A quasi-local Gross–Pitaevskii equation for attractive Bose–Einstein condensates

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Abstract

We study a quasi-local approximation for a nonlocal nonlinear Schrödinger equation. The problem is closely related to several applications, in particular to Bose–Einstein condensates with attractive two-body interactions. The nonlocality is approximated by a nonlinear dispersion term, which is controlled by physically meaningful parameters. We show that the phenomenology found in the nonlocal model is very similar to that present in the reduced one with the nonlinear dispersion. We prove rigorously the absence of collapse in the model, and obtain numerically its stable soliton-like ground state.

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1. Introduction

One of the basic model equations in the field of nonlinear waves with a wider range of applications, is the nonlinear Schrödinger equation (NLSE). It arises, in different forms, in nonlinear optics, polymer-molecule dynamics, plasma physics, many-body quantum systems treated in the Hartree approximation, Bose–Einstein condensation (BEC), and many other problems [1].

A little explored type of NLSE is

\[ i\frac{d\psi(r)}{dt} = \left[ -\frac{1}{2}\Delta + V(r,t) + \int K(r-r')|\psi(r')|^2 \, dr' \right] \psi(r), \]

which includes a nonlocal kernel $K(r-r')$ and an external potential $V(r,t)$. In the case of the local kernel, $K(r-r') = \delta(r-r')$, Eq. (1) goes over into the usual NLSE with an external potential.

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Nonlocal models of this type appear in different contexts: nonrelativistic baryon models, quantum gravity [2], fundamentals of quantum mechanics, thermal self-focusing of laser beams, liquid-helium BEC, and, more recently, BEC with ultracold atomic gases [3–6] and other problems. On the mathematical side, most of the work has concentrated on a specific instance of Eq. (1) which is usually referred to as the Schrödinger–Poisson [7,8] or Schrödinger–Newton [2] system.

It is known that when a weakly interacting boson gas with dominating two-body interactions is cooled down below a certain temperature, it undergoes a phase transition to a collective state which is called a BEC. The theoretical description of such a BEC is provided by the so called Gross–Pitaevskii equation (GPE) [9]

\[ i\hbar \frac{\partial \Psi}{\partial t} = -\frac{\hbar^2}{2m} \nabla^2 \Psi + V(r)\Psi + U_0|\Psi|^2\Psi, \]  

where \( m \) is the boson mass, \( V(r) \) the trapping potential, and \( U_0 = \frac{4\pi \hbar^2 a}{m} \) is proportional to the scattering length \( a \) and characterizes the two-body interaction. The case \( a > 0 \), corresponds to repulsion between the bosons. In this situation solutions to Eq. (2) are well-defined for all times. However, in the case of attractive interactions, \( a < 0 \), collapse (blow-up) may take place in the 2D and 3D cases. The presence of the collapse means that there is a generic set of initial conditions such that the solution \( \Psi(r, t) \) ceases to exist after a finite of time. The evolution of collapsing solutions is a fundamental point in the theory of multidimensional nonlinear Schrödinger (NLS) equations [10]. Many results on collapse in BEC systems (i.e. including the trap) have been obtained previously both in the theoretical (see [11–13] and references therein) and experimental sides (see [14] and references therein).

As it has been mentioned above, Eq. (2) is a local model which approximates the more realistic case of nonlocal interactions in which the potential of the two-body interaction is given by:

\[ U[\Psi] = \int dr \int d^3r' K(r' - r)|\Psi(r, t)|^2|\Psi(r', t)|^2. \]  

The nonlocal kernel \( K(r' - r) \) contains the details of the interaction. The Hamiltonian then reads

\[ H[\Psi] = \int \bar{\Psi} \left[ -\frac{\hbar^2}{2m} \Delta + V(r) \right] \Psi \, dr + U[\Psi], \]  

so that the wave function satisfies a nonlocal NLSE which is [15]

\[ i\hbar \frac{\partial \Psi(r)}{\partial t} = -\frac{\hbar^2}{2m} \nabla^2 \Psi(r) + V_{\text{ext}}(r)\Psi(r) + \int V(r - r')|\Psi(r')|^2 \, dr'. \]  

In accordance with the common situation in BEC we choose the trapping potential to be \( V(r) = V_0/2 (\lambda_x x^2 + \lambda_y y^2 + \lambda_z z^2) \), where \( V_0 \) is a characteristic frequency, and \( \lambda_\alpha \in \mathbb{R} \) (\( \alpha = x, y, z \)) describe the asymmetry of the trapping potential. However, many of our results are also applicable to the case when \( \lambda_j = 0 \), as it will be discussed later.

For positive scattering lengths the nonlocality of the interactions manifests itself only as small corrections [5], but in the case of attractive interactions the nonlocality of the potential is essential. For particularly simple kernels it has been proved in Ref. [16] that the Hamiltonian is bounded below, which is the first step towards a full proof of the global existence of solutions. Qualitative arguments in favor of preventing collapse by nonlocal interactions were also proposed in Ref. [3]. Besides that, in Ref. [4] it has been argued and shown numerically that nonlocality gives rise to oscillations of a wave-packet between
the large scale defined by the trap potential $V$ and a small scale determined by the interaction radius. Indeed, it has been found [4] that at the point when the development of collapse stops, the wave-packet width is still significantly larger than the intrinsic size of the kernel $K$ (3). This raises the question whether it is important to keep the nonlocality in its exact form, or it can be modeled by a simplified quasi-local model. Another reason for the interest of this type of models will be given later.

It is our intention in this paper to provide a general and simple description of the nonlocal interaction using a quasi-local model which retains essentials of the dynamics of the problem.

2. The quasi-local model

We first transform Eq. (5) into a renormalized form by defining new variables, $\tilde{r} = (\tilde{x}, \tilde{y}, \tilde{z}) = (x, y, z)/a_0$, $\tilde{t} = \nu t$, $\tilde{\psi}(\tilde{r}) = \Psi(r)/a_0 = \sqrt{\hbar/m \nu}$, $K(r) = (\hbar^2/m) \tilde{K}(r/a_0)$. Since we will only be using the rescaled variables, we omit the tildes attached to them, so that accordingly transformed Eq. (5) takes the form

$$\frac{i}{\hbar} \frac{\partial \psi}{\partial t} = \frac{1}{2} \nabla^2 \psi + \frac{1}{2} (\lambda^2_{xx} + \lambda^2_{yy} + \lambda^2_{zz}) \psi + \int K(r - r') |\psi(r')|^2 \, dr' \psi. \tag{6}$$

Note that the normalization of the rescaled wave function gives the number of particles in a given BEC state,

$$\|\tilde{\psi}\|_2^2 = \int |\tilde{\psi}|^2 \, dr = N.$$  

The standard local GPE (2) is an approximation to a nonlocal model obtained in the limit of zero interaction radius, replacing the nonlocal potential kernel with a delta-function,

$$K'(r - r') = \delta(r - r'), \quad \text{with} \quad a_0 = 4\pi a/a_0. \tag{8}$$

An exact form of the nonlocal kernel, $K(r)$, can rarely be found, which suggests to introduce an approximate interaction term which reproduces essential dynamical features of the nonlocal model based on Eq. (5). Along with the fact that, in most cases, the finite interaction radius remains small compared to a characteristic scale $\lambda$ of the spatial variation of the wave function, this leads us to a model which takes into account the next term of the expansion in the small parameter $a/\lambda$.

In this paper we consider isotropic interactions, which is the most natural case (other possibilities have also been considered in the literature [5,6]), i.e., $K(r' - r) = K(|r' - r|)$, hence the expansion leads to the following approximation for the interaction energy

$$U[\psi] \approx U_0[\psi] + U_2[\psi], \tag{7}$$

a local part of which is represented by (hereafter $r = |r|$)

$$U_0 = -g_0 \int |\psi|^4 \, dr, \quad g_0 = -\int K(r) \, dr, \tag{8}$$

and the residual nonlinearity is accounted by a term

$$U_2 = \frac{1}{2} g_2 \int |\nabla(|\psi(r)|^2)|^2 \, dr, \quad g_2 = -\int K(r) r^2 \, dr, \tag{9}$$

with positive coefficients $g_0$ and $g_2$. This expansion requires finiteness of $g_2$, i.e., that the interaction kernel has a fast enough decay at infinity, necessary for the convergence of the integral which defines $g_2$ in Eq. (9). Note that, in the framework of the renormalized Eq. (6), the length $\lambda = 2\pi/Q_0$, where
\( Q_0 = \sqrt{g_0/g_2} \), determines a range of the interaction, while the parameter \( g_0 \) determines the strength of the interaction.

In a (near)-collapse situation not only the nonlocality of the two-body collisions, but also three-body interactions should be, generally speaking, taken into account. It is natural to assume that the three-body interactions are repulsive, and in the lowest approximation they may be assumed local, being accounted for by another extra term in the potential of the form 

\[ U_\gamma = \frac{1}{3} \gamma |\psi|^4 \int |\psi|^6 \, d\mathbf{r}, \]

with \( \gamma > 0 \). The local equation with a contribution from this term, which is usually called a cubic–quintic NLS equation, has recently attracted considerable attention in nonlinear optics (see [19] and references therein). It is easy to estimate that the extra quintic term in GPE is negligible provided that \( g_4 \ll g_0 g_2 \), which will be assumed here to hold. There is another reason for neglecting this term: in usual condensates, losses are due to three-body collisions, which means that, if quintic terms are relevant, they should correspond to dissipative perturbations and thus lead to condensate extinction in a finite time. Since we are interested on effect of the nonlocality, we do not consider the quintic terms.

The application of the standard variational procedure to the terms in the Hamiltonian (7) yields a uniquely defined quasi-local modified GPE

\[ i \frac{\partial \psi}{\partial t} = -\frac{1}{2} \nabla^2 \psi + V(\mathbf{r}) \psi - g_0 |\psi|^2 \psi - g_2 \psi \nabla^2 (|\psi|^2). \tag{10} \]

In this model we have a single parameter \( g_2 \) accounting for the nonlocal interaction, replacing the (usually unknown) full interaction potential. Of course, to completely examine the validity of the new model, it is necessary to show that it reproduces basic the dynamical features generated by the full Eq. (5).

Similar models without an external potential term appear in different physical situations [20–22]. The one-dimensional version of Eq. (10) has been studied in Ref. [17] and some limited results were given in [22] for the two-dimensional case. Here we concentrate on a detailed analysis of multidimensional problems \((D = 2, 3)\).

3. Radially symmetric solutions

3.1. Self-similar solutions

The simplest version of Eq. (10) is that with the radial symmetry. Radially symmetric solutions are interesting since they allow direct insight into the collapse process [10,18]. Thus we will look for solutions \( \psi(\mathbf{r}, t) = \psi(r, t) \) in two \((D = 2)\) or three \((D = 3)\) dimensions. In this case, Eq. (10) reads

\[ i \frac{\partial \psi}{\partial t} = \frac{1}{2} r^{D-1} \frac{\partial}{\partial r} \left( r^{D-1} \frac{\partial \psi}{\partial r} \right) + \frac{1}{2} r^{D-1} \psi - g_0 |\psi|^2 \psi - g_2 \frac{1}{r} \frac{\partial}{\partial r} \left( r^{D-1} |\psi|^2 \right) \psi. \tag{11} \]

To analyze the existence of collapsing solutions it is customary to renormalize the radially symmetric solution with a scale factor \( L(t) \) [18]

\[ \psi = L(t) \xi, \quad \xi = \frac{r}{L}, \quad \tau = \frac{t}{L^2}. \tag{12} \]

The evolution equation is then reduced to the form

\[ i \frac{\partial u}{\partial \tau} = -\Delta u + L^4 \xi^2 u - g_0 |u|^2 u - g_2 L^{-2} \Delta (|u|^2), \]
$\Delta$ standing for the standard Laplacian in the radially symmetric case. The scaling with regard to $L$ shows that, in the limit $L \to 0$, which corresponds to the collapse, the nonlinear dispersion term becomes the dominant one, while the contribution of the confining potential is negligible. This simple analysis suggests that the role of the nonlinear dispersion term could be the same as that already found in the analysis of fully nonlocal models \[4\], i.e., the term under consideration may suppress the collapse.

As a side result, we notice that, since the nonlinear model is not invariant under the renormalization \(12\), any symmetric ground state having the form $\psi(r,t) = \phi(r) \exp(-i\mu t)$ must have a uniquely defined radius (in other words, a scale-invariant family of ground states cannot exist in this model).

To check the expected collapse inhibition and oscillations, similar to those already observed in the full nonlocal model \[4\], we have simulated Eq. (11) in different situations. A typical result is shown in Fig. 1 where we have simulated the evolution of Gaussian initial data for $g_0 = 8.0, g_2 = 0.2$. When $g_2 = 0$ this initial profile leads to collapse. However, it is seen from Fig. 1(c) that the nonlinear dispersion term indeed stops the collapse even when $g_2$ is small and the wave functions performs oscillations (Fig. 1(b) and (c)).

3.2. The variational approximation

To get a deeper insight into the behavior of the radially symmetric solutions to Eq. (11), it is customary to study the behavior of solutions, assuming a fixed functional form for them, and approximating the dynamics by evolution equations for a few parameters which determine the functional form. In this subsection, we restrict our analysis to radially symmetric solutions in two or three spatial dimensions.

Once the radial symmetry is imposed, the Hamiltonian for Eq. (10) takes the form

$$H(\psi) = \frac{1}{2} \int |\nabla \psi|^2 \, dr + \frac{1}{2} \int r^2 |\psi|^2 \, dr - \frac{g_0}{2} \int |\psi|^4 \, dr + \frac{g_2}{2} \int (\nabla |\psi|^2)^2 \, dr.$$ Substituting a Gaussian ansatz, $\psi(r,t) = A(t) \exp(-r^2/(2\sigma(t))^2 + i\beta(t)r^2)$, into the Hamiltonian and imposing the constraint stating that $N$ is

Fig. 1. Oscillatory behavior of solutions of Eq. (11) for Gaussian initial data and parameter values $g_0 = 8.0, g_2 = 0.2$: (a) spatial profile $|\psi(r,t = 7.6)|^2$; (b) solution’s width, $W = (1/2\pi) \int r^2 |\psi|^2 \, dr$, vs. time $t$; (c) amplitude vs. time, $|\psi(0,t)|^2$. 

[Diagram and calculations]
fixed, we find the following expression for the effective Hamiltonian:

$$H(w) = N\kappa_1 \left( \frac{1}{w^2} + w^2 - \frac{g_0 N_2}{w^2} + \frac{g_2 N_3}{w^{1+D}} \right),$$  \hspace{1cm} (13)

where $\kappa_1, \kappa_2$ and $\kappa_3$ are the three positive numerical constants, and $D$ is the dimensionality of the space. From Eq. (13), we see that the term proportional to $g_2$, which is produced by the nonlinear dispersion term in (13), is the dominant one for $w \to 0$, preventing collapse in this approximation.

A simple estimate of the minima of $H(w)$ provides $w_{\text{min}} \sim \sqrt{g_2/g_0}$ as $g_2$ approaches zero. This result is consistent with the analysis of Ref. [4], where the minimum was found to be related to the effective radius (range) of the potential.

4. Exact results

While the variational approach is intuitively appealing, one cannot make any definite statements based on this approximation. Also, up to now, our analysis has been restricted to solutions with radial symmetry. In this section we present more rigorous arguments supporting the idea that collapse is prevented in Eq. (10). We note that it was previously argued in Ref. [22] that a quasi-local model of the present type is collapse-free in 2D. Here we present a more rigorous proof of this assertion and consider the physically relevant 3D case.

Since the density $\rho(r) \in L^2(\mathbb{R}^D)$ its Fourier transform

$$\hat{\rho}(k) = (2\pi)^{-D/2} \int \rho(r) \exp(ikr) \, dr,$$  \hspace{1cm} (14)

is well-defined. The Parseval identity in this case is

$$\int \rho^2(r) \, dr = \int |\hat{\rho}(k)|^2 \, dk.$$  \hspace{1cm} (15)

If $(\nabla \rho)^2$ exists as well and it is integrable, we can perform a similar Fourier transformation to get

$$\int (\nabla \rho(r))^2 \, dr = \int k^2 |\hat{\rho}(k)|^2 \, dk.$$  \hspace{1cm} (16)

It is clear that the integrand of Eq. (16) is always larger than that of Eq. (15), except inside the sphere $|k| \leq 1$. Let us then define a sphere of a radius $Q$ and arrive to the following inequality:

$$\int \rho^2(r) \, dr \leq \frac{1}{R^2} \int (\nabla \rho(r))^2 \, dr + \int_{|k| \leq 1} \left( 1 - \frac{k^2}{Q^2} \right) |\hat{\rho}(k)|^2 \, dk.$$

Bounding the Fourier transform as

$$|\hat{\rho}(k)| = (2\pi)^{-D/2} \int \rho(r) \exp(-ikr) \, dr \leq (2\pi)^{-D/2} \int \rho(r) \, dr = (2\pi)^{-D/2} N.$$  \hspace{1cm} (18)

We can impose a bound on the first nonlinear term

$$\int |\psi(r)|^4 \, dr \leq \frac{1}{Q^4} (\int |\psi|^2 \, dr + (2\pi)^{-D/2} N^2 \chi(Q)).$$  \hspace{1cm} (19)
Here $\mathcal{V}(Q)$ is a positive function

$$\mathcal{V}(Q) = \int_{k \leq Q} \left(1 - \frac{k^2}{Q^2}\right) dk,$$

(20)

which is always smaller than the volume $V(Q)$ of the $D$-dimensional ball of the radius $Q$: $0 < \mathcal{V}(Q) < V(Q)$.

Transferring all the bounds back to the nonlinear quasi-local interaction potential $U[\psi]$ and choosing $Q = Q_0$, defined above, we obtain the result

$$U[\psi] = \frac{1}{2} \mathcal{B} \left[ -\int |\psi(r)|^4 \, dr + \frac{1}{K_0} \int (\nabla|\psi|^2)^2 \, dr \right] \geq -\frac{g_0}{2(2\pi)^{D/2}} N^2 \mathcal{V}(Q_0) = -C^2(Q_0).$$

(21)

Let us notice that

$$E[\psi] \equiv \langle -\frac{1}{2} \Delta \rangle + \langle V_{\text{ext}}(r) \rangle \geq 0,$$

(22)

is always nonnegative and represents the kinetic plus the potential energy in the trap (here we use the usual definition of averaging $\langle f \rangle = \int \bar{\psi} f \psi \, dr$). However the contribution of $U[\psi]$, may be negative. Nevertheless, as we have found above, there is also a lower bound for this term.

Combining the inequalities (21) and (22), we obtain the estimate

$$H[\psi] \geq U[\psi] \geq -C^2(Q_0).$$

(23)

From here it also follows that the kinetic energy of any given solution is bounded by the sum of the net energy of that solution (which is an integral of motion) and the bound from Eq. (21)

$$\langle -\frac{1}{2} \Delta \rangle \leq H + C^2(Q_0).$$

(24)

The last result proves that the $H^1$ norm of the solution, defined as $\|\psi\|_{H^1}^2 = \int (\nabla|\psi|^2 + |\psi|^2) \, dr$, is bounded, which means that the solution does not develop singular gradients and there is no collapse.

Strictly speaking, to complete the rigorous proof, it is necessary to formally prove the local existence of solutions in $H^1$. Although the latter technical point is mathematically difficult, it is physically clear that this must be true for the present model.

We will now show that the width of the wave-packet is bounded away from zero (i.e., that a catastrophic self-compression of the state, which is the most typical feature of the collapse, does not occur here). This fact alone does not prevent the collapse [10], although it is considered as an indication of collapse suppression. The proof begins with the Heisenberg’s uncertainty relation, which leads us to the following inequality:

$$\frac{1}{2} \left| \int \bar{\psi}(r \cdot \nabla - \nabla \cdot r) \psi \, dr \right|^2 \leq (-\Delta)(r^2).$$

(25)

It is not difficult to realize that our final result is tantamount to the following lower bound for the width of the wave-packet

$$\langle r^2 \rangle \geq \frac{1}{4} \mathcal{B} + \frac{N^2}{H + C^2(Q_0)} > 0.$$

(26)

It is important to remark that the inverse of the wavenumber $Q_0$ gives the length scale $\lambda$ at which the nonlinear dispersive term becomes dominant. The length scale may also be interpreted as a typical width of the ground state wave-packet, hence we conclude that the collapse is stopped at a scale $\lambda \sim \sqrt{\mathcal{B}/g_0}$. 


5. Solitary waves: ground states

Let us consider solitary wave solutions to Eq. (10) in the form
\[ \psi(r, t) = \phi(r) e^{-i\mu t}. \] (27)

These solutions are critical points of the Hamiltonian given by Eq. (4). The fact that they are critical points means that the variational derivative of \( H[\psi] \), for a fixed norm, vanishes, i.e., \( \delta H(\phi)\big|_{\|\phi\|^2 = N} = 0 \).

It is interesting to characterize these solutions since they correspond to stationary configurations of BEC with the nonlocal attractive self-interaction. In particular we will be interested in the solution minimizing \( H \) globally, i.e., the ground state. The fact that the ground state corresponds to a minimum of the energy implies its dynamical stability, which rules out the possibility of collapse of this configuration.

We have searched numerically for the ground state by using a steepest descent method modified using the so called Sobolev gradients technique. The details of the technique may be found in [23].

We have applied this method to the 2D and 3D versions of Eq. (10). For fixed \( g_0 (g_0 = 9.0 \) in the 2D trap, \( g_0 = 20.0 \) in the 3D case), we varied \( g_2 \) within the range [0.01,1.0], finding the ground state. In Fig. 2(a) we plot several examples of such solutions. From Fig. 2(b), it is clear that the ground state width scales according to a power law of the type \( X \sim \sqrt{g_2} \).

We have performed this minimization both in radially symmetric traps (\( \lambda_x = \lambda_y = \lambda_z = 1 \)), in asymmetric ones (\( \lambda_{x,z} = 1, \lambda_y = 1.5 \)), and in free space (\( \lambda_{x,y,z} = 0 \)) with periodic boundary conditions, observing no significant difference, neither in the asymptotic behavior of the wave-packet’s width for small \( g_2 \), nor onset of any type of instability.

In accordance with what was said above, we arrive at a general conclusion that, because the ground state has a small size and it is supported by the balance between the kinetic energy and self-interaction (including its dispersive part), it is expected to be practically independent of the external trapping potential, i.e., this ground state is, as a matter of fact, a BEC “soliton”, similar to stable multidimensional optical solitons in the form of “light bullets”.

![Fig. 2. (a) Density profiles of a radially symmetric three-dimensional ground state solutions for \( g_0 = 20.0, g_2 \in \{0.0, 0.7, 0.5, 0.3\} \) and \( N = 1 \) (dashed and solid lines). Solid curve corresponds to \( g_2 = 0 \), and the dotted line represents a solution with \( g_0 = g_2 = 0 \). (b) Ground state width \( X = \langle \psi^4 \rangle^{1/4} \) for \( D = 2 (g_0 = 9.0; \) upper solid line), and \( D = 3 (g_0 = 20.0; \) lower solid line), as a function of \( g_2 \). The dashed lines represent asymptotic behavior, \( X \sim g_2^\alpha \), with \( \alpha = 0.5(0) \) and 0.5(5) for \( D = 2 \) and 3, respectively.]
6. Conclusions and discussion

In this paper we have proposed a quasi-local model with a nonlinear dispersion term which approximates the nonlocal term describing interactions between bosons in a Bose–Einstein condensate. Our quasi-local description retains all the essential features of the full nonlocal model: collapse prevention, dependence of the width of the ground state on the interaction range, oscillatory behavior, and insensitivity of the eventually established soliton-like state to the particular trapping potential.

Our simplified description of the nonlocal interaction has the advantage that only the knowledge of the scattering length and the range of interaction are necessary to introduce the model, while the full consideration of the nonlocal term requires the knowledge of the precise form of the interaction potential. Of course, by using this approximation some information on the interaction is lost, but we expect the model to be quite accurate when the scattering length is smaller than the interaction range.

Although the motivation for our simplified model originated in the analysis of condensate with radially symmetric interactions between particles, its extension to a more complex situation with dipole–dipole forces, which occur in several experimental realizations of the BEC [5], will be a subject of a future work. In fact, the model used here is not restricted to the BEC phenomena; it can also be quite useful in any physical situation where nonlocal self-interactions appear.

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