain data *)
V0 = 1; alp = 1.; (* strength and width of the potential *)
V[x_] := V0 * Exp[-alp * x^2]; (* Gaussian well *)
vel = 1; (* soliton velocity *)
x0 = -10.; (* soliton initial position *)
u0[x_] := Sech[1. * (x - x0)] * Exp[I * vel * x];

In[19]= (* Gross-Pitaevskii equation *)
tend = 20.;
gpe = I * D[u[x, t], t] + 0.5 * D[u[x, t], x, x] + V[x] * u[x, t] + Abs[u[x, t]]^2 * u[x, t];
(* absorbing boundary function *)
sink = I * 20. * (Sech[1. * (x - L)]^2 + Sech[1. * (x + L)]^2) * u[x, t];
s = NDSolve[{gpe + sink == 0, u[x, 0] == u0[x], u[-L, t] == u[L, t]},
  u, {t, 0, tend}, {x, -L, L}, MaxSteps -> Infinity, StartingStepSize -> dx,
  Method -> {"MethodOfLines", "SpatialDiscretization" ->
    {"TensorProductGrid", "MinPoints" -> np}}, PrecisionGoal -> Infinity];

In[23]= Manipulate[Plot[{-V1[x], Abs[u[x, t] /. s[[1]]]^2},
  {x, -L, L}, PlotPoints -> 200, PlotRange -> {{-L/2, L/2}, {-1.1, 1.25}},
  Axes -> {True, True}, AxesLabel -> {"t", Abs[ψ]^2}, LabelStyle -> Directive[14],
  TicksStyle -> Directive[14], PlotStyle -> {{Dashed, Thick}, Thick},
  PlotLabel -> Row[{Text[Style["t = ", Large, Bold, Red]],
    Text[Style[ToString[t], Large, Bold, Red]]}], ImageSize -> Scaled[0.8]],
  {t, 0, tend, tend/200.}, {{k, 1, ""}, 1, Length[list], 1, ControlType -> Animator},
  AnimationRate -> 15, AnimationRunning -> True, AppearanceElements -> {},
  AppearanceElements -> None, Paneled -> False];

In[30]= (* single Gaussian well *)
t1 = 20;
norm = NIntegrate[Abs[u[x, t1] /. s[[1]]]^2, {x, -5, 5}]
b0 = 0.3742;
Amp = Sqrt[Sqrt[2 * b0 / Pi]] * Sqrt[norm];
gs[x_, t_] := Amp^2 * Exp[-2 * b0 * x^2];
Plot[{gs[x, t1], Abs[u[x, t1] /. s[[1]]]^2}, {x, -4, 4}, PlotRange -> All,
  AxesLabel -> {"x", Abs[ψ]^2}, LabelStyle -> Directive[14], TicksStyle -> Directive[14],
  Ticks -> {Automatic, Automatic}, PlotStyle -> {{Dashed, Thick}, Thick}]

```

Figure 2.4: The Mathematica-7 program for numerical simulation of the scattering of a matter-wave soliton by Gaussian potential well.

2.5 Numerical results for Gaussian potential well

Dynamics of the soliton interacting with the external potential $V(x)$ is described by the dimensionless one-dimensional Gross-Pitaevskii equation

$$i\psi_t + \frac{1}{2}\psi_{xx} - V(x)\psi + |\psi|^2\psi = 0 \quad (2.21)$$

One soliton solution of this equation

$$\psi(x) = A \operatorname{sech}[A(x - x_0)] \cdot e^{iv(x-x_0)}, \quad (2.22)$$

with amplitude A placed at some distance x_0 from the potential well and set in motion with velocity v , is used as initial condition. Occupation of the ground state of the potential well as a result of soliton scattering is illustrated in Fig. 2.5

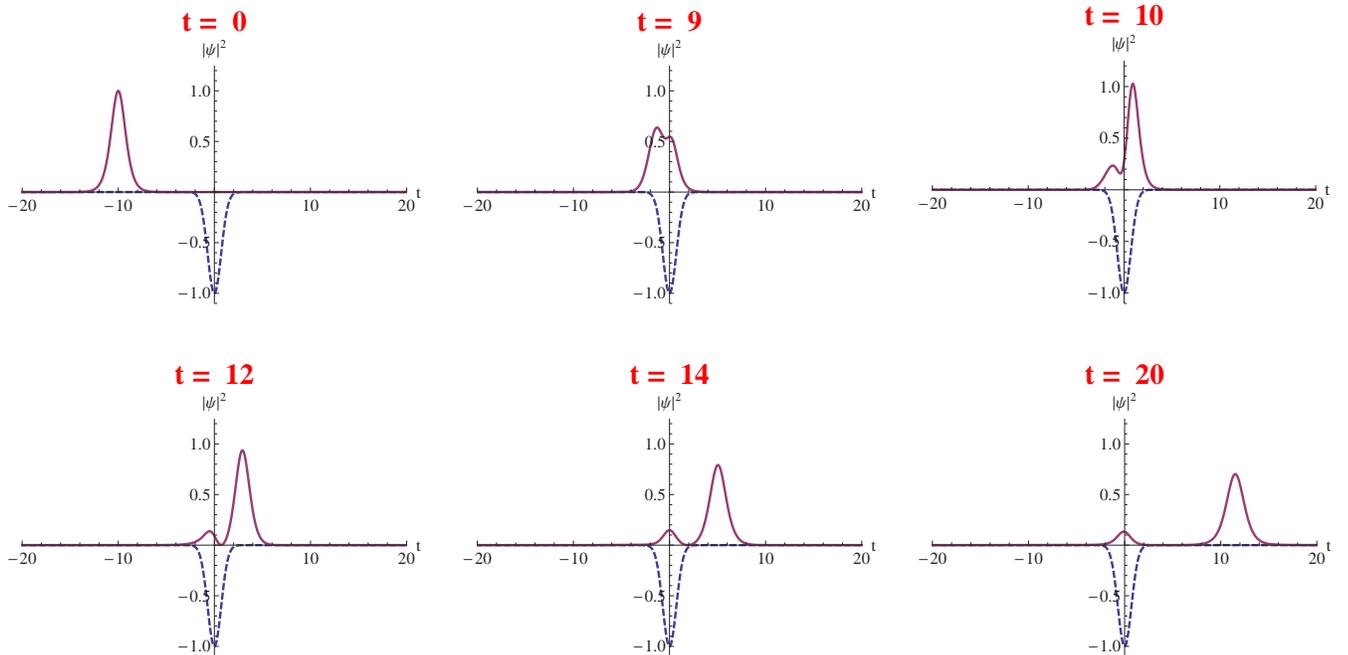


Figure 2.5: Snapshots of the soliton (represented by a solid line) scattering by a Gaussian potential well (shown by dashed line). The quantum bound state in the potential well becomes occupied when soliton traverses it. Some part of the matter wave is trapped by the potential well. Parameters for the soliton and potential well: $A = 1$, $v = 1$, $x_0 = -10$, $V_0 = 1$, $\alpha = 1$.

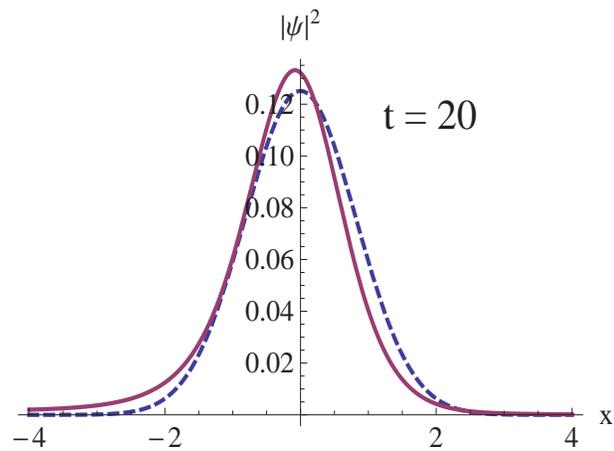


Figure 2.6: Comparison of the ground state wave function, calculated using the variational method (dashed line) and as found from numerical solution of the GPE (2.21) (solid line) for $t = 20$. The amount of matter wave trapped by the potential well has the norm $N_0 = 0.256$. Parameters for the variational ground state: $V_0 = 1$, $\alpha = 1$, $b = 0.3742$, $A_0 = (2b/\pi)^{1/4}N_0^{1/2}$.

Chapter 3

Scattering on the Dirac delta function potential well

The Dirac delta function is defined as follows:

$$\delta(x) = \begin{cases} 0, & \text{if } x \neq 0 \\ 1, & \text{if } x = 0 \end{cases} \quad \text{and} \quad \int_{-\infty}^{\infty} \delta(x) dx = 1. \quad (3.1)$$

We will consider a potential well of the form

$$V(x) = -V_0 \cdot \delta(x), \quad (3.2)$$

where V_0 is the strength of the delta function.

3.1 Calculation of bound state energy

The time dependent Schrödinger equation has the form

$$-\frac{\hbar^2}{2m} \frac{d^2\psi}{dx^2} - V_0\delta(x)\psi = E\psi. \quad (3.3)$$

If $E < 0$ then we will have a bound states, and if $E > 0$ we will have scattering states.

First consider bound states ($E < 0$) in the region where $x < 0$. Here $V(x) = 0$, so we have

$$\frac{d^2\psi}{dx^2} = -\frac{2mE}{\hbar^2}\psi = k^2\psi, \quad \text{with } k = \frac{\sqrt{-2mE}}{\hbar}. \quad (3.4)$$

A general solution to this equation has the form

$$\psi(x) = Ae^{-kx} + Be^{kx}. \quad (3.5)$$

But we know that k is positive (because E is negative), so the Ae^{-kx} term becomes infinite as $x \rightarrow -\infty$. Therefore, we have for $x < 0$

$$\psi(x) = Be^{kx}. \quad (3.6)$$

Now we look at the area where $x > 0$. In this region we have the general solution of the form

$$\psi(x) = Fe^{-kx} + Ge^{kx}, \quad (3.7)$$

which reduces to

$$\psi(x) = Fe^{-kx}, \quad (3.8)$$

since $Ge^{kx} \rightarrow \infty$ as $x \rightarrow \infty$.

We now have two solutions for $\psi(x)$, for $x < 0$ and $x > 0$. We can find the solution at $x = 0$ by noting the following boundary conditions: ψ is always continuous, and $d\psi/dx$ is continuous everywhere, except the origin, where $V(x)$ is infinite.

The continuity of ψ tells us that $F = B$ at $x = 0$. From normalization we can find F and B :

$$F^2 \int_0^\infty e^{2kx} dx = \frac{1}{2}, \quad F = \sqrt{k}. \quad (3.9)$$

Finally we need to consider the region containing the delta function potential. We will try to solve the Schrödinger equation by integrating from $-\varepsilon$ to ε , either side of $x = 0$:

$$-\frac{\hbar^2}{2m} \int_{-\varepsilon}^{\varepsilon} \frac{d^2\psi}{dx^2} dx + \int_{-\varepsilon}^{\varepsilon} V(x)\psi(x)dx = E \int_{-\varepsilon}^{\varepsilon} \psi(x)dx. \quad (3.10)$$

The right hand side becomes zero as $\varepsilon \rightarrow 0$, so we have

$$\frac{d\psi}{dx} \Big|_{-\varepsilon}^{\varepsilon} = \frac{2m}{\hbar^2} \cdot \int_{-\varepsilon}^{\varepsilon} V(x)\psi(x)dx \quad (3.11)$$

The result of the integration is

$$\Delta \left(\frac{d\psi}{dx} \right) = -\frac{2mV_0}{\hbar^2} \psi(0).$$

We know that

$$\psi(x) = \sqrt{k}e^{-kx} \text{ for } x > 0, \text{ so } \left. \frac{d\psi}{dx} \right|_+ = -k\sqrt{k}, \quad (3.12)$$

and

$$\psi(x) = \sqrt{k}e^{kx} \text{ for } x < 0, \text{ so } \left. \frac{d\psi}{dx} \right|_- = k\sqrt{k}, \quad (3.13)$$

So

$$\Delta \left(\frac{d\psi}{dx} \right) = -2k\sqrt{k}, \quad \text{and at } x = 0 \quad \psi(0) = \sqrt{k}.$$

Combining the last results we get

$$-2k\sqrt{k} = -\frac{2mV_0}{\hbar^2} \sqrt{k}, \quad k = \frac{mV_0}{\hbar^2}.$$

The corresponding energy is

$$E = -\frac{\hbar^2 k^2}{2m} = -\frac{mV_0^2}{2\hbar^2} \quad (3.14)$$

The wave function can be written as

$$\psi(x) = \frac{\sqrt{mV_0}}{\hbar} e^{-mV_0|x|/\hbar^2}. \quad (3.15)$$

There is only one bound state for any given value of V_0 .

3.2 Numerical results for Dirac delta function well

Dynamics of the soliton interacting with the Dirac delta function potential well $V(x) = -V_0\delta(x)$ is described by the dimensionless one-dimensional Gross-Pitaevskii equation

$$i\psi_t + \frac{1}{2}\psi_{xx} - V_0\delta(x)\psi + |\psi|^2\psi = 0 \quad (3.16)$$

As initial condition to Eq. (3.16) we use again one soliton solution

$$\psi(x) = A \operatorname{sech}[A(x - x_0)] \cdot e^{iv(x-x_0)}, \quad (3.17)$$

with amplitude A placed at some distance x_0 from the potential well and set in motion with velocity v .

Snapshots of the scattering process is shown in Fig. 3.1.

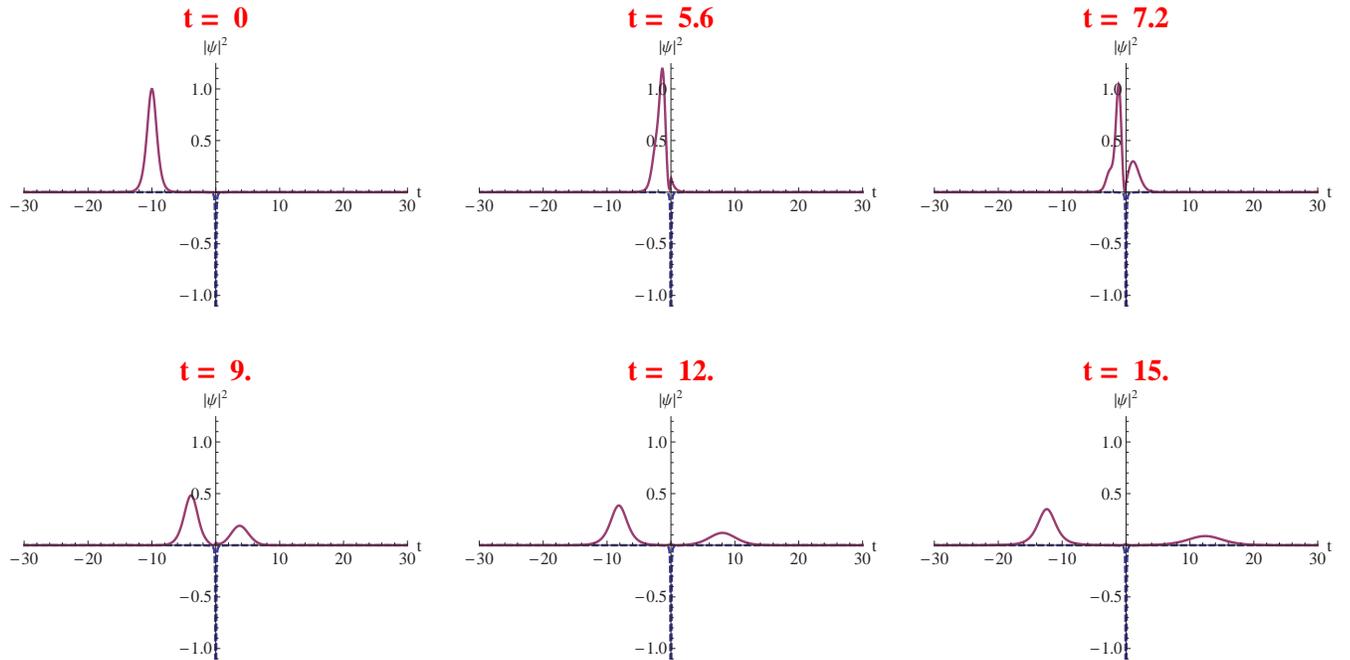


Figure 3.1: Snapshots of the soliton (represented by a solid line) scattering by a Dirac delta function well (shown by dashed line). The quantum bound state in the potential well becomes occupied when soliton traverses it. Some part of the matter wave is trapped by the potential well. Parameters for the soliton and potential well: $A = 1$, $v = 1.5$, $x_0 = -10$, $V_0 = 1$.

Occupation of the single bound state of the delta function potential well as a result of soliton scattering is illustrated in Fig. 3.2.

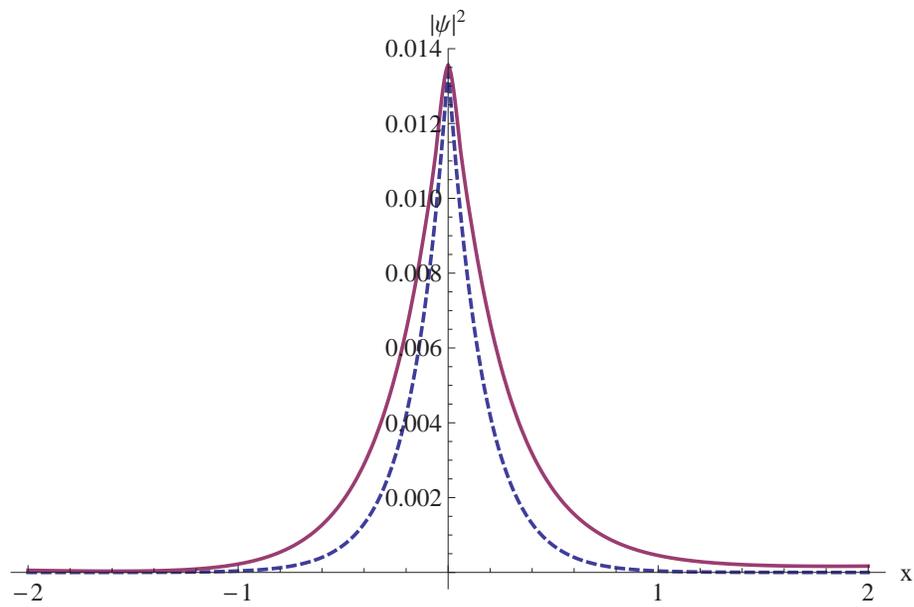


Figure 3.2: Comparison of the bound state wave function (3.15) of the Dirac delta function potential well (red solid line) with the result of numerical solution of the GPE (3.16) (blue dashed line) for $t=20$ in units of $\hbar = m = 1$. The amount of matter wave trapped by the potential well has the norm $N_0 = 0.0096$.

Conclusions

In the result of investigations conducted in this work we came to following conclusions:

1. Scattering of a matter wave soliton by potential well gives rise to population of quantum states in this potential well.
2. Numerical simulation of the soliton scattering by Gaussian potential well shows, that population of the ground state takes place.
3. There is only one bound state in the delta function potential well for any given value of the strength V_0 . Population of this state during scattering of a matter wave soliton has been investigated.

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