Temporal evolution of attractive Bose-Einstein condensate in a quasi 1D cigar-shape trap modeled through the semiclassical limit of the focusing Nonlinear Schrödinger Equation

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One-dimensional (1D) Nonlinear Schrödinger Equation (NLS) provides a good approximation to attractive Bose-Einstein condensate (BEC) in a quasi 1D cigar-shaped optical trap in certain regimes. 1D NLS is an integrable equation that can be solved through the inverse scattering method. Our observation is that in many cases the parameters of the BEC correspond to the semiclassical (zero dispersion) limit of the focusing NLS. Hence, recent results about the strong asymptotics of the semiclassical limit solutions can be used to describe some interesting phenomena of the attractive 1D BEC. In general, the semiclassical limit of the focusing NLS exhibits very strong modulation instability. However, in the case of an analytical initial data, the NLS evolution does display some ordered structure, that can describe, for example, the bright soliton phenomenon. We discuss some general features of the semiclassical NLS evolution and propose some new observables to the attractive 1D BEC.

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1D BEC as a semiclassical limit of the focusing NLS. It is generally accepted that the temporal evolution of the BEC is governed by the Gross-Pitaevskii (GP) equation for the condensate wave function \( \Psi(\mathbf{r}, t) \), given by

\[
i\hbar \frac{\partial}{\partial t} \Psi = \left[ -\frac{\hbar^2}{2m} \nabla^2 + V_{\text{ext}}(\mathbf{r}) + g|\Psi|^2 \right] \Psi,
\]

where: \( m \) is the single atom mass; \( V_{\text{ext}} \) is an external trapping potential that we consider to be a harmonic oscillator potential, and \( g \) is the coupling constant determined by the scattering length. Negative values of \( g \) correspond to the attractive BEC. If the characteristic energies of the radial excitations are much greater than the energy of the nonlinear term (see estimate (5) below), the 3D GP equation (1) can be approximated by a 1D GP in the longitudinal (axial) direction ([1])

\[
i\hbar \frac{\partial}{\partial t} \psi = \left[ -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial \xi^2} - V_{\text{ext}}(\xi) - \frac{g}{2}\left| \psi(\xi, t) \right|^2 \right] \psi(\xi, t) = 0,
\]

where \( \xi \) is the axial variable and

\[
V_{\text{ext}}(\xi) = \frac{1}{2} m \omega_{\xi}^2 \xi^2
\]

is the axial part of the harmonic trapping potential. Here \( g = \frac{\pi \hbar^2 a_s}{m \omega_{\xi}^2}, \) \( \ell_\perp = \frac{\hbar}{m \omega_{\perp}} \) and \( \omega_{\perp} \) are the trap frequencies in the radial and the axial directions respectively. Taking as an example the bright solitons experiment with Lithium (\(^7\)Li, Sreckker et al., [10]), we have \( m \approx 10^{-26}\text{kg}, \) \( a_s \approx -3a_0 \approx -16 \cdot 10^{-11}\text{m} \) (here \( a_0 \) denotes Bohr radius) and \( \omega_{\perp} = 2\pi \cdot 640\text{Hz} \approx 4 \cdot 10^4\text{Hz}; \) in the first approximation, we put \( \omega_{\xi} = 0. \) The axial wave function \( \psi(\xi, t) \) is assumed to have a shape of Gaussian and is normalized by

\[
\int_{\mathbb{R}} \left| \psi(\xi, 0) \right|^2 d\xi = N,
\]

where \( N \approx 3 \cdot 10^5 \) is the total number of the atoms in the trap.

Considering \( |\Psi|^2 \sim \frac{N}{|\tau|^3} \), the 1D GPE (2) is applicable ([1]) under the condition

\[
\frac{N|a_s|}{s_{\parallel}} \ll 1,
\]

where \( s_{\parallel} \) is the order of magnitude of the size of the condensate in the axial direction. Assuming \( s_{\parallel} \approx 3 \cdot 10^{-4}m, ([10]), \) the left hand side of (5) becomes 0.16, which may give some justification for the use of (2).

Equation (2) with zero external potential is a 1D NLS, which can be integrated through the inverse scattering technique. We start our discussion by showing that the GP equation (2) with zero external potential that describes the attractive BEC in a cigar-shaped trap can be rescaled to

\[
i\varepsilon \frac{\partial}{\partial \tau} + \left( \frac{s^2}{2} \right) \frac{\partial^2}{\partial x^2} + |q|^2 q = 0,
\]

where \( \varepsilon \) is a small positive parameter, \( x, \tau \) are scaled space - time variables and the initial data \( |q(x,0)| \) has a shape of Gaussian with a typical length of order 1 is normalized by

\[
\int_{\mathbb{R}} |q(x, 0)|^2 dx = 1.
\]

Equation (6) is the standard form of the focusing NLS in the semiclassical (zero dispersion) limit. Substitution of expressions for \( g, l_\perp \) into (2) yields

\[
i\frac{\partial}{\partial \tau} + \frac{\hbar}{2m} \frac{\partial^2}{\partial \xi^2} + 2|a_s|\omega_{\perp} \left| \psi(\xi, t) \right|^2 \psi(\xi, t) = 0.
\]

Equation (6) can be obtained from (8) through the change of variables

\[
\psi(\xi, t) = \beta q(x, \tau), \quad \xi = \Delta x, \quad t = k\tau,
\]
where the coefficients $\beta$, $\Delta$ and $k$ are to be determined. The comparison of the norming conditions (4) and (7) yields $\beta^2 = \frac{N}{\Delta}$. Substituting (9) into (8) one gets
\[ i \frac{\Delta}{2|a_s|\omega N k} q_\tau + \frac{1}{2} \left( \frac{h}{2|a_s|\omega N m \Delta} \right) q_{xx} + |q|^2 q = 0. \] (10)

Comparison of equations (10) and (6) yields
\[ \varepsilon = \frac{\Delta}{2|a_s|\omega N k} \quad \text{and} \quad \frac{\Delta^2}{2|a_s|\omega N k^2} = \frac{\hbar}{m \Delta}, \] (11)
so that
\[ k = \Delta \sqrt{\frac{m \Delta}{2|a_s|\omega N \hbar}} \quad \text{and} \quad \varepsilon = \frac{\sqrt{\hbar}}{\sqrt{2|a_s|\omega N m \Delta}}. \] (12)

Comparison of the typical size of Gaussian distributions for $|\phi(\xi,0)|$ and $|q(x,0)|$ gives
\[ \Delta \sim 10^{-4}. \] (13)

Using numerical values $\hbar \approx 10^{-34} \text{m}^2 \text{kg} / \text{s}$, we calculate
\[ \varepsilon \approx 1.6 \times 10^{-2} \quad \text{and} \quad k \approx 5 \times 10^{-3}. \] (14)

Equation (14) shows that the time evolution of attractive BEC, governed by equation (8), can be described by the semiclassical limit of the focusing NLS (6) with normalization (7). (Normalization of $\int |q|^2 dx = n$ instead of (7), where $n = O(1)$, leads to the replacement of $N$ by $N/n$ in equations (10)-(12). Thus, in this case $\varepsilon, k$ has to be multiplied by $\sqrt{n}$.)

**Semiclassical limit solutions to the focusing NLS (6).** The focusing Nonlinear Schrödinger equation (6), where $x \in \mathbb{R}$ and $\tau \geq 0$ are space-time variables, is a basic model for self-focusing and self-modulation; it describes the evolution of the envelope of modulated wave in general nonlinear systems. It is also one of the most celebrated nonlinear integrable equations that was first integrated by Zakharov and Shabat [16], who produced a Lax pair for it and used the inverse scattering procedure to describe general decaying solutions ($\lim_{|x| \to 0} q(x,0) = 0$) in terms of radiation and solitons.

In the semiclassical limit ($\varepsilon \to 0$) the focusing NLS (6) exhibits *modulationally unstable* behavior (see Fig. 1), as was first shown in [6]. This is in drastic contrast to the case of the defocusing NLS equation ([2], [7]) in which the semiclassical theory shows regions of modulated periodic or quasiperiodic oscillation. These two very different types of behavior can be explained through modulation equations, which are elliptic in the focusing and hyperbolic in the defocusing cases. The corresponding initial value problems are, therefore, ill-posed and well-posed respectively. As a result, a plane wave with amplitude modulated by $A(x)$ and phase modulated by $S(x)$, taken as an initial data
\[ q(x,0,\varepsilon) = A(x)e^{iS(x)/\varepsilon} \] (15)

for the focusing NLS (6), is expected to break immediately into disordered oscillations of both the amplitude and the phase. However, in the case of an analytic initial data, the NLS evolution displays some orderly structure instead of the disorder suggested by the modulational instability, see [2], [9] and [3]. Throughout this work, we will use the abbreviation NLS to mean “focusing Nonlinear Schrödinger equation”.

FIG. 1: Absolute value $|q(x,\tau,\varepsilon)|$ of a solution $q(x,\tau,\varepsilon)$ to the focusing NLS (6) versus $x,\tau$ coordinates from [2]. Here $A(x) = \varepsilon^{-1/2}$, $S'(x) = -\tanh x$ and $\varepsilon = 0.02$.

In some very few special cases, for example, when $A(x) = \text{sech} x$ and $S'(x) = -\mu/2 \tanh x, \mu \geq 0$, the scattering data for (6) can be calculated explicitly. Then the modulated amplitude and phase of (16), (17) can be
obtained from the system of transcendental equations for 
\( \alpha(x, \tau) = a(x, \tau) + ib(x, \tau) \):
\[
\begin{align*}
\sqrt{(a - T)^2 + b^2} + \sqrt{(a + T)^2 + b^2} &= \mu + 4\tau b^2 \\
|a + T + \sqrt{(a + T)^2 + b^2}| a - T + \sqrt{(a - T)^2 + b^2} &= b^2 e^{2(x+4\tau)} 
\end{align*}
\]
(18)
where \( T = \sqrt{\frac{2}{\mu}} - 1 \). In the particular case \( \mu = 2 \) (the borderline value of \( \mu \) between the pure radiational case \( \mu > 2 \) and radiation with solitons case \( \mu < 2 \)), introducing the implicit time \( u = u(x, \tau) \) at each point \( x \in \mathbb{R} \) by \( \tau = \frac{(u-x)|\sinh 2u-(u-x)|}{8\sinh^2 u} \), one can obtain an explicit solution ([11])
\[
a = \frac{2\sin^2 u}{\sinh 2u - (u-x)} , \quad b = \frac{2\sin u}{\sinh 2u - (u-x)} \quad (19)
\]
for \( A(x, \tau) = b \) and \( S'(x, \tau) = -2a \). Similar expressions are available for the case \( \mu = 0 \).

Notice that the amplitude \( A(x, t) \) of the solution on Fig. 1 at first contacts (accumulates) towards the point of maximum \( (x = 0) \) of \( |q(x, 0)| \) and then suddenly bursts into rapid (order 1) and violent oscillations in amplitude (transition to genus two regime). This is the typical behavior ([12]) for an analytic one-bump initial data (provided that \( S'(x) \) does not decrease too fast) The very first point of this transition, which is the tip-point of the first breaking curve (see Fig. 1), is called a point of gradient catastrophe, or elliptic umbilical singularity ([4]). At the point \( (x_0, \tau_0) \) of gradient catastrophe the semiclassical solution (16) of (6) losses its smoothness (15), i.e., \( \alpha_x(x_0, \tau_0) = \infty \) (either \( A_x(x, \tau_0) \) or \( S_{xx}(x, \tau_0) \) or both become infinite).

The Theta-function expression for higher genus solutions is somewhat cumbersome for this paper (see, for example, [11]). This expression gives an \( O(\varepsilon) \) approximation for the solution of (6), (15) in the corresponding region. For a fixed time snapshot in the genus two region (Fig. 1, around \( \tau = 1 \)), the graph of \( |q(x, \tau, \varepsilon)| \) can be identified with bright solitons, that were experimentally observed, for example, in [10]. If the BEC with a Gaussian shaped initial data is governed by 1D NLS (8), the region filled with solitons is spreading off in the axial direction. According to Fig. 1, the onset of soliton-like (genus two) behavior in the semiclassical limit happens at \( \varepsilon = \frac{1}{\varepsilon} \) or \( t = k\tau \approx 2.5 \times 10^{-3}s \), which does not contradict observations of [10], were bright solitons were first observed at \( t = 5ms \). Since the “effective” axial size of the condensate \( s_0 \) shrinks considerably near the time of gradient catastrophe (see Fig. 1), condition (5) may be violated during this period. This is consistent with the fact that the total number of atoms observed in the soliton region in the experiment of [10] is less than 20% of the number of atoms \( N \approx 3 \times 10^5 \) at the beginning of the experiment. (The NLS evolution preserves the \( L^2 \) norm of the solution, i.e., evolution governed by equation (8) would preserve the total number of atoms \( N \).) Moreover, the evolution of the Fourier transform of \( q(x, t, \varepsilon) \), which can be calculated explicitly form (16) through the stationary phase method, shows that the portion of atoms in the condensate with high axial momentum significantly increases (see Fig. 2) as the point of gradient catastrophe is approached.

Note that breaking curves (boundaries between the regions of different genera) depend on both the amplitude and the phase of the initial condition \( q(x, 0, \varepsilon) \), but do not depend on \( \varepsilon \). Within a region of genus \( 2n, n > 0 \), the semiclassical limit solution can be viewed as modulated \( 2n \)-phase nonlinear wave, with \( 2n + 1 \) complex \( (4n + 2) \) real wave parameters, which slowly vary (in \( x, \tau \) ) in the region. (Fig. 1 depicts consequitive regions with \( n = 0, 2, 4 \).) Complex wave parameters can be interpreted as a set of branchpoints of the Schwarz-symmetrical hyperelliptic surface \( R(x, \tau) \), whose evolution in the \( x, \tau \) plane is defined by modulation (Whitham) equations. (Here we want to mention that regions of genus four (see Fig. 1 after \( \tau = 1.5 \)) and of higher genera are associated with the initial data (15) that support solitons, see [11]: in the semiclassical limit solutions the number of solitons has order \( O(1/\varepsilon) \).

Calculation of semiclassical solutions to (6). Equation (6), as an integrable NLS, can be solved by inverse scattering technique. However, the semiclassical limit solutions require the semiclassical limit of the scattering transform. Let \( z \) be a point on the curve \( \Sigma \) in the upper halfplane, that is defined parametrically by the analytic initial data (15) as \( \alpha(x) = -\frac{1}{2}S'(x) + iA(x) \), \( x \in \mathbb{R} \). (Here \( A(x) \) and \( S'(x) \) have sufficient decay to zero or to some finite values \( \pm \mu \) at \( \pm \infty \) respectively.) Assuming for

FIG. 2: Evolution of the Fourier transform of the initial data (15) with \( A(x) = \text{sech} \ x \) and \( S'(x) = -2\tan x \) in the limit \( \varepsilon \to 0 \) from \( \tau = 0 \) to the time of gradient catastrophe \( \tau = 0.125 \).
simplicity that \( \alpha(x) \) is invertible, the semiclassical scattering data limit \( f_0(z) \), \( z \in \Sigma \), is defined ([15]) through a generalized Abel integral transform as

\[
f_0(z) = \int_{R}^{R+} \left[ z - \mu + \sqrt{(z - \mu)(z - \bar{\mu})} \right] x'(u) du + (z - \mu_+) x(z),
\]

where \( x(\alpha) \) is inverse to \( \alpha(x) \) and the integral is taken along \( \Sigma \). The analytic extension of \( f_0(z) \) from \( \Sigma \) to \( \mathbb{R} \) (which can have logarithmic branchcuts) has a meaning of the leading order term of \( \frac{1}{2} i \kappa \ln r_0(z, \varepsilon) \) as \( \varepsilon \to 0 \), where \( r_0(z, \varepsilon) \), \( z \in \mathbb{R} \), is the reflection coefficient of (15). Once \( f_0(z) \) is known, the complex wave parameters are defined through the modulation equations. In particular, in the genus zero region, the modulation equation for \( \alpha(x, \tau) \) is given by a system of two real equations ([11])

\[
\int_{\gamma_m} f'(\zeta) d\zeta = 0, \quad \int_{\gamma_m} \zeta f'(\zeta) R(\zeta) d\zeta = 0,
\]

(21)

where \( f(z) = f(z; x, t) = f_0(z) - xz - 2tz^2 \) and \( R(z) = \sqrt{(z - \alpha)(z - \bar{\alpha})} \). It defines \( q(x, \tau, \varepsilon) \) through (16)-(17). (Here \( f_0(z) \) is Schwarz symmetrically extended into the lower halfplane; typically, \( \Im f_0(z) \) has a jump along \( \mathbb{R} \).)

Define function \( h(z) = h(z; x, \tau) \) as

\[
h(z) = \frac{i}{\pi} \int_{\gamma_m} f(\zeta) R(\zeta) (\zeta - z) d\zeta - f(z),
\]

(22)

where \( \gamma_m \) is a Shwarz-symmetrical contour connecting \( \alpha \) and \( \alpha_+ \), and such that \( \gamma_m \cup \mathbb{R} = \mu_+ \). Because of the analyticity of \( f(z) \), a particular shape of \( \gamma_m \) is not important. However, it is possible to fix \( \gamma_m \) by the condition \( \Im h(z) = 0 \) on \( \gamma_m \). According to the Deift-Zhou nonlinear steepest descent method, the genus zero anzatz (16) approximates the actual solution of the NLS (6) with the reflection coefficient \( r_0(z, \varepsilon) = e^{-\frac{i}{2} \kappa f_0(z)} \) if ([11])

\[
\Im h(z; x, \tau) < 0 \text{ on both sides of } \gamma_m^+;
\]

\[
\Im h(z; x, \tau) > 0 \text{ on } \gamma_m^+,
\]

(23)

where \( \gamma_m^+ \) is a contour in the upper halfplane \( \mathbb{C} \) connecting \( \alpha_+ \) and \( \mu_- \) and \( \gamma_m^+ = \gamma_m \cup \mathbb{C}^+ \). We have a freedom to deform the contour \( \gamma_m^+ \) so that the inequalities (23) are satisfied along it. The first breaking curve consists of points \( (x, \tau) \) where at least one of the inequalities (23) turns into equality at some \( z_0 \). Thus, equation for the first breaking curve can be written as a system of three real equations for \( z_0 \in \mathbb{C} \) and \( (x, \tau) \in \mathbb{R}^2 \)

\[
\Im h(z_0; x, \tau) = 0 \quad \text{and} \quad h_z(z_0; x, \tau) = 0.
\]

(24)

For the initial data (15) with when \( A(x) = \text{sech} x \) and \( S'(x) = - \tanh x \), the expression

\[
h(z) = z \ln \sqrt{a^2 + b^2 R(z) - a(z - a) + b^2} - 2 \tau (z - a) R(z) + (1 - z) \left[ \ln b - \frac{i\pi}{2} \right] - \ln[R(z) - (z - a)]
\]

(25)

was found in [11]. Modulation equations, as well as expressions for \( h(z; x, \tau) \) for higher genus regions, can be written in the explicit determinantal form (see [13], [14]), however, since these expressions are somewhat involved, they will not be given in this paper.

**Suggestions and conclusions.** Semiclassical limit of the focusing 1D NLS (6) provides a new, mathematically rigorous tool to study modulationally unstable evolution of the attractive 1D BEC. Evolution of the BEC with a one-hump initial data that is governed by the NLS (8) is expected to show two or more qualitatively different regimes (regions of different genera) within \( O(k) \) (see eq. (12)) time interval. Bright soliton experiment of [10] is an example of a typical higher genera region behavior (apparently, for the genus 2 region), attained within the time period of 5ms, where \( k \approx 4 \)ms. In general, any macroscopic characteristic of the evolving condensate can be suggested as an observable. That include (see Fig. 1):

- space-time location of the breaking curves (exact location of a breaking curve is given by (24));
- slowly modulated amplitude \( A(x, \tau) \) in the genus zero (the exact value of \( A(x, t) \) is given through the modulation equation (21));
- the upper and lower envelopes of the high-frequency amplitude oscillations in the genus two region (the envelopes are defined through the Riemann-theta functions).

Calculation of the observables, mentioned above, is based on the semiclassical limit of the scattering data \( f_0(z) \), which, in its turn, can be obtained from \( g(x, 0, \varepsilon) \) through (20), i.e., through the initial amplitude \( A(x) \) and the phase \( S(x) \). However, accurate measurement of the initial phase is often a difficult task. We can turn the question around and ask whether the phase \( S(x) \) can be somehow reconstructed from \( A(x) \) and some observables. Continuation of this line of argument leads to the question of designing some NLS-data, initial or scattering, whose evolution will have certain desired properties and/or fit within some required parameters. Generally speaking, formulae (20)-(24) are valid for a large class of analytic initial data, including, for example, cases of the multi-hump initial data \( A(x) \), and experimental data about evolution of the BEC with multi-hump initial density might be interesting.

1D NLS approximation of the evolving attractive BEC in a cigar-shaped trap may be valid during certain intervals of the total period of observation and not valid during the others. The atoms lost in the experiment of [10] (probably, near the point of the gradient catastrophe), seem to indicate that this is an example of such situation. Perhaps, some other model is needed to trace the evolution of the BEC through the point of the gradient catastrophe into the soliton regime, where the 1D NLS approximation will be working again.
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