



GEORG-SIMON-OHM
HOCHSCHULE NÜRNBERG

- Project work

Gross Pitaevskii equation for the description of Bose-Einstein condensate.

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1. Introduction:

In 1924-1925, a theory about a new state of matter was proposed by Albert Einstein and Satyendra Nath Bose called Bose-Einstein condensate (BEC). It is the condensed state of the gaseous particles, which upon cooled low enough, such that the sub-atomic or the constituent particles attains the same quantum state. And thus, this new state of matter is obtained. To attain such a state, certain condition must be fulfilled. In the first part of this work, the physics BEC is discussed.

The second part of the work discusses the Gross-Pitaevskii equation (GPE). It is the extended theory of the BEC. Here, the necessary requirement for the nonlinearity is discussed and the Gross-Pitaevskii equation is derived.

Since GPE is a nonlinear Schrödinger equation. It can be solved for both time dependent and nondependent cases. One of each cases is then discussed under condensed (Thomas- Fermi approximation) and dynamics of the condensed state (Soliton) is discussed. There are two cases, how the soliton arises, one considering the attraction between the bosons and another considering the repulsion between the bosons. Soliton developed by the repulsion between the bosons is discussed in this work and a MATLAB simulation of this soliton is presented.

2. Bose- Einstein condensate:

Before defining the physics and deriving the mathematical equation for the theory of the condensed state. It is insightful to discuss the nature of the sub-atomic particle, their characteristics and how are they distributed over an equilibrium state. Below are some terms discussed.

Bosons: Subatomic particles whose spin quantum number has integer value (0,1, 2...) are called Bosons. They are indistinguishable particles. we can't differentiate one Boson from another, and they have symmetric wave function.

$$(\psi_1 \cdot \psi_2) = (\psi_2 \cdot \psi_1) \quad 1$$

Fermions: Subatomic particles whose spin quantum number has half integer value (1/2, 3/2, ...) are called Fermions. Like Bosons they are also indistinguishable particles, but they have anti-symmetric wave function.

$$(\psi_1 \cdot \psi_2) = - (\psi_2 \cdot \psi_1) \quad 2$$

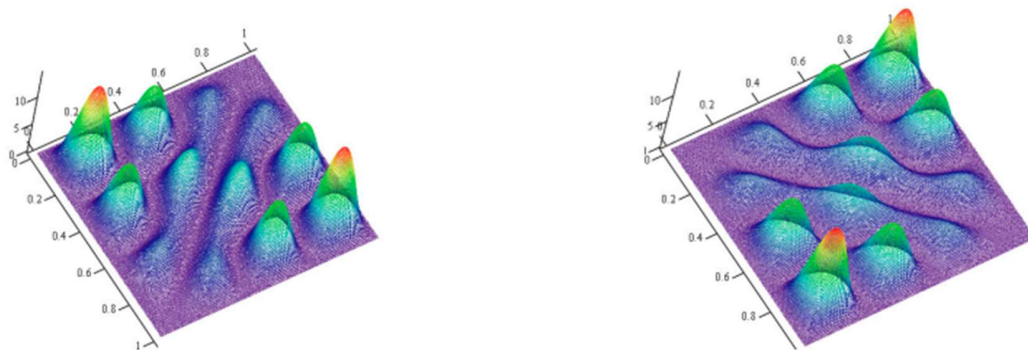


Figure 1: symmetric and anti-symmetric wave function.[1]

Chemical potential (μ): Chemical potential of a substance can be understood as the energy released or absorbed due to a change of particle number of the given species or during the phase transition.

$$\mu: \frac{dU}{dN} \quad 3$$

The density of molecules in air at normal temperature and atmospheric pressure is 10^{19} per cubic centimeter. To observe Bose-Einstein condensate, the particle density should be of around 10^{13} to 10^{15} per cubic meter. This kind quantum mechanical phenomena occurs at very low temperature around 10^{-5} K. In such lower temperature and low density, the gaseous state becomes more condensed, condensed enough to share the same quantum state. The particles in a system are distributed accordance to their energy level of a quantum state they occupied. Such a function is called partition function (Z). Certain particles sharing the same energy level makes this partition function. And is defined for a particular state (ϵ_i) as,

$$Z = \sum_i \exp(-\beta \epsilon_i) \quad 4$$

When the system is cooled enough, the chemical potential enters the equation. As the system gets cooled the particle tends to occupy the lowest energy states as well. Under such condition, the chemical potential needs to be considered. Chemical potential can be defined as energy per particle number for a given energy state. And there are limited number of particles in the lowest energy state. Chemical potential eventually becomes the energy posed by the collection of these particles.

Bosonic cloud when cooled to very low temperature, tends to get very condensed. When the temperature is sufficiently low enough, the energy of the occupied quantum state is low. Bosons whose spin quantum number is integer value can occupy the same quantum state unlike fermions. For non-interacting bosonic cloud with taking chemical potential in account, the total distribution function is then given by [2],

$$f^0(\epsilon_v) = \frac{1}{\exp(\epsilon_v - \mu/kT) - 1} \quad 5$$

The following distribution gives the number of particles occupied for a given energy state. If we consider the minimum energy to be 0, then chemical potential approaches the minimum value of the energy level.

$$\text{As, } \epsilon_v \longrightarrow 0$$

$$\mu \longrightarrow \epsilon_{min}$$

Then the distribution becomes the function the energy of the state,

$$f^0(\epsilon_{min}) = \frac{1}{\exp(\epsilon_{min}/kT) - 1} \quad 6$$

The term $\exp(\epsilon_{min}/kT)$ can be defined as the fugacity and the distribution function tends to be maximum when fugacity is unity.

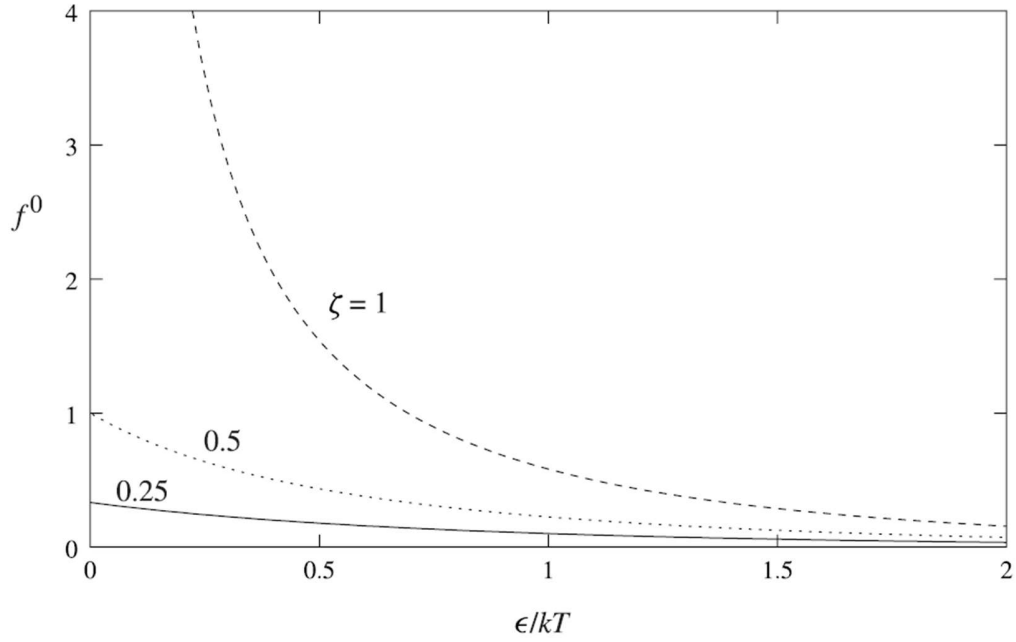


Figure 2: Distribution function per fugacity:[2]

The maximum occupancy is thus seen when fugacity is unity, and this phenomenon is the Bose-Einstein condensate. And the temperature corresponding is called the critical temperature. Above critical temperature the system loses the condensed state. This critical temperature depends on the particle density and the expression is given by: [2]

$$T_C = C \frac{\hbar^2 n^{2/3}}{mk} \quad 7$$

Where C is a numerical constant and has approximate value of 3.3. Above this temperature the chemical potential is much less than minimum energy and thus can be neglected. This critical temperature is depending upon the molecule and is different for the different system.

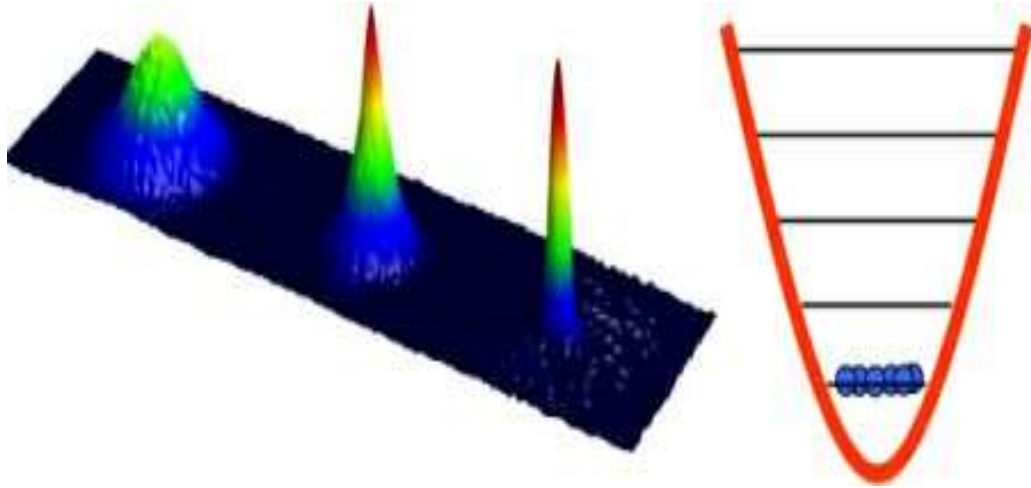


Figure 3: Figurative representation of the accumulation of bosons in the lowest energy state. [3]

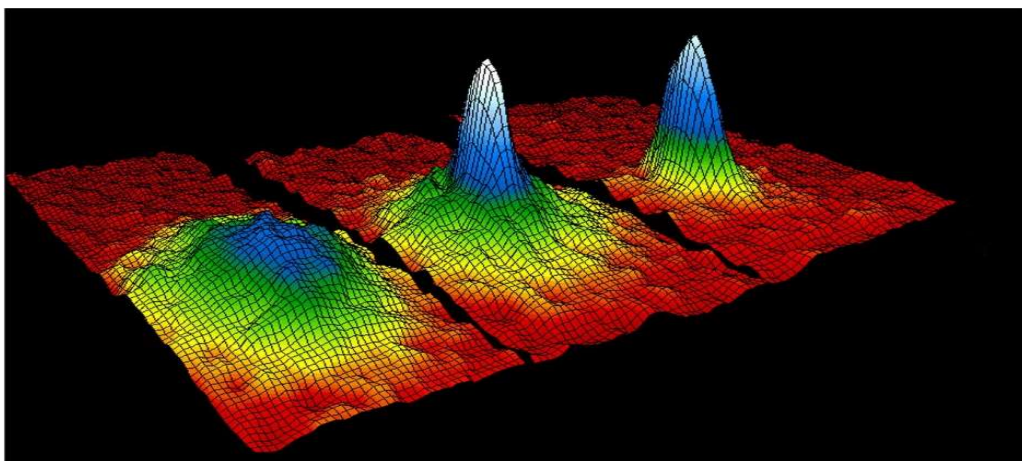


Figure 4: Bose-Einstein condensate for rubidium atom, just before condensed state(left) and condensed state (center and right). [4]

3. Gross-Pitaevskii Equation:

Bose-Einstein condensate described above is the theory for the non-interacting Bosons. But the theory is insufficient to describe the condensed state for non-uniform interacting bosonic gas. In order to describe the theory of non-uniform, interacting bosons, the interacting potential between the bosons need to be considered. When the scattering length of the trapped boson under a given potential is much less than the interspacing between them, then there is a considerable interacting potential between them. This interacting potential additional to the applied potential makes the Schrödinger equation non-linear and thus formed Non-linear Schrödinger equation is defined as Gross-Pitaevskii equation.

Gross-Pitaevskii equation (GPE) is based on the Hartree approximation. In this approximation a wave function for a single particle is considered and since all the particles share the same quantum state, the overall wavefunction of the condensed state is taken as the sum of the single wave function.

Let, ϕ_r be the wave function of a single particle, and from Hartree approximation,

$$\psi_{(r_1, r_2, r_3, \dots, r_N)} = \prod_{i=1}^N \phi_{(ri)} \quad 8$$

Here the single particle wave function is naturally a normalized wavefunction.

Having defined the wavefunction of the collection of particles, we can now define the interacting potential for the system. The interacting potential from mean field theory is calculated to be:[2]

$$U_0 = \frac{4\pi\hbar^2 a}{m} \quad 9$$

Where a is the scattering length of the trapped bosons.

With the interacting potential and applied potential, the Schrödinger equation becomes nonlinear as: [2]

$$-\frac{\hbar^2}{2m} \nabla^2 \psi(r) + V(r)\psi(r) + U_0[\psi(r)]^2\psi(r) = \mu\psi(r) \quad 10$$

Which is the Gross-Pitaevskii equation and is nonlinear due to presence of interacting potential produced by the trapped bosons. For non-uniform interacting bosons, the energy eigen value is the total chemical potential unlike uniform.

Equation 10, is the nonlinear equation, which does not have any specific solution, but solutions depending on the case that we consider. Depending on the condition of

the state and nature of Bosons there are solution on the condensed and dynamic state. Solution to each of the state is discussed below.

3.1 Thomas-Fermi approximation:

The bosons that undergo BEC are densely condensed and it's appropriate to neglect the kinetic energy posed by them. What we are left then is a system of particles with chemical potential and the nonlinear term. [2]

$$V(r)\psi(r) + U_0[\psi(r)]^2\psi(r) = \mu\psi(r) \quad 11$$

In such condition the bosonic cloud, the force exerted on the cloud is the gradient of the potential,

$$F = - \nabla V(r_0) \quad 12$$

Where, $V(r_0)$ is the chemical potential at the surface of the cloud.

Here represented are the trapped bosons under BEC, the center of the system the potential is maximum and as it goes up the surface of the cloud X_0 . At surface, $V(r_0)$ is the maximum potential equals the chemical potential and outside of the surface, it vanishes outside the surface.

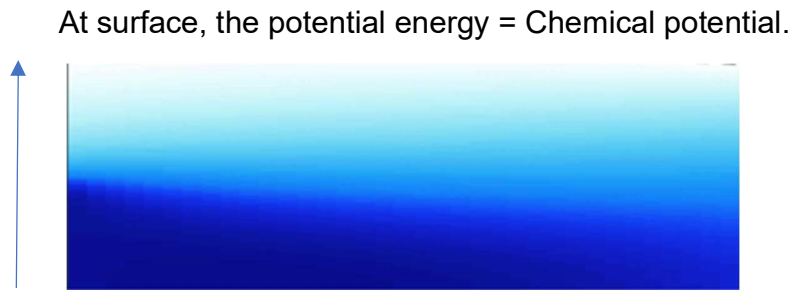


Figure 5: figurative representation of TF approximation. At bottom the density of high and it fades out as it goes upward.

Then the final expression for the wave function is given by,

$$n(r) = [\psi(r)]^2 = [\mu - V(r)] / U_0 \quad 13$$

In terms of the gradient,

$$\psi(r) = [F \cdot (r - r_0) / U_0]^{1/2} \quad 14$$

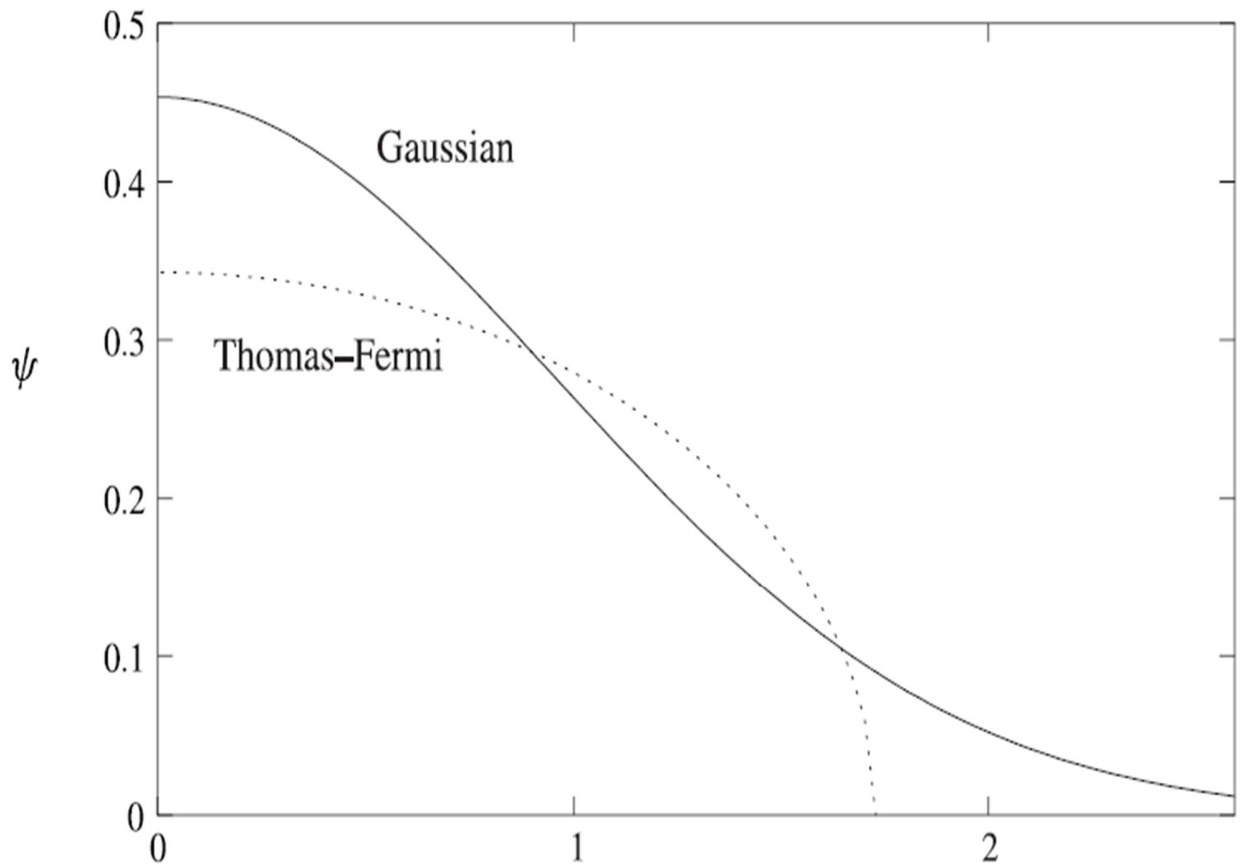


Figure 6: Showing the Thomas-Fermi approximation. The dashed line represents the T-F approximation, and the dark line represents the non-interacting Bose-Einstein condensate.[2]

Time dependent solution of the Gross-Pitaevskii equation.

3.2 Soliton:

Solitons are the solution to the time dependent GPE. In order to derive the expression and cases for the solitons, the time dependent Schrödinger needs to be developed. [5]

The time dependent Gross-Pitaevskii Schrödinger equation is given as,

$$-\frac{\hbar^2}{2m} \nabla^2 \psi(r) + V(r)\psi(r) + U_0[\psi(r)]^2\psi(r) = i\hbar \frac{\partial \psi(r,t)}{\partial t} \quad 15$$

Unlike time independent Schrödinger equation, the energy eigenvalue is no longer related to chemical potential. Since the wavefunction propagates with time, a relationship between time independent and dependent Schrödinger needs to be developed. This can be done by coupling the energy phase factor with the stationary solution to the Schrödinger equation as:

$$\psi_{(r,t)} = \psi_{(r)} \exp(-i \mu t/\hbar) \quad 16$$

Here, the chemical potential is acts as a phase with which the wave propagates, which agrees with the Schrödinger equation as the chemical potential can be expressed in terms of the energy and the particle number as:

$$\mu = \frac{\partial E}{\partial N} \quad 17$$

Having defined the time dependent Schrödinger equation, the physics of solitons can be described.

When the Bosonic clouds are trapped and the Bose-Einstein condensate is observed, then the concept of solitons arises. Solitons are the solitary waves and does not change shape when collided with another wave. They have a small amplitude, and they travel within a confined space called coherence length. Coherence length can be defined as the shortest distance over which the wavefunction can change its extreme value, or it's the length over which the wavefunction can obtain its maximum value at vortex and minimum at the center. The expression for the wavefunction and its corresponding healing length obtained from time independent Schrödinger equation as: [2]

$$\psi_{(x)} = \psi_0 \tanh(x/\sqrt{2}\xi) \quad 18$$

And,

$$\xi = \frac{\hbar}{(2mn_0U_0)^{1/2}} \quad 19$$

Healing length or coherence length being defined, the dynamics of solitons can be described. In solitons the attraction and repulsion between the bosons are taken in consideration. Above expression for the healing length in time independent GPE can be considered as the soliton but with zero velocity. When the system evolves in time, the solitary waves (Solitons) are formed based on the repulsion and attraction of bosons. The solution to the soliton can be obtained by solving the wave displacement $x-ut$, in the direction of propagation. As the wave progress, we look for a solution in which the density of the particles reaches to a non-zero value.

As,

$$x \rightarrow \pm\infty$$

$$n \rightarrow n_0$$

With the following Boundary condition, the final expression of the healing length in terms of density and coherence length is given by,

$$n(x, t) = n_{min} + (n_0 - n_{min}) \tanh^2[(x - ut)/\sqrt{2}\xi_u] \quad 20$$

Here,

$$\xi_u = \xi / (1 - (u/s)^2)^{1/2}$$

is now the width of the soliton with,

$$s = (\frac{n_0 U_0}{m})^{1/2}$$

being the velocity of sound in the uniform gas. The velocity of the soliton is therefore equal to the bulk sound velocity evaluated when there are minimum bosons trapped in the system.

4.Simulation:

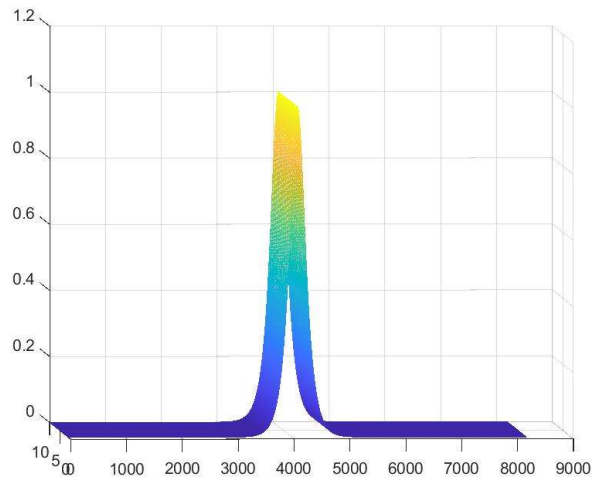


Fig: Soliton simulation in 3-D space.

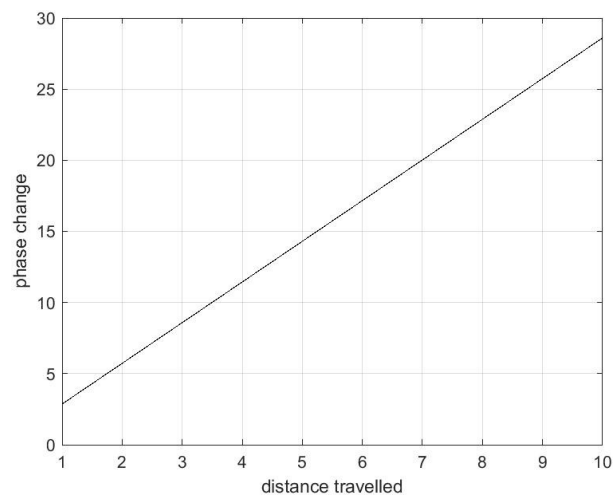


Fig: phase change vs distance travelled.

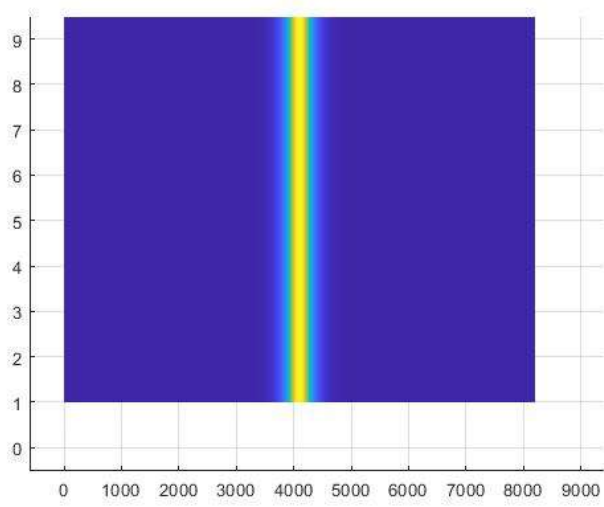


Fig: Soliton from Top view.

4 Reference:

[1]Figure 1: skript Bernd Braun, vielteichen physics.

[2]Bose-Einstein condensation in Dilute Gases C.J Pethick and H.Smith. Cambridge university press 2002.

[3]uni-ulm.de/nawi/institut-fuer-quantenmaterie/forschung/rubidium-bec-project/atom-molecule-dark-states-in-a-bose-einstein-condensate/

[4]fineartamerica.com/featured/bose-einstein-condensate-nistjilacuboulder.html?product=acrylic-print.

[5] N. N. Bogoliubov, J. Phys. (USSR) 11, 23 (1947), reprinted in D. Pines, The Many-Body Problem, (W. A. Benjamin, New York, 1961), p. 292.

MATLAB code:

```

clc; clear all; close all; clf;
cputime=0;
tic;
%%%%%%%%%%%%
ln=1;
%%%%%%%%%%%%
i=sqrt(-1);
s=-1;
alpha=0; % Fiber loss value in dB/km
alpha=alpha/(4.343); %Ref page#55 eqn 2.5.3
g=0.003; %fiber non linearity in /W/m
N=1; %soliton order
to=125e-12; %initial pulse width in second
pi=3.1415926535;
Po=0.00064; %input pwr in watts
Ao=sqrt(Po); %Amplitude
Ld=(N^2)/(g*Po); %dispersion length for corresponding soliton order
b2=-(to)^2/Ld; %2nd order disp. (s^2/m)
tau =- 4096e-12:1e-12: 4095e-12;% dt=t/to
dt=1e-12/to;
hl=1000;% step size
for ii=0.1:0.1:1.0
z=ii*Ld;
u=N*sech(tau/to); %fundamental soliton pulse
figure(1)
plot(abs(u), 'r');
grid on;
hold on;
h=hl/Ld; %soliton conditions
Z=z/Ld; %soliton conditions
l=max(size(u));
%%%%%%%%%%%%
fwhm1=find(abs(u)>abs(max(u)/2));
fwhm1=length(fwhm1);
spectrum=fft(fftshift(u)); %Pulse spectrum
dw=(1/l)/dt*2*pi;
w=(-1*l/2:1:l/2-1)*dw;
w=fftshift(w);
d=0;
for jj=h:h:Z
spectrum=spectrum.*exp(-alph*(h/2)+i*s/2*w.^2*(h/2)) ;
f=ifft(spectrum);
f=f.*exp(i*(N^2)*((abs(f)).^2)*(h));
% f=fftshift(f);
spectrum=fft(f);
spectrum=spectrum.*exp(-alph*(h/2)+i*s/2*w.^2*(h/2)) ;
d=d+1;
end
f=ifft(spectrum);
f=fftshift(f);
op_pulse(ln,:)=abs(f); %saving output pulse at all intervals
fwhm=find(abs(f)>abs(max(f)/2));
fwhm=length(fwhm);
ratio=fwhm/fwhm1 %PBR at every value
pbratio(ln)=ratio; %saving PBR at every step size

```



```

dd=atand((abs(imag(f)))/(abs(real(f))));
phadisp(ln)=dd;%saving pulse phase
ln=ln+1;
end
toc;
cputime=toc;
figure(2);
mesh(op_pulse(1:1:ln-1,:));
figure(3)
plot(pbratio(1:1:ln-1),'k');
xlabel('Number of steps');
ylabel('Pulse broadening ratio');
grid on;
hold on;
figure(4)
plot(phadisp(1:1:ln-1),'k');
xlabel('distance travelled');
ylabel('phase change');
grid on;
hold on;
disp('CPU time:'), disp(cputime);

```