Similarity solutions and collapse in the attractive Gross-Pitaevskii equation

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We analyze a generalized Gross-Pitaevskii (GP) equation involving a paraboloidal trap potential in D space dimensions and generalized to a nonlinearity of order $2n+1$. For *attractive* coupling constants collapse of the particle density occurs for $Dn\geqslant 2$ and typically to a δ function centered at the origin of the trap. By introducing a special variable for the spherically symmetric solutions, we show that all such solutions are self-similar close to the center of the trap. *Exact* self-similar solutions occur if, and only if, $Dn=2$, and for this case of $Dn=2$ we exhibit an exact but rather special $D=1$ analytical self-similar solution collapsing to a δ function which, however, recovers and collapses periodically, while the ordinary GP equation in two space dimensions also has a special solution with periodic δ function collapses and revivals of the density. The relevance of these various results to attractive Bose-Einstein condensation in spherically symmetric traps is discussed.

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The experimental discovery of Bose-Einstein condensation in trapped vapors of cooled alkali-metal atoms [1–4] has opened up unique possibilities for the investigation of collective many-body effects in dilute gases. In the experiments the cloud of atoms is isolated from the environment by a magnetic trap. After cooling, the cloud exhibits Bose-Einstein condensation, i.e., the existence of a macroscopically populated quantum state. The study of the dynamics of this quantum state is an important fundamental problem in many-body quantum physics. For three space dimensions $D=3$, the dynamics of the condensate can be described within the Hartree-Fock approximation by the Gross-Pitaevskii equation

$$i\hbar\Phi_t+\frac{\hbar^2}{2m}\Delta_x\Phi-\frac{4\pi\hbar^2 a_s}{m}\Phi|\Phi|^2-V(\vec{x})\Phi=0, \qquad (1)$$

where $\Phi(\vec{x},t)$ is the wave function of the condensate, the external potential $V(\vec{x})$ models the wall-less confinement (the trap), m is the mass of an individual atom, a_s is the scattering length, and $\Delta_x=\Sigma_i^3\partial^2/\partial x_i^2$ is the Laplace operator. A convenient choice for the confining trap is the paraboloidal potential, assumed here to be spherically symmetric for simplicity, i.e., $V=(m\omega_0^2/2)\vec{x}^2$.

In this paper we are concerned with condensates in $D=3$ and $D=2$ dimensions. The Bose-Einstein condensate in two space dimensions is only marginally stable in that below the critical temperature correlations decay, but decay only as a power law [5,6]. Recent experimental techniques allow realization of a two-dimensional trap for, e.g., spin-polarized hydrogen adsorbed on a helium surface [7,8]. The dynamics of trapped Bose-Einstein condensates and the search for the related solitonlike solutions of the Gross-Pitaevskii equations is thus an interesting and relevant problem also in two dimensions. In this paper we concentrate on some aspects of this dynamics and on the existence of self-similar solutions of the Gross-Pitaevskii equation in particular. Self-similarity is an important and useful concept in nonlinear dynamics, particularly so when collapsing systems are being considered [9,10] as they are below. This phenomenon of collapse appears in Bose-Einstein condensates with negative scattering length, as for example in ^{7}Li (see, e.g., [11]). In this paper we show that self-similar behavior appears only in two-dimensional traps although "attractive" condensates ($a_s<0$) collapse for all $D\geqslant 2$.

To begin with we consider a generalized D-dimensional Gross-Pitaevskii (GP) equation, which for units such that $\hbar=1$, $m=1/2$ can be expressed in the form

$$i\psi_t+\Delta_x\psi-2\kappa\psi|\psi|^{2n}-\frac{\omega^2}{4}r^2\psi=0. \qquad (2)$$

Here Δ_x is the D-dimensional Laplace operator and $r^2=\Sigma_i^D x_i^2$. Notice that "generalization" means here an exponent $2n$ instead of the 2 that appears in the ordinary GP equation. We consider only the attractive case of Eq. (2) $\kappa<0$, and the boundary conditions are vanishing at infinity. An observation is that a symmetry that leaves Eq. (2) invariant is

$$\psi(\vec{x},t)\rightarrow e^{i\{\omega/4\,\sin(\omega t+\varphi_0)[2\vec{x}\cdot\vec{\eta}_0+\vec{\eta}_0\cdot\vec{\eta}_0\cos(\omega t+\varphi_0)]\}}\times\psi(\vec{x}+\vec{\eta}_0\cos(\omega t+\varphi_0),t), \qquad (3)$$

in which $\vec{\eta}_0$ is an arbitrary vector in D dimensions and φ_0 is an arbitrary phase. This symmetry reveals the, in general, *oscillatory* character of the wave packet dynamics of Eq. (2) whether $\kappa>0$ or $\kappa<0$. In Ref. [9] and its references "collapse" was demonstrated for $\omega=0$ and $\kappa<0$. Solutions become singular in a final time interval if the condition

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$$nD \geqslant 2 \tag{4}$$

is fulfilled. We show here how the same condition arises in the present context, where $\omega \neq 0$ (and $\kappa < 0$). Reference [12] has addressed the same problem (of $\omega \neq 0$) for $n=1$ and $D=2$ and 3. Following both [9] and [12] we use the functional $U[\psi] = \int_{R^D} r^2 |\psi|^2 d^D x$ in which $r = |\vec{x}|$: $U[\psi] \geqslant 0$. From Eq. (2) this functional satisfies a second order ordinary differential equation whose solution is

$$U[\psi] = \frac{4\sin^2(\omega t)}{\omega^2} E_{NLS} + U_0 \cos^2(\omega t) + J_0 \frac{\sin(2\omega t)}{2\omega} + \frac{4\kappa(Dn-2)}{\omega(n+1)} \int_0^t \sin[2\omega(t-t')] I_{2n+2}[\psi] dt' \tag{5}$$

with

$$U_0 = U[\psi]|_{t=0}, \quad J_0 = \frac{d}{dt} U[\psi]\bigg|_{t=0},$$

$$E_{NLS} = E[\psi] - \frac{\omega^2}{4} U_0, \tag{6}$$

$$I_q[\psi] = \int_{R^D} |\psi|^q d^D x,$$

where

$$E[\psi] = \int_{R^D} \left(|\nabla \psi|^2 + \frac{2\kappa}{n+1} |\psi|^{2n+2} + \frac{\omega^2}{4} r^2 |\psi|^2 \right) d^D x \tag{7}$$

is an obvious ''energy'' functional and is the Hamiltonian of Eq. (2) with the bracket $\{\psi(\vec{x}), \psi^*(\vec{y})\} = i\delta(\vec{x} - \vec{y})$.

The Hamiltonian Eq. (7) is a constant of the motion fixed by the initial data. For $\kappa < 0$ and smooth enough initial data it is not bounded below, while E_{NLS} as defined in Eqs. (6) has the same properties. The condition $E_{NLS} \leqslant 0$, for example, still admits a large amount of physically accessible initial data. A second constant of the motion is $\int_{R^D} |\psi|^2 d^D x \equiv \mathcal{N}$, the total number of bosons (atoms). Careful scrutiny of $U[\psi]$ of Eq. (5) then shows (see also [9,12]) that, provided that

$$\kappa < 0, \quad Dn \geqslant 2, \quad E_{NLS} \leqslant 0, \tag{8}$$

with the exception of the special case $Dn = 2$, $E_{NLS} = J_0 = 0$, there is always at least one point $t = t_* \in (0, \pi/2\omega]$ such that the right hand side of Eq. (5) becomes negative for $t > t_*$. Since by its definition the functional $U[\psi]$ is nonnegative, this contradiction leads to the conclusion that ψ cannot be continued beyond the point $t = t_*$ and must exhibit a singularity. We show below that this singularity is typically $|\psi|^2 \to \mathcal{N}\delta(\vec{x})$. However, for the special case $Dn = 2$, $E_{NLS} = J_0 = 0$, the functional $U[\psi] = U_0 \cos^2(\omega t)$ never becomes negative. We show below that collapse in $|\psi|^2$ occurs with $|\psi|^2 \to \mathcal{N}\delta(\vec{x})$ as $t \to t_*$, but now this can be followed by revival and periodic collapse of period π/ω. There is some evidence that a form of collapse could occur in general even when $U[\psi]$ apparently remains positive, i.e. at some point $t < t_*$ (see [14,15] and references therein where $\omega \equiv 0$). We shall assume here that collapse occurs only at a zero of $U[\psi]$.

Thus the conditions Eq. (8) are sufficient for $U[\psi]$ to reach a zero at $t = t_* \leqslant \pi/2\omega$ and, generically at least, $|\psi|^2 \to \mathcal{N}\delta(\vec{x})$ there. These conditions are sufficient but not necessary: for given such evolution for $E_{NLS} \leqslant 0$, the transformation Eq. (3) can increase E_{NLS} to > 0 while the evolution remains singular. This is true, for example, for the exact analytical solution Eq. (25) for $Dn = 2$ that we give below. The formation of these singularities may be very sensitive to the initial conditions and the values of the parameters. Evidently these results mean that for $E_{NLS} \leqslant 0$ initially collapse and blow-up will occur for all $\mathcal{N} \geqslant \mathcal{N}_c$ [12] (see also [13] and references therein).

We turn to the problem of similarity solutions which within the terms of our analysis arise only for $Dn = 2$. We seek spherically symmetric solutions of Eq. (2) in the form $\psi(r,t) = A(r,t) e^{i\phi(r,t)}$ in which $r = |\vec{x}|$. From Eq. (2) we arrive at the set of equations

$$\frac{\partial A^2}{\partial t} + \frac{2}{r^{D-1}} \frac{\partial}{\partial r}\left(r^{D-1} A^2 \frac{\partial \phi}{\partial r} \right) = 0, \tag{9}$$

$$\frac{1}{r^{D-1}} \frac{\partial}{\partial r}\left(r^{D-1} \frac{\partial A}{\partial r} \right) - \left[\frac{\partial \phi}{\partial t} + \left(\frac{\partial \phi}{\partial r} \right)^2 + \frac{\omega^2}{4} r^2 \right] A - 2\kappa A^{2n+1} = 0. \tag{10}$$

It is not evident how similarity solutions could be constructed from this set of equations in the general case, and we therefore choose to make an ansatz for the amplitude variable $A(r,t)$:

$$A(r,t) = \left(\frac{\eta(r,t)}{r} \right)^{(D-1)/2} \left(\frac{\partial \eta(r,t)}{\partial r} \right)^{1/2} A_0(\eta(r,t)). \tag{11}$$

This ansatz solves Eq. (9) provided that the function η satisfies

$$\frac{\partial \eta}{\partial t} + 2 \frac{\partial \eta}{\partial r} \frac{\partial \phi}{\partial r} = 0. \tag{12}$$

Notice that the function $A_0(\eta)$ is arbitrary and the ansatz Eq.(11) describes an *arbitrary* spherically symmetric solution. The gradient $\partial\phi/\partial r$ is related to the velocity of the particles of the condensate, and, through Eq. (12), $\eta(r,t)$ is then related to the local time dependent concentration of condensate particles. In fact $\eta(r,t)$ completely determines this concentration as is evident from the number of particles $n(r,t)$ in the interval $[0,r]$, which is

$$n(r,t) \equiv \Omega_D \int_0^r r^{D-1} A^2(r,t) dr = \Omega_D \int_0^\eta \eta^{D-1} A_0^2(\eta) d\eta,$$

$$\Omega_D = \frac{2\pi^{D/2}}{\Gamma(D/2)}, \tag{13}$$

while $n(\infty,t)=\mathcal{N}$ is independent of t. From the ansatz Eq. (11) we can deduce that $\eta(r,t)$ is a monotonically increasing function of r, i.e., $\partial\eta/\partial r>0$, and $\eta\to\infty$ when $r\to\infty$. Also, in the vicinity of the origin $r=0$, η behaves as

$$\eta(r,t)=r/\rho(t)+O(r^2), \tag{14}$$

where $\rho(t)$ is a function of time. The solution for $\eta(r,t)$ is self-similar if $\eta=r/\rho(t)$ exactly. This ''self-similarity'' is in the sense that the function η depends now on a single variable $\eta=r/\rho(t)$. From Eq. (12) it follows immediately that in this case the *phase* $\phi(r,t)$ is quadratic in r,

$$\phi(r,t)=\phi_0(t)+\frac{1}{4}\frac{\rho'(t)}{\rho(t)}r^2. \tag{15}$$

Equation (10) should now be understood as an equation for A_0. Consider first the case $nD=2$. Separating the variables in this equation we find that

$$\frac{1}{\eta^{D-1}}\frac{\partial}{\partial\eta}\left(\eta^{D-1}\frac{\partial A_0}{\partial\eta}\right)-2\kappa A_0^{2n+1}-(\mu+\lambda\eta^2)A_0=0, \tag{16}$$

$$\phi_0'+\frac{\mu}{\rho^2}=0, \tag{17}$$

$$\rho''+\omega^2\rho-\frac{4\lambda}{\rho^3}=0. \tag{18}$$

Here λ and μ are arbitrary constants.

A solution of Eq. (18) can easily be found in the form

$$\rho(t)=\sqrt{\cos^2(\omega t)+\frac{4\lambda}{\omega^2}\sin^2(\omega t)}. \tag{19}$$

Other solutions can be obtained through the transformation $t\to t+t_0$ and $\rho(t)\to h(t)\rho(s(t))$, where

$$h(t)=[\sqrt{1+\alpha^2}+\alpha\cos(2\omega t)]^{1/2},$$
$$s(t)=\frac{1}{\omega}\tan^{-1}[(\sqrt{1+\alpha^2}-\alpha)\tan(\omega t)]. \tag{20}$$

We have thus demonstrated that, for $nD=2$, $\eta(r,t)=r/\rho(t)$ with $\rho(t)$ given by Eqs. (19) and (20) is indeed a solution, and Eqs. (11) and (15) now provide the corresponding self-similar solution of the Gross-Pitaevskii equation Eq. (2). For the explicit form of this solution one still needs to solve Eq. (16) for $A_0(\eta)$.

In the case $nD\neq 2$ there are no self-similar solutions (except the trivial case $\rho=\text{const}$). Indeed, for the existence of such solutions we need to require that both A_0^{2n} and $\Delta_\eta A_0/A_0$ are functions quadratic in η. These conditions obviously cannot be satisfied. This means that, even though the solution given by Eq. (11) is locally self-similar for any D in the vicinity of $r=0$, the exact self-similarity is only realized for $Dn=2$.

For the self-similar solutions there are two integral identities. Multiplying Eq. (16) by $\eta^{D-1}A_0$ and by $\eta^D\partial A_0/\partial\eta$, respectively, and integrating by parts, we find after a little algebra that

$$\int_0^\infty d\eta\,\eta^{D-1}\left[\left(\frac{\partial A_0}{\partial\eta}\right)^2+\frac{2\kappa}{n+1}A_0^{2n+2}-\lambda\eta^2A_0^2\right]=0, \tag{21}$$

$$\int_0^\infty d\eta\,\eta^{D-1}\left[\left(\frac{\partial A_0}{\partial\eta}\right)^2+\kappa\frac{n+2}{n+1}A_0^{2n+2}+\frac{1}{2}\mu A_0^2\right]=0. \tag{22}$$

Using the identity Eq. (21) we easily find that the total energy of the solution, $E[\psi]$ [Eq. (7)] is given by

$$E[\psi]=\frac{1}{4}e(\rho)\int_0^\infty\eta^{D+1}A_0^2(\eta)d\eta,$$
$$e(\rho)=(\rho')^2+\omega^2\rho^2+\frac{4\lambda}{\rho^2}. \tag{23}$$

As an example of an exact solution of Eq. (16) we consider here the attractive generalized GP equation in one dimension: $D=1$, $(n=2)$, $\lambda=0$, and $\kappa<0$. In this case we find that

$$A_0(\eta)=\frac{p_0}{\sqrt{\cosh\left(\frac{2}{3}\sqrt{6|\kappa|}p_0^2\eta\right)}},\quad \mu=\frac{2}{3}|\kappa|p_0^4, \tag{24}$$

and the solution of Eq. (2) can be expressed in the form

$$\psi(x,t)=\frac{p_0}{\sqrt{\cos(\omega t)}}\times\frac{\exp\{-i\tan(\omega t)[(\omega/4)x^2-(2/3\omega)|\kappa|p_0^4]\}}{\sqrt{\cosh\left[\frac{2}{3}\sqrt{6|\kappa|}p_0^2x/\cos(\omega t)\right]}}. \tag{25}$$

For an attractive condensate ($\kappa<0$) we expect the solution to become singular at a finite time. But it is indeed obvious that the solution Eq. (25) becomes singular for $t\to\pi/2\omega$ when its amplitude diverges as $1/\sqrt{\pi/2\omega-t}$. In this limit $|\psi|^2\to(\pi/2)\sqrt{3/2|\kappa|}\delta(x)=\mathcal{N}\delta(x)$, which is the convergence to the δ function expected. Notice that $|\psi|^2$ from Eq. (25) is now periodic of period π/ω while the solution Eq. (25) itself has jumps in phase, compounded by branch point singularities, when crossing the singularities of $|\psi|$ at $t=(\pi/2\omega)(2k+1)$, $k\in\mathbf{Z}$ [16].

If now we simply assume that the point of collapse is $t=t_*$ defined below Eq. (8), it can still be shown that the collapse occurs to a δ function centered on the trap. A consideration leading to this conclusion is the following. The equality $U[\psi]=0$ means that $|\psi(\vec{x},t_*)|=0$ for any $\vec{x}$ except possibly at the origin. Since $\mathcal{N}=\int d^Dx|\psi|^2$ is a constant of motion identified as the total number of bosons (atoms), the obvious physical solution is $|\psi|^2=\mathcal{N}\delta(\vec{x})$, excluding other possible generalized functions. The spherically symmetric case can be treated rigorously. Consider for this the functional $U[\psi]$ taken on the ansatz Eq. (11), i.e.,

$$U[\psi]=\int_0^\infty d\eta r^2(\eta,t)\eta^{D-1}A_0^2(\eta). \tag{26}$$

For $U[\psi]=0$ it immediately follows from Eq. (26) that $r(\eta,t_*)=0$. For an appropriate arbitrary test function $\varphi(r)$, consider now the limit

$$\lim_{t\to t_*}\Omega_D\int_0^\infty dr r^{D-1}|\psi(r,t)|^2\varphi(r)$$
$$=\lim_{t\to t_*}\Omega_D\int_0^\infty d\eta\eta^{D-1}|A_0(\eta)|^2\varphi(r(\eta,t))=\mathcal{N}\varphi(0). \tag{27}$$

This result means rigorously that for spherically symmetric solutions for which $U[\psi]$ evolves to a zero at $t=t_*$ the system blows up to the δ function singularity

$$\lim_{t\to t_*}|\psi(r,t)|^2=\mathcal{N}\delta(r).$$

This result is particularly evident for the self-similar solutions for which $\eta=r/\rho$. In this case,

$$U[\psi]=\left(\cos^2(\omega t)+\frac{4\lambda}{\omega^2}\sin^2(\omega t)\right)\int_0^\infty d\eta\eta^{D+1}A_0^2(\eta)$$

and the point of collapse for $\lambda\leqslant 0$ ($E_{NLS}\leqslant 0$) can be readily found as $t_*=(1/\omega)\tan^{-1}(\omega/2\sqrt{|\lambda|})$. Notice again that when $\lambda=0$ the functional U never becomes negative and there is a possibility of periodic δ function collapses and revivals of the condensate density in this case of two-dimensional traps.

Even though the methods are different, some part of the results reported here is analogous to those obtained in Refs. [9,14,15] for the nonlinear Schrödinger equation (NLS), which is the Gross-Pitaevskii equation with $\omega\equiv 0$. This analogy is related to the fact that for $Dn=2$ the generalized NLS and GP equations are equivalent. For the change of variables [17]

$$\theta=\frac{1}{\omega}\tan(\omega t),\quad z_i=\frac{x_i}{\cos(\omega t)}, \tag{28}$$

$$\psi(x,t)=[\cos(\omega t)]^{-D/2}\exp\left\{-i\frac{\omega}{4}\tan(\omega t)r^2\right\}p(z,\theta) \tag{29}$$

maps Eq. (2) to

$$ip_\theta+\Delta_z p-\frac{2\kappa}{(1+\omega^2\theta^2)^{-Dn/2+1}}p|p|^{2n}=0, \tag{30}$$

and it is clear that for $Dn=2$ the θ dependence of the effective ''coupling constant'' disappears and the NLS system is recovered. This means in particular that the whole variety of results available for the two dimensional NLS equation for $n=1$ is directly applicable to the Gross-Pitaevskii equation for $n=1$ in two space dimensions. It is interesting that the Gross-Pitaevskii equation allows a self-similar solution of the type considered in this paper only in this case, when it can be exactly transformed to the NLS equation.

It is worth mentioning that for $Dn=2$ all self-similar solutions of the Gross-Pitaevskii equation are invariant under the transformation

$$\psi(x,t)\to h(t)^{-D/2}\exp\left(\frac{ih'(t)}{4h(t)}r^2\right)\psi\left(\frac{x}{h(t)},s(t)\right). \tag{31}$$

For the solution Eq. (25) this transformation means a mere rescaling $p_0\to p_0/(\alpha+\sqrt{1+\alpha^2})^{1/4}$.

We emphasize that our similarity analysis of the Gross-Pitaevskii equation is based on the ansatz Eq. (11). This approach is applicable to the Gross-Pitaevskii equation in D space dimensions and with an arbitrary external potential $V(\vec{x})$. It can also be shown that the dynamics described by the Gross-Pitaevskii equation for an arbitrary initial condition that has an extremum is effectively equivalent to a system describing a D-dimensional classical particle. This dynamical system generalizes that found in [18] for Gaussian initial profiles through a variational approach. These results will be reported in a forthcoming publication.

We showed in this paper that for $Dn=2$ alone the generalized Gross-Pitaevskii equation [Eq. (2)] allows self-similar solutions, and that in this case it can be exactly transformed to the NLS equation with no trap potential. An explicit solution was given for $D=1$, $n=2$, $\kappa<0$ which displayed a δ function divergence at a finite time. We further showed, for $Dn\geqslant 2$ and $\kappa<0$, that *all* spherically symmetric solutions with $E_{NLS}\leqslant 0$ collapse in a finite time to a δ function centered at the origin of the trap, while we showed generally that even without such symmetry evolution may be to the δ function singularity. The ordinary Gross-Pitaevskii equation in two space dimensions and with $\kappa<0$, $E_{NLS}=0$, was shown to have periodic δ function collapses and subsequent *revivals* of the particle density.

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