Practical Nonlinear Physics

A Collection of Interesting Problems
in Modelling Nonlinear Optics, Cold Atoms
and Polariton Condensates

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Contents

Preface

Nonlinear Physics is a newly developed field which had attracted much attention from community of physicists over the second half of the last century. Many interesting phenomena (e.g. solitons, modulational instability, symmetry breaking, ...) were realized universal properties of nonlinear systems as they were observed in many different fields in physics such as plasma physics, optics, hydrodynamics, condensed matters, Bose-Einstein condensates.
In the theoretical point of view, the detail analysis of nonlinear phenomena is very difficult because the superposition principle is not valid. There are only few exact analytical approaches have been developed for nonlinear systems (Inverse Scattering Transform, Hirota bilinear method, Painleve test,...). These methods are limited and only applied to fully integrable systems. For more general cases, some approximated analytical techniques should be used. The popular tools for studies of nonlinear systems are numerical methods.
The aim of this lecture is to give brief introduction about nonlinear phenomena to undergraduate students, and then, provided them some selected projects for practice. The students mainly focus on analyzing nonlinear effects in optics, Bose-Einstein Condensates and Polariton condensates which are the subjects of our research group. The phenomena discussed in this lecture are usually observed in nonlinear systems, each is presented with clearly physical explanation, detail derivation and provided programs with Python codes. After this lecture, the students will be familiar with some popular techniques for dealing with nonlinear systems, such as the imaginary time propagation method, the split-step Fourier method, linear stability analysis, variational approximation,... If some of them are interested in nonlinear physics, they can join our group and start doing research works very quickly.
This lecture is a collection of projects which were selected from research results of our group in the Faculty of Physics - University of Warsaw along the last two decades.

Prof. *Marek Trippenbach* (Warsaw, Poland),

Dr. *Nguyen Viet Hung* (Hanoi, Vietnam).

Chapter 1

1. Fourier methods in numerical studies

The aim of this chapter is to give an introduction to numerical and analytical methods which are mostly used in the following chapters of the book.

1.1 Fourier transform

We present briefly the definition of the Fourier transform, Fast Fourier Transform algorithm and applications of the Fourier transform to find numerically derivatives and solve partial differential equations. Fourier transform is defined here as follows

$$F(k) \equiv \mathcal{F}(f)(k) = \int_{-\infty}^{+\infty} f(x) \exp(-2\pi ikx)\, dx.$$

$$f(x) = \int_{-\infty}^{+\infty} \mathcal{F}(f)(k) \exp(2\pi ikx)\, dk = . \int_{-\infty}^{+\infty} F(k) \exp(2\pi ikx)\, dk$$

Basic properties include:

i) *linearity*

ii) *Dirac'c Function*

$$\delta(x) = \int_{-\infty}^{+\infty} e^{2\pi ikx}\, dk$$

iii) *Fourier transform of the product of functions*

$$\int f_1(x) f_2(x) \exp(-2\pi ikx)\, dx = \int F_1(k_1) F_2(k - k_1)\, dk_1.$$

Fourier transform of the product of functions is called convolution.

iv) Transform of real functions

$$f(x) = f^*(x)$$

$$f(x) = \int e^{2\pi ikx} F(k)\, dk = \int e^{-2\pi ikx} F^*(k)\, dk$$

$$F(k) = F^*(-k)$$

v) *Fourier transform of the Gaussian function* Consider Gaussian function

$$f(x) = \sqrt[4]{2\sigma/\pi} e^{-x^2\sigma}$$

. This function is normalized to one; integral of the modulus square is equal to 1

$$\int_{-\infty}^{+\infty} |f(x)|^2 \, dx = 1$$

and we are using property $\int_{-\infty}^{\infty} exp(-x^2)dx = \sqrt{\pi}$. It is easy to obtain

$$F(k) = \sqrt[4]{2\pi/\sigma} \exp(-\pi^2 k^2/\sigma)$$

This function is normalized to one, as expected. useful formula

$$\frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} e^{-\lambda x^2 + i\mu x} \, dx = \frac{1}{2\lambda} e^{-\mu^2/4\lambda}$$

vi) *Normalization in the configuration space and Fourier space, Parseval's theorem*

$$\int_{-\infty}^{+\infty} |f(x)|^2 \, dx$$

$$\begin{aligned}
&= \int_{-\infty}^{+\infty} dx \int_{-\infty}^{+\infty} F^*(k_1) e^{-2\pi i k_1 x} \, dk_1 \int_{-\infty}^{+\infty} F(k_2) e^{-2\pi i k_2 x} \, dk_2 \\
&= \int_{-\infty}^{+\infty} dk_1 \int_{-\infty}^{+\infty} dk_2 F^*(k_1) F(k_2) \int e^{-2\pi i (k_1 - k_2) x} \, dx \\
&= \int_{-\infty}^{+\infty} dk_1 \int_{-\infty}^{+\infty} dk_2 F^*(k_1) F(k_2) \delta(k_1 - k_2) \\
&= \int dk_1 F^*(k_1) F(k_1)
\end{aligned}$$

vii) *Rectangular Pulse of the length* Δt

$$f(t) = \begin{cases} A & \text{if } -\Delta t/2 \le t \le \Delta t/2; \\ 0 & \text{otherwise.} \end{cases}$$

In this case

$$F(\omega) = \int_{-\infty}^{+\infty} f(t) e^{-2\pi i \omega t} \, dt$$

and we obtain

$$\int_{-\infty}^{+\infty} f(t) e^{-2\pi i \omega t} \, dt = \int_{-\Delta t/2}^{+\Delta t/2} A e^{-2\pi i \omega t} \, dt$$

$$= -\frac{A}{2\pi i \omega} \, e^{-2\pi i \omega t} \Big|_{-\Delta t/2}^{+\Delta t/2} = \frac{A}{\pi \omega} \sin \pi \omega \Delta t$$

If the signal f(t) is normalized to one:

$$\int_{-\infty}^{+\infty} f(t)\,dt \Rightarrow A.\Delta t = 1 \Rightarrow A = \frac{1}{\Delta t}$$

$$F(\omega) = \frac{\sin(\omega\pi\Delta t)}{\pi\omega\Delta t}$$

Note that the first zeros occurs when $\pi\Delta t\omega_0 = \pm\pi \Rightarrow \omega_0 = \pm\frac{1}{\Delta t}$. If we take it for the width in the Fourier space we obtain "Heisenberg principle" $\omega_0\Delta t = constant$.

In the limit $\Delta t \to 0$ we obtain Dirac's delta function.

viii) *Lorentz's Spectrum*
Consider function $f(t) = e^{-\Gamma|t|}$. It's Fourier transform reads

$$F(\omega) = \int_{-\infty}^{+\infty} e^{-\Gamma|t|}e^{-2\pi i\omega t}\,dt = \int_{-\infty}^{0} e^{\Gamma t-2\pi i\omega t}\,dt + \int_{0}^{+\infty} e^{-\Gamma t-2\pi i\omega t}\,dt$$

$$\frac{1}{\Gamma-2\pi i\omega}\,e^{(\Gamma-2\pi i\omega)t}\Big|_{-\infty}^{0} + \frac{-1}{\Gamma+2\pi i\omega}\,e^{-(\Gamma+2\pi i\omega)t}\Big|_{0}^{+\infty}$$

$$\frac{1}{\Gamma-2\pi i\omega} + \frac{1}{\Gamma+2\pi i\omega} = \frac{2\Gamma}{\Gamma^2+(2\pi\omega)^2}$$

This is so-called Lorentz's function (or Lorentz spectrum, very important in optics), $F(0) = \frac{2}{\Gamma}$. Its full width at half maximum (FWHM) can be found as

$$F(\omega_0) = \frac{1}{2}F(0) = \frac{1}{\Gamma} = \frac{2\Gamma}{\Gamma^2+(2\pi\omega_0)^2}$$

It occurs when $2\pi\omega_0 = \Gamma$.

ix) *Infinite pulse* $f(t) = \cos(\omega_0 t)$

$$F(\omega) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{+\infty} \cos(\omega_0 t)e^{-i\omega t}\,dt = \frac{1}{2\sqrt{2\pi}}\int_{-\infty}^{+\infty} [e^{i\omega_0 t}e^{-i\omega t} + e^{-i\omega_0 t}e^{-i\omega t}]\,dt$$

$$= \frac{1}{2\sqrt{2\pi}}\int_{-\infty}^{+\infty} [e^{i(\omega_0-\omega)t}e^{-i(\omega_0+\omega)t}]\,dt = \frac{1}{2}[\delta(\omega_0-\omega)+\delta(\omega_0+\omega)]$$

x) $f(t) = M(t)\cos(\omega_0 t)$ where

$$M(t) = \begin{cases} A & -\Delta t/2 \le t \le \Delta t/2 \\ 0 & \text{otherwise} \end{cases}$$

$$\sqrt{2\pi}F(\omega) = \frac{A}{2}\int_{-\Delta t/2}^{+\Delta t/2} [e^{i(\omega_0-\omega)t} + e^{-i(\omega_0+\omega)t}]\,dt$$

$$= \frac{A}{2}\,\frac{e^{i(\omega_0-\omega)t}}{i(\omega_0-\omega)}\Bigg|_{-\Delta t/2}^{+\Delta t/2} + \frac{A}{2}\,\frac{e^{-i(\omega_0+\omega)t}}{-i(\omega_0+\omega)}\Bigg|_{-\Delta t/2}^{+\Delta t/2}$$

$$= A\left\{\frac{\sin(\omega_0-\omega)\Delta t/2}{(\omega_0-\omega)} + \frac{\sin(\omega_0+\omega)\Delta t/2}{(\omega_0+\omega)}\right\}$$

xi) *differentiation.*

$$\mathcal{F}\left(\frac{d}{dx}f(x)\right(k) = (ik)\mathcal{F}(f)(k)$$

$$\frac{d}{dx}f(x) = \frac{1}{\sqrt{2\pi}}\int (ik)e^{ikx}\mathcal{F}(f)(k)\,dk$$

This formula is important for FFT!

1.2 Using FFT for solving PDE

1.2.1 Split Step Method I: evolution

In this section we demonstrate split-step Fourier method for hermitean evolution.

We use split - Fast Fourier method (FFT) to solve Schrodinger equation. The SSF probably is the most widely used method for numerical solution of the NLS like equations [24, 25] because it is stable scheme and it can be performed very fast by means of the Fast Fourier Trasform. We again consider the NLS equation in the abstract form

$$\partial\Psi(x,t)/\partial t = -(iD(x) + iV(x))\Psi. \tag{1.1}$$

Here $D(x)$ stands for operator of partial derivatives in the temporal variables (as we have seen above, dispersion terms are of this kind) and $V(x)$ represents potential term in the equation of motion. We can rewrite it to show explicitly small step change in time of the wavefunction

$$\Psi(x, t+\delta t) \approx -i\left(D(x) + V(x)\right)\delta t\Psi + \Psi(x,t). \tag{1.2}$$

There is however better approximation. We can integrate equation (2.3)and using Baker Hausdorf formula we can write

$$\Psi(x,t+\delta t) = \exp[-i\left(D(x)+V(x)\right)\delta t]\Psi \approx \exp[-iD(x)\delta t]\ \exp[-iV(x)\delta t]\ \Psi(x,t) =$$
$$= \exp[-iD(x)\delta t]\ \Psi'(x,t) = \exp[-iD(x)\delta t]\int dk\ \Psi'(k)\,exp(ikx) = \int dk\,\Psi'(k)\ exp(-i\delta t k^2)\ \exp(ikx).$$

We can even find eigenstate of the system and eigen-energy using similar method. Take reasonable initial state normalized to one $\int|\Psi_0(x)|^2dx = 1$. Propagate over the distance δt, omitting factor i in Eq. (1.3). Norm will not be preserved. So we renormalize, restoring norm equal to one. Ane we continue this procedure iteratively. See what you get. Try another potential.

1.2.2 Imaginary Time Method. Ground state.

In this part we will present basics of the so-called *imaginary time method* (ITM). This is an important numerical tool used to generate stationary states of nonlinear systems. In this section we will interchange the role of z and t variables. We will consider time evolution of the system that depends on z, at each instant of time. Well, after all this method is called "imaginary time"!

Here we first describe background of this algorithm for the linear cases and then extend it to the nonlinear situations. There is no rigorous proof for the extension but in fact the ITM works very efficiently :).

For a Hamiltonian $\widehat{H}$ (assumed to be bounded from below), the eigenvalue problem is written as follows

$$\widehat{H}\phi_j(x) = E_j\phi_j(x). \tag{1.3}$$

Applying the ITM for that Hamiltonian, we start by introducing an "ansatz" wavefunction $\Psi_0(x)$. The algorithm drives this wavefunction into the ground state $\phi_0(x)$. The formal expansion of $\Psi_0(x)$ in the complete set of $\{\phi_j(x)\}$ is

$$\Psi_0(x) = \sum_{j=0}^{\infty} a_j\phi_j(x). \tag{1.4}$$

Assuming $\Psi_0(x) = \Psi_0(x, t = 0)$ the time evolution is performed by an unitary operator $\widehat{U}$

$$\begin{aligned} \Psi(x,t) = \widehat{U}(t)\Psi_0(x) &= e^{-\frac{i}{\hbar}\widehat{H}t}\sum_{j=0}^{\infty} a_j\phi_j(x) \\ &= \sum_{j=0}^{\infty} a_j e^{-\frac{i}{\hbar}E_j t}\phi_j(x). \end{aligned} \tag{1.5}$$

The idea is to implement "time evolution" in the imaginary time: $it \Rightarrow \tau$ (t is real time)

$$\Psi(x,\tau) = \sum_{j=0}^{\infty} a_j e^{-E_j\tau/\hbar}\phi_j(x). \tag{1.6}$$

Unlike real time evolution, the "imaginary time evolution" is introducing exponential damping - factors: $E_j\tau/\hbar$. The terms correspond to higher energies are damped faster than low energy ones and the ground state is damped least. For $\tau \to \infty$ all components approach zero, therefore, to avoid this trivial result, one has to renormalize the wavefunction after each time step $\Delta\tau$. By doing so, the wavefunction after each time steps reads

$$\Psi(x,\Delta\tau) = \sum_{j=0}^{\infty} \frac{a_j e^{-E_j\Delta\tau/\hbar}}{\sqrt{\sum_{k=0}^{\infty}|a_k|^2 e^{-2E_k n\Delta\tau/\hbar}}}\phi_j(x). \tag{1.7}$$

Thus, this algorithm converges any initial wavefunction $\Psi_0(x)$ to the ground state $\phi_0(x)$, in other words it "purifies" the state.

Now we desribe the algorithm.

$$i\Psi_t = -\beta\Psi_{xx} + V(x)\Psi, \tag{1.8}$$

which can be rewritten as

$$\Psi_t = -i\left(\widehat{D} + V(x)\right)\Psi \tag{1.9}$$

Here $\widehat{D}$ is linear operator given by

$$\widehat{D} = -\beta\left(\frac{\partial^2}{\partial x^2}\right), \tag{1.10}$$

Applying the ITM for the equation (1.9), we introduce an trial wavefunction $\Psi_0(x)$ with given norm

$$\int_{-\infty}^{\infty} |\Psi_0(x)|^2 \mathrm{d}x = 1. \tag{1.11}$$

Notice that if the norm of the wavefunction is equal to A, then we can reformulate the whole problem using nonlinear coefficient equal to Ag. Evolution of the system in small interval time Δt is approximated to

$$\Psi(x, \Delta t) \approx e^{-i\Delta t\left(\widehat{D}+V(x)\right)}\Psi_0(x) \approx e^{-i\Delta t\widehat{D}}e^{-i\Delta tV(x)}\Psi_0(x). \tag{1.12}$$

The basic idea of this approximation is that over sufficiently small interval Δt the linear and non-linear terms can be assumed to act independently. Analogously to the linear case, if we implement "time evolution" in the imaginary regime: $i\Delta t \Rightarrow \Delta\tau$ then the result takes

$$\Psi(x, \Delta\tau) \approx e^{-\Delta\tau\widehat{D}}e^{-\Delta\tau V(x)}\Psi_0(x). \tag{1.13}$$

Again, we observe exponential damping of amplitude of the wavefunction. To avoid this fact, we renormalize the wavefunction as the following way

$$\widetilde{\Psi}(x, \Delta\tau) = \sqrt{\frac{1}{\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}|\Psi(x, \Delta\tau)|^2 \mathrm{d}x\mathrm{d}y}}\Psi(x, \Delta\tau). \tag{1.14}$$

This new wavefunction is used as $\Psi_0(z)$ for evolution in next iteration and propagation by the next interval of time $\Delta\tau$. In applications, we repeated the computations (1.13) and (1.14) until convergence is reached.

1.3 Linear propagation of Gaussian pulses. Exactly solvable model

The linear propagation for the envelope function $A(z, \tau)$ reads

$$\frac{\partial A}{\partial z} = -\frac{1}{v_g}\frac{\partial A}{\partial \tau} - i\beta_2\frac{\partial^2 A}{\partial \tau^2} \tag{1.15}$$

We will show here detail analytical calculations for the special case, when the initial pulse $A(0, \tau)$ takes the Gaussian form. The results of this calculation of linear propagation of the Gaussian pulse will be compared with numerical simulation using the split-step Fourier method. We observe very good agreement between them.

We write an optical impulse in the form of central frequency and slowly varying envelope $E(z, t) = A(z, t)\exp(i(\frac{n(\omega_0)\omega_0}{c}z - \omega_0 t))$. where we used dispersion relation - relation between central k vector and central frequency. Next we do the decomposition of our wave - pulse - into plane waves. It is called Fourier Transform :)

$$E(z, t) \;=\; \frac{1}{2\pi}\int d\omega E(\omega)\exp\left[i\left(\frac{n(\omega)\omega}{c}z - \omega t\right)\right] \tag{1.16}$$

and we can write envelope of the pulse as

$$A(z,t) = \frac{1}{2\pi}\int d\omega E(\omega)\exp\left[i\left(\frac{n(\omega)\omega - n(\omega_0)\omega_0}{c}z - (\omega-\omega_0)t\right)\right] \tag{1.17}$$

To obtain equation of motion for the wavepacket - pulse we can evaluate derivative in the direction of propagation (or in time if we talk about the dynamics) Superposition of waves from above equation gives us

$$\frac{\partial}{\partial z}A(z,t) = \frac{i}{2\pi c}\int d\omega E(\omega)(n(\omega)\omega - n(\omega_0)\omega_0) \times \\ \times \exp\left[i\left(\frac{n(\omega)\omega - n(\omega_0)\omega_0}{c}z - (\omega-\omega_0)t\right)\right]. \tag{1.18}$$

We can rewrite RHS of this equation, $E(\omega)$ which has narrow maximum at ω_0 ; we can expand $[n(\omega)\omega - n(\omega_0)\omega_0]$ in the Taylor series $[n(\omega)\omega - n(\omega_0)\omega_0] = \beta_1(\omega_0)(\omega-\omega_0) + \beta_2(\omega_0)(\omega-\omega_0)^2 + \beta_3(\omega_0)(\omega-\omega_0)^3 + ...$ where β_l are defined as $\beta_l = \frac{d\beta_{l-1}}{d\omega} = \frac{d^l\beta_0}{d\omega^l}$ for $l > 0$ and condition $\beta_0 = \frac{\omega n}{c}$. It does not have zero order (constant) term in variable $(\omega-\omega_0)$ and we notice that in the Fourier domain we can get each of the polynomial term by differentiation according to the rule $(\omega-\omega_0)^n \equiv i^n\frac{\partial^n}{\partial t^n}$ and we finally obtain differential equation

$$\frac{\partial}{\partial z}A(z,t) = \left(-\beta_1\frac{\partial}{\partial t} - \frac{i}{2}\beta_2\frac{\partial^2}{\partial t^2} + \frac{1}{6}\beta_3\frac{\partial^3}{\partial t^3} + ...\right)A(z,t) \tag{1.19}$$

To understand β_1 owe restrict to the first

$$\frac{\partial}{\partial z}A(z,t) + \beta_1\frac{\partial}{\partial t}A(z,t) = 0 \tag{1.20}$$

It describe one dimensional motion without change of shape $\frac{1}{\beta_1}$ When we add second term

$$\frac{\partial}{\partial z}A(z,t) + \beta_1\frac{\partial}{\partial t}A(z,t) + \frac{i}{2}\beta_2\frac{\partial^2}{\partial t^2}A(z,t) = 0 \tag{1.21}$$

$$\frac{\partial}{\partial z}A(z,\omega) = \frac{i}{2}\beta_2\omega^2 A(z,\omega), \tag{1.22}$$

which has easy solution

$$A(z,\omega) = \exp(\frac{i}{2}\beta_2\omega^2 z)A(0,\omega). \tag{1.23}$$

In the last part we find $A(0,\omega)$, which is Ft of initial pulse. For Gaussian pulse $A(0,t) = A_0\exp(-\frac{1}{2}\frac{t^2}{t_0^2})$ is known and equal to $A(0,\omega) = \frac{A_0 t_0}{\sqrt{2\pi}}\exp(-\frac{1}{2}\omega^2 t_0^2)$. If we apply it in Eq (1.23) and calculate inverse FT

$$A(z,t) = A_0\frac{t_0}{\sqrt{t_0^2 - i\beta_2 z}}\exp\left(-\frac{1}{2}\frac{(t-\beta_1 z)^2}{t_0^2 - i\beta_2 z}\right) \tag{1.24}$$

Problem

i) Compare solution (2.10) with numerical solution obtained by split step method.

ii) Do analytical calculations for `chirp`, described by $A(0,\omega) = \frac{A_0 t_0}{\sqrt{2\pi}}\exp\left(-\frac{1}{2}(1+i\alpha)\omega^2 t_0^2\right)$

iii) Find the shape of the impulse at distance L, when $\beta_2(\omega_0) = 0$ and we need to include $\beta_3(\omega_0)$.

Solving harmonic oscillator.

In this section we practice solving Schrodinger equation. We start with harmonic oscillator. We will do time evolution according to Schrodinger equation and will find ground state. Eventually we can observe oscillation of quantum wave-packet trapped in a harmonic potential and solve dynamics in different type of potentials.

Scattering of wave-packets from wells and barriers

We show here the way to determine the bound states of particles in well potentials (single well and double well).
We also show here the results of simulation for scattering of particles through step barriers.

Chapter 2

Nonlinear Schrodinger equation and optical solitons

2.1 Propagation equation of pulses in optical media

Starting from Maxwell equations, we apply the so called Slowly-Varying-Envelope-Approximation (or paraxial approximation) to derive linear propagation equations of pulses (or beams) in isotropic (bulk) optical media.
Secondary, assuming the weak (and instantaneous) nonlinear response of the isotropic (Kerr) media, we derive the nonlinear propagation equation for pulses (or beams). These equations take the Nonlinear type-Schrodinger equation.

2.2 Nonlinear propagation of pulses in Kerr media

The nonlinear propagation equation of pulses is written as the following

$$i\frac{\partial A}{\partial z} = \frac{1}{v_g}\frac{\partial A}{\partial \tau} + i\beta_2\frac{\partial^2 A}{\partial \tau^2} + n_2|A|^2 A. \tag{2.1}$$

The important quantity is the norm of pulse

$$N = \int_{-\infty}^{\infty} |A(z,\tau)|^2 d\tau. \tag{2.2}$$

2.3 Numerical methods for the Nonlinear Schrodinger equation. Split Step Method II. Nonlinearity

In this section we show here the split-step Fourier method for NLSE which is the tool for numerical study of nonlinear propagation.

We use split - step Fourier method (SSF) to test stability and to model soliton collisions. The SSF probably is the most widely used method for numerical solution of the NLS like equations [24, 25] because it is stable scheme and it can be performed very fast by means of the Fast Fourier Trasform. We again consider the NLS equation in the abstract form

$$\partial\Psi(z,t)/\partial z = -(iD(t) + ig|\Psi|^2)\Psi. \tag{2.3}$$

Here $D(t)$ stands for operator of partial derivatives in the temporal variables (as we have seen above, dispersion terms are of this kind) and $g|\Psi|^2$ is representing nonlinear term in the equation of motion. We can rewrite it to show explicitly small step in time change of the wavefunction

$$\Psi(z+\delta z,t) \approx -i\left(D(t) + g|\Psi|^2\right)\Psi \times \delta z \Psi(z,t) + \Psi(z,t). \tag{2.4}$$

There is however better approximation. WE can integrate equation (2.3)and using Baker Hausdorf formula we can write

$$\Psi(z+\delta z,t) = \exp[-i\left(D(t) + g|\Psi|^2\right)\delta z]\Psi \approx \exp[-iD(t)\delta z]\ \exp[-ig|\Psi|^2\delta z]\ \Psi(z,t). \tag{2.5}$$

Chapter 3

Bose-Einstein Condensations within mean-field theory

3.1 The Gross-Pitaevskii equation

Starting from full Hamiltonian of the system of weakly-interacting (identical) bosons and applying variational ansatz for the many-body wave function (minimizing the energy functional), we end up with the Gross-Pitaevskii equation for the wave function $\Psi(x,t)$ of condensates (in the dimensionless form)

$$i\frac{\partial \Psi}{\partial t} = -\frac{1}{2}\frac{\partial^2 \Psi}{\partial x^2} + V(x)\Psi + g|\Psi|^2\Psi. \tag{3.1}$$

where $V(x)$ is external potential. In this case when you apply split step method you have to add potential $V(x)$ to the nonlinear part, since they both "act" in the configuration space.

3.2 The case of attractive interaction: Matter-wave solitons

In the situation when the interaction between atoms is attractive we have $g < 0$. In this case the Gross-Pitaevskii supports bright-soliton solutions.

We put extenal potental $V(x) = 0$ and find stable solution. Soliton wil be described by

$$\Psi(x,t) = Asech(Ax)\exp(iA^2/2t) \tag{3.2}$$

3.3 The case of repulsive interaction: Thomas-Fermi approximation

In the case of repulsive interaction we have $g > 0$ and we consider harmonic potential $V(x) = ax^2$. For the situation when the energy associated with nonlinear interaction is much bigger than the kinetic energy, we can neglect the kinetic term and obtain the analytic (parabolic) form of the density of condensate. This is the so-called Thomas-Fermi approximation.

We will show here some analytic calculations to obtain approximated wave function, and then, perform numerical calculation for full Gross-Pitaevskii equation (using imaginary time method) to get stationary state. Finally we compare these two results. If we neglect kinetic energy term and look for stationary solutions we need to consider

$$\mu\Psi = V(x)\Psi + g|\Psi|^2\Psi, \tag{3.3}$$

which, after we devide by Ψ will give

$$|\Psi| = \sqrt{\frac{\mu - V(x)}{g}} \tag{3.4}$$

when expression under the square root is positive ($|x| \leq R$, and $\mu = aR^2$) and zero otherwise. Now we need to find μ. To this end we notice that Ψ is normalized to one,

$$1 = \int |\Psi(x)|^2 dx. \tag{3.5}$$

Integral is only extended over the region where wavefunction is positive. After simple algebra we obtain $R^3 = 3g/4a$ and $\mu = \sqrt[3]{a(3g/4)^2}$. Now we can use imaginary time method (starting from Gaussian function to obtain Ψ and compare it with analytic expression found above.