Formation of soliton trains in Bose-Einstein condensates as a nonlinear Fresnel diffraction of matter waves

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Abstract

The problem of generation of atomic soliton trains in elongated Bose-Einstein condensates is considered in framework of Whitham theory of modulations of nonlinear waves. Complete analytical solution is presented for the case when the initial density distribution has sharp enough boundaries. In this case the process of soliton train formation can be viewed as a nonlinear Fresnel diffraction of matter waves. Theoretical predictions are compared with results of numerical simulations of one- and three-dimensional Gross-Pitaevskii equation and with experimental data on formation of Bose-Einstein bright solitons in cigar-shaped traps.

Discovery of Bose-Einstein condensate (BEC) \cite{1, 2, 3} has created new active field of research of quantum macroscopical behavior of matter. Among most spectacular evidences of such macroscopic behavior one can mention formation of interference fringes between two condensates \cite{4} and creation of dark \cite{5, 6} and bright \cite{7, 8} solitons. The interference phenomenon is usually considered in framework of a linear wave theory, whereas solitons are treated as a nonlinear wave effect. At the same time, basically, these two phenomena have much in common. For example, formation of bright soliton trains in nonlinear wave systems is often explained as a result of modulational instability, where selection of the most unstable mode is a result of interplay of interference and nonlinear effects (see, e.g. \cite{9, 10}). Such
interconnection of interference and soliton phenomena is demonstrated most spectacularly
in formation of solitons in vicinity of a sharp edge of density distribution. In this case, at
linear stage of evolution the linear diffraction provides an initial modulation of the wave and
further combined action of interference and nonlinear effects leads to formation of soliton
trains. Without nonlinear effects, such kind of time evolution of a sharp wave front would
be a temporal counterpart of usual spatial Fresnel diffraction and therefore soliton train
formation at the sharp front of nonlinear wave can be called a nonlinear Fresnel diffraction.

Similar formation of oscillatory structures at sharp wave front or after wave breaking in
modulationally stable systems described by the Korteweg-de Vries equation is well known
as a “dissipationless shock wave” (see, e.g. [10]). Its theoretical description is given [11, 12]
in framework of Whitham theory of nonlinear wave modulations [13], where the oscillatory
structure is presented as a modulated nonlinear periodic wave which parameters change little
in one wavelength and one period. Then slow evolution of the parameters of the wave is
governed by Whitham equations obtained by averaging of initial nonlinear wave equations
over fast oscillations of the wave. Application of this method to modulationally unstable
systems has been given for important particular case of soliton train formation at the sharp
front of a long step-like initial pulse [14, 15, 16, 17]. Here we shall consider by this method
formation of solitons in BEC with negative scattering length (attractive interaction of atoms).

We suppose that condensate is confined in a very elongated cigar-shaped trap whose axial
frequency $\omega_z$ is much less than the radial frequency $\omega_{\perp}$. In the first approximation we can
neglect the axial trap potential and suppose that condensate is contained in a cylindrical
trap ($\omega_z = 0$) and its initial density distribution has a rectangular form. Evolution of BEC
is governed by three-dimensional (3D) Gross-Pitaevskii (GP) equation

$$i\hbar \psi_t = -\frac{\hbar^2}{2m_a} \Delta \psi + \frac{1}{2} m_a \omega_{\perp}^2 (x^2 + y^2) \psi + g|\psi|^2 \psi,$$

for the condensate wave function $\psi$, where we use standard notation $g = 4\pi \hbar^2 a_s / m_a$ for
the effective nonlinear coupling constant, $a_s < 0$ is the s-wave scattering length, and $\psi$ is
normalized on the number of particles in BEC, $\int |\psi|^2 d\mathbf{r} = N$. For analytical treatment of
nonlinear Fresnel diffraction it is important to determine conditions when the 3D equation
(1) can be reduced to its one-dimensional (1D) approximation (see, e.g. [18])

$$i\hbar \Psi_t = -\frac{\hbar^2}{2m_a} \Psi_{zz} + g_{1D}|\Psi|^2 \Psi, \quad \int |\Psi|^2 dz = N,$$

where

$$g_{1D} = \frac{g}{2\pi a_{\perp}^2} = \frac{2\hbar^2 a_s}{m_a a_{\perp}^2}, \quad a_{\perp} = \sqrt{\frac{\hbar}{m_a \omega_{\perp}}}.$$

that is the transversal degrees of freedom are frozen. It is well known (see, e.g. [10])
that a homogeneous distribution with linear density $n_0 = |\Psi|^2 = \text{const}$ described by (2)
with negative $g_{1D}$ ($a_s < 0$) is unstable with respect to self-modulation with increment of
instability equal in our present notation to

$$\Gamma = \frac{\hbar K}{2m_a a_{\perp}} \sqrt{8|a_s|n_0 - (a_{\perp} K)^2},$$
where \( K \) is a wavenumber of small periodic modulation. The most unstable mode has the wavenumber

\[
K_{\text{max}} = 2\sqrt{|a_s|n_0/a_\perp}
\]

and the corresponding increment is equal to

\[
\Gamma_{\text{max}} = 4|a_s|n_0\omega_\perp.
\]

This means that after time \( \sim 1/(|a_s|n_0\omega_\perp) \) the homogeneous condensate splits into separate solitons (diffraction fringes) and each soliton (diffraction fringe) contains about \( N_s \sim n_0/K_{\text{max}} \) atoms. If in 3D GP equation (1) the nonlinear energy \( gN_sK_{\text{max}}/a_\perp^2 \sim gn_0/a_\perp^2 \) in each solitons is much less than the kinetic energy in the transverse direction, \( \sim \hbar^2/m_\perp a_\perp^2 \), then the transverse motion is reduced to the ground state oscillations and the 3D condensate wave function can be factorized into \( \psi = \phi_0(x,y)\Psi(z,t) \), where \( \phi_0 = (\sqrt{\pi a_\perp})^{-1} \exp[-(x^2 + y^2)/(2a_\perp^2)] \) is the ground state wave function of transverse motion, and \( \Psi(z,t) \) obeys to the effective 1D nonlinear Schrödinger (NLS) equation (2). Thus, the condition of applicability of 1D equation (2) for description of solitons formation is

\[
n_0|a_s| \ll 1,
\]

which means that the instability wavelength \( \sim 1/K_{\text{max}} \) is much greater than the transverse radius \( a_\perp \) of BEC. If (7) is not satisfied, then the transverse motion has to be taken into account which may lead to collapse of BEC inside each separate soliton. Therefore we shall confine ourselves to the BEC described by the 1D NLS equation under supposition that the initial distribution satisfies the condition (7).

To simplify formulae in the analytic theory, we transform (2) to dimensionless variables

\[
\tau = 2(|a_s|n_0)^2\omega_\perp t, \quad \zeta = 2|a_s|n_0z/a_\perp, \quad \Psi = \sqrt{2|a_s|n_0u},
\]

so that (2) takes the form

\[
iu_\tau + u_{\zeta\zeta} + 2|u|^2u = 0,
\]

and \( u \) is normalized to the effective length \( L \) of the condensate \( \int |u|^2d\zeta = L/a_\perp \) measured in units of \( a_\perp \). We are interested in the process of formation of solitons (nonlinear Fresnel diffraction fringes) at the sharp boundary of initially rectangular distribution. Since this process takes place symmetrically at both sides of the rectangular distribution, we can confine ourselves to the study of only one boundary. This limitation remains correct until the nonlinear waves propagating inside the condensate collide in its center. If the initial distribution is long enough, this time is much greater than the time of solitons formation. Thus, we consider the initial distribution in the form

\[
u(\zeta,0) = \begin{cases} \gamma \exp(-2i\alpha\zeta), & \text{for } \zeta < 0 \\ 0, & \text{for } \zeta > 0, \end{cases}
\]

where \( \gamma \) is the height of initial step-like distribution and \( \alpha \) characterizes the initial homogeneous phase. The problem of this kind has already been considered in some other problems of nonlinear physics \[14, 15, 16, 17, 10\] and we shall present here only the main results.

Due to dispersion effects described by the second term in Eq. (8), the sharp front transforms into slightly modulated wave which describes usual Fresnel diffraction of atoms. In our
case the diffraction pattern evolves with time rather than is “projected” on the observation
plane. The linear stage of evolution is followed by the nonlinear one in which combined
action of dispersion and nonlinear terms yields the pattern which can be represented as a
modulated nonlinear periodic wave or, in other words, a soliton train. We suppose that this
soliton train contains large enough number of solitons, so that their parameters change little
in one wavelength and one period. Then, in framework of Whitham theory, the density of
BEC can be approximated by a modulated periodic solution of Eq. (8) (see [17, 10])

\[ n = |u(\zeta, \tau)|^2 = (\gamma + \delta)^2 - 4\gamma \delta \text{sn}^2(\sqrt{(\alpha - \beta)^2 + (\gamma + \delta)^2} \theta, m), \]  

where \( \text{sn}(x, m) \) is the Jacobi elliptic function,

\[ \theta = \zeta - V\tau, \quad V = -2(\alpha + \beta), \]  

\[ m = 4\gamma \delta/[(\alpha - \beta)^2 + (\gamma + \delta)^2], \]  

the parameters \( \alpha \) and \( \gamma \) are determined by the initial condition (9), and \( \beta \) and \( \delta \) are slow
functions of \( \zeta \) and \( \tau \). Their evolution is governed by the Whitham equation

\[ \frac{\partial(\beta + i\delta)}{\partial\tau} + v(\beta, \delta) \frac{\partial(\beta + i\delta)}{\partial\zeta} = 0, \]  

where Whitham velocity \( v(\beta, \delta) \) is given by the expression

\[ v(\beta, \delta) = -2(\alpha + \beta) - \frac{4\delta[\gamma - \delta + i(\beta - \alpha)]K}{(\beta - \alpha)(K - E) + i[(\delta - \gamma)K + (\delta + \gamma)E]}, \]  

\( K = K(m) \) and \( E = E(m) \) being the complete elliptic integrals of the first and second kind,
respectively. Since our initial condition (9) does not contain any parameters with dimension
of length, the parameters \( \beta \) and \( \delta \) can only depend on the self-similar variable \( \xi = \zeta/\tau \). Then
Eq. (13) has the solution

\[ \zeta/\tau = \xi = v(\beta, \delta) \]  

with \( v(\beta, \delta) \) given by (14). Separation of real and imaginary parts yields the formulae

\[ \zeta/\tau = -4\beta - 2(\gamma^2 - \delta^2)/(\beta - \alpha), \]  

\[ (\alpha - \beta)^2 + (\gamma - \delta)^2 = \frac{E(m)}{K(m)}, \]  

which together with Eq. (12) determine implicitly dependence of \( \beta \) and \( \delta \) on \( \xi = \zeta/\tau \). It is
central to express this dependence in parametric form

\[ \beta(m) = \alpha - \gamma \sqrt{4A(m) - (1 + mA(m))^2}, \]  

\[ \delta(m) = \gamma mA(m), \]  

where

\[ A(m) = \frac{(2 - m)E(m) - 2(1 - m)K(m)}{m^2E(m)}. \]  

Substitution of these expressions into (10), (11) yields the density \( n \) as a function of \( m \).
Since the space coordinate \( \zeta \) defined by Eq. (16) is also a function of \( m \) at given moment
we arrive at presentation of dependence of $n$ on $\zeta$ in parametric form. The limit $m \to 0$ corresponds to a vanishing modulation, and this edge point moves inside the condensate according to the law

$$\zeta_- = (-4\alpha + 4\sqrt{2}\gamma)\tau.$$  
(21)

The other edge with $m \to 1$ moves according to the law

$$\zeta_+ = -4\alpha\tau,$$  
(22)

and corresponds to the bright solitons (or fringes of nonlinear diffraction pattern) at the moment $\tau$. The whole region $\zeta_- < \zeta < \zeta_+$ describes the oscillatory pattern arising due to nonlinear Fresnel diffraction of the BEC with initially sharp boundary at $\zeta = 0$.

We have performed numerical simulation of 1D and 3D GP equations with the aim to compare approximate Whitham theory with numerical results. The 1D density distributions calculated numerically from (8) and analytically are shown in Fig. 1. We see excellent agreement between the theoretical and numerical predictions of the height of the first soliton generated from initially step-like pulse, but its position given by analytical formula is slightly shifted with respect to numerical result. This is well-known feature of asymptotic Whitham approach [11, 12] which accuracy in prediction of location of the oscillatory pattern cannot be much better than one wavelength. Thus, we see that the above theory reproduces the numerical results quite well for period of time $\tau \simeq 2$. For much greater time values some other unstable modes different from one-phase periodic solution (10) can also give considerable contribution into wave pattern. Nevertheless, the qualitative picture of soliton pattern remains the same.

For 3D numerical simulation, the GP equation (1) was transformed to dimensionless form by means of substitutions $x = a_\perp x'$, $y = a_\perp y'$, $z = a_\perp z'$, $t = 2t' / \omega_\perp$, $\psi' = (N^{1/2} / a_\perp^{3/2})\psi$, so that it takes the form

$$i\psi_t = -\Delta \psi + r^2 \psi - (8\pi N |a_s| / a_\perp) |\psi|^2 \psi,$$  
(23)

where primes are omitted for convenience of the notation and $\int |\psi|^2 2\pi r dr dz = 1$, $r^2 = x^2 + y^2$. Evolution of the density distribution $\rho(z) = \int_0^\infty |\psi(r,z)|^2 2\pi r dr$ along the axial direction is shown in Fig. 2 for the values of the parameters corresponding to the experiment [8] $(a_s = -3a_0, \omega_\perp = 2\pi \cdot 625$ Hz, $L = 300 a_\perp)$ except for the number of atoms which was chosen to be $N = 5 \cdot 10^3$ in order to satisfy the condition (17), so that $|a_s|n_0 = 1.7 \cdot 10^{-3}$. We see that diffraction (soliton) pattern arises after the dimensionless time $t \simeq 400$ which corresponds after appropriate scaling transformation to $\tau \simeq 2$ in Fig. 1. The width of solitons in Fig. 2 also agrees with the width predicted by 1D analytical theory and numerics. The spatial distribution of the condensate density $|\psi(r,z)|^2$ is illustrated by Fig. 3. The 3D nonlinear interference pattern is clearly seen. For greater values of the condensate density, when 1D theory does not apply, numerical simulation demonstrates similar evolution of the diffraction pattern up to the moment when collapse starts in each separate soliton. Thus, formation of solitons in the experiment [8] with large initial number of atoms $N \simeq 10^5$ goes through collapses with loss of atoms until the remaining atoms can form stable separate soliton-like condensates. The present theory emphasizes the importance of the initial stage of evolution with formation of the nonlinear Fresnel diffraction pattern.
Formation of soliton trains in BEC confined in a cigar-shaped trap has also been studied numerically in [19, 20]. The results of 1D simulation in [19] agree qualitatively with our results. In numerics of [20] strong losses were introduced to prevent fast collapse of BEC with large number of atoms. Nevertheless, formation of soliton trains was also observed.

The above theory is correct for evolution time much less than period of oscillations $2\pi/\omega_z$ in the axial trap. When the axial trap is taken into account, solitons acquire velocities in axial direction even if initial phase is equal to zero. The number of solitons produced ultimately from some finite initial BEC distribution can be found by means of quasiclassical method applied to an auxiliary spectral problem associated with the NLS equation [8] in framework of the inverse scattering transform method [12, 21]. If the initial wave function is represented in the form $u_0(\zeta) = \sqrt{n_0(\zeta)} \exp(i\phi_0(\zeta))$, then the total number of solitons is equal approximately to

$$N_s = \frac{1}{\pi} \int \sqrt{n_0(\zeta) + \frac{v_0^2(\zeta)}{4}} d\zeta - \frac{1}{2}, \quad (24)$$

where $v_0(\zeta) = \partial\phi_0(\zeta)/\partial\zeta$ is the initial velocity distribution of BEC. If there is no initial phase imprinted in BEC, then the total number of solitons is given by the formula

$$N_s = (\sqrt{2|a_s|/\pi a_\perp}) \int |\Psi| dz, \quad (25)$$

which is written in dimensional units and we have neglected a “one-half” term in (24).

In experiment, the initial stage is usually obtained by sudden change of the sign of the scattering length from positive to negative one, so that initial density distribution has, for large enough number of atoms, the Thomas-Fermi form

$$|\Psi|^2 = \frac{3N}{4Z} \left(1 - \frac{z^2}{Z^2}\right), \quad (26)$$

where $Z$ is the Thomas-Fermi half-length of the condensate. Then substitution of (26) into (25) gives

$$N_s = \sqrt{3N|a_s|L/(4a_\perp)}, \quad (27)$$

where $L = 2Z$ is the total length of the condensate. Up to constant factor, this estimate coincides with one obtained in [20] by division of $L$ by the instability wavelength $1/K_{max}$. Note that this estimate includes also very small solitons which cannot be observed in real experiments, so that it must be considered as an upper limit of the number solitons which can be produced from a given initial distribution. The same property of this kind of estimate for number of dark solitons has been observed in comparison of analytical theory with numerical simulations in [21]. The axial potential influences mainly on velocities of solitons, so the above estimate can be applied to the condensate in a cigar-shape trap under condition that inequality (7) is fulfilled.

In conclusion, we have studied theoretically and numerically the process of formation of soliton trains near the sharp edges of the density distribution of BEC. The arising oscillatory regions can be considered as nonlinear Fresnel diffraction fringes of matter waves.

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Figure 1: Density distributions of BEC calculated by numerical solution of 1D GP equation (8) and given by Whitham theory with initial step-like wave function (9) with $\gamma = -1$, $\alpha = 0$. 
Figure 2: Density distributions of BEC $\rho(z)$ along axial direction for different moments of time calculated by numerical solution of 3D GP equation \cite{23} with cylindrical initial distribution.
Figure 3: Dependence of the density distributions on radial, $r$, and axial, $z$, coordinates at time $t = 400$. 

$|\psi(r,z)|^2$ 

$t=400$