SIMILARITY SOLUTIONS AND COLLAPSE IN THE ATTRACTIVE GROSS-PITAEVSIIKII EQUATION

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Abstract

We analyse a generalised Gross-Pitaevskii equation involving a paraboloidal trap potential in D space dimensions and generalised to a nonlinearity of order $2n + 1$. For attractive coupling constants collapse of the particle density occurs for $Dn \geq 2$ and typically to a $\delta$-function centered at the origin of the trap. By introducing a new dynamical 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 $\delta$-function which however recovers and collapses periodically, while the ordinary G-P equation in 2 space dimensions also has a special solution with periodic $\delta$-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 (BEC) in trapped vapours of cooled alkali atoms 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

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

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 $\Delta_x = \sum_i \frac{\partial^2}{\partial x_i^2}$ 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. $V = \frac{m\omega_0^2}{2} x^2$.

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. Recent experimental techniques allow realisation of a two-dimensional trap for e.g. spin-polarized hydrogen adsorbed on a helium surface. The dynamics of trapped Bose-Einstein condensates and the search for the related soliton-like 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 as they are below. This phenomenon of collapse appears in Bose-Einstein condensates with negative scattering length, as for example in $^7\text{Li}$ (see e.g. [11]). In this paper we show that self-similar behaviour only appears in two-dimensional traps although 'attractive' condensates ($a_s < 0$) collapse for all $D \geq 2$.

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

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

Here $\Delta_x$ is the $D$-dimensional Laplace operator and $r^2 = \sum_i^D x_i^2$. Notice that "generalisation" means here an exponent $2n$ instead of the $2$ which appears in the ordinary G-P 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 which leaves Eq. (2) invariant is

$$\psi(\vec{x}, t) \rightarrow e^{i\left\{\frac{n}{4}\sin(\omega t + \varphi_0)(2\vec{x} \cdot \vec{\eta}_0 + \vec{\eta}_0 \cdot \vec{\eta}_0 \cos(\omega t + \varphi_0))\right\}} \psi(\vec{x} + \vec{\eta}_0 \cos(\omega t + \varphi_0), t). \quad (3)$$

in which $\vec{\eta}_0$ is an arbitrary vector in $D$ dimensions, $\varphi_0$ 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

$$nD \geq 2 \quad (4)$$

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

$$U[\psi] = \frac{4\sin^2(\omega t)}{\omega^2}E_{NLS} + U_0 \cos^2(\omega t) + J_0 \frac{\sin(2\omega t)}{2\omega}$$

$$+ \frac{4\kappa(Dn - 2)}{\omega(n + 1)} \int_0^t \sin(2\omega(t - t'))I_{2n+2}[\psi]dt'$$

with

$$U_0 = U[\psi]|_{t=0}, \quad J_0 = \frac{d}{dt}U[\psi]|_{t=0}, \quad E_{NLS} = E[\psi] = \frac{\omega^2}{4}U_0, \quad (6)$$

$$2$$
\[ I_q[\psi] = \int_{R^D} |\psi|^q d^Dx, \]

where

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

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

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 \( E_{NLS} \leq 0 \), for example, still admits a large amount of physically accessible initial data.

A second constant of the motion is \( \int_{R^D} |\psi|^2 d^Dx \equiv N \), the total number of bosons (atoms). Careful scrutiny of \( U[\psi] \) of Eq. (5) then shows (see also [9], [12]) that provided that \( \kappa < 0 \), \( Dn \geq 2 \), \( E_{NLS} \leq 0 \),

(8)

with the exception of the special case \( Dn = 2 \), \( E_{NLS} = J_0 = 0 \), there is always at least one point \( t = t_* \in (0, \frac{\pi}{2\omega}] \) 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 \( \psi \) cannot be continued beyond the point \( t = t_* \) and must exhibit a singularity. We show below that this singularity is typically \( |\psi|^2 \to N\delta(\vec{x}) \). 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 \( |\psi|^2 \to N\delta(\vec{x}) \) as \( t \to t_* \), but now this can be followed by revival and periodic collapse of period \( \pi/\omega \). 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 \( t = t_* \leq \frac{\pi}{2\omega} \) and, generically at least, \( |\psi|^2 \to N\delta(\vec{x}) \) there. These conditions are sufficient but not necessary: for given such evolution for \( E_{NLS} \leq 0 \), 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 \( Dn = 2 \) 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 $E_{NLS} \leq 0$ initially collapse and blow-up will occur for all $N \geq N_c$ [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 $D n = 2$. 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

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

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

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 $A(r,t)$:

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

This ansatz solves Eq. (9) provided that the function $\eta$ satisfies

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

Notice that the function $A_0(\eta)$ is arbitrary and the ansatz Eq. (11) describes an arbitrary spherically symmetric solution. The gradient $\frac{\partial \phi}{\partial r}$ 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

$$n(r,t) \equiv \Omega_D \int_0^r r^{D-1} A^2(r,t) \, dr = \Omega_D \int_0^\eta \eta^{D-1} A_0^2(\eta) \, d\eta, \quad \Omega_D = \frac{2\pi^{D/2}}{\Gamma(D/2)}. \quad (13)$$

while $n(\infty, t) = N$ 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. $\frac{\partial \eta}{\partial r} > 0$, and $\eta \to \infty$ when $r \to \infty$. Also, in the vicinity of the origin $r = 0$, $\eta$ behaves as

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

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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 $\eta$ 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 $r$,

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

The Eq. (10) should now be understood as an equation for $A_0^0$. Consider first the case $nD = 2$. Separating the variables in this equation we find that

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

$$\phi' + \frac{\mu}{\rho^2} = 0$$ \hfill (17)

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

Here $\lambda$ and $\mu$ are arbitrary constants.

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

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

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

$$h(t) = (\sqrt{1 + \alpha^2 + \alpha \cos(2\omega t)})^{\frac{1}{2}}, \quad s(t) = \frac{1}{\omega} \tan^{-1} \left( (\sqrt{1 + \alpha^2} - \alpha) \tan(\omega t) \right).$$ \hfill (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. (10) 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 $\eta$. These conditions cannot
obviously 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 realised 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

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

and

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

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

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

As an example of an exact solution of Eq. (16) we consider here the attractive generalised G-P equation in one dimension: $D = 1, n = 2, \lambda = 0$ and $\kappa < 0$.

In this case we find that

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

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

$$
\psi(x, t) = \frac{p_0}{\sqrt{\cos(\omega t)}} \exp \left\{ -i \tan(\omega t) \left( \frac{2}{3} x^2 - \frac{2}{3 \omega |\kappa| p_0^2} x \right) \right\} \frac{1}{\sqrt{\cosh \left( \frac{2}{3} \sqrt{6|\kappa| p_0^2 \cos(\omega t)} \right)}}. \quad (25)
$$

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. (23) becomes singular for $t \to \frac{\pi}{2\omega}$ when its amplitude diverges as $1/\sqrt{\frac{\pi}{2\omega} - t}$. In this limit $|\psi|^2 \to \frac{2}{\sqrt{2|\kappa|}} \delta(x) = N\delta(x)$ which is the convergence to the $\delta$-function expected. Notice that $|\psi|^2$ from Eq. (23) is now periodic of period
\[ \pi \omega \]

while the solution Eq. (25) itself has the jumps in phase, compounded by branch point singularities, when crossing the singularities of \(|\psi|\) at \(t = \frac{\pi}{2\omega}(2k + 1), \, k \in \mathbb{Z}\).

If now we simply assume that the point of collapse is \(t = t_\ast\) defined below Eq. (8), it can still be shown that the collapse occurs to a \(\delta\)-function centered on the trap. A consideration leading to this conclusion is the following: the equality \(U[\psi] = 0\) means that \(|\psi(\vec{x}, t_\ast)| = 0\) for any \(\vec{x}\) except possibly at the origin. Since \(\mathcal{N} = \int d^D x |\psi|^2\) 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 generalised 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 \(r(\eta, t_\ast) = 0\). For an appropriate arbitrary test function \(\varphi(r)\) consider now the limit

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

This result means rigorously that for spherically symmetric solutions for which \(U[\psi]\) evolves to a zero at \(t = t_\ast\), the system 'blows-up' to the \(\delta\)-function singularity

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

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 \(\lambda \leq 0\) (\(E_{NLS} \leq 0\)) can be readily found as \(t_\ast = (1/\omega)\tan^{-1}\left(\omega/2\sqrt{\lambda}\right)\).

Notice again that when \(\lambda = 0\) the functional \(U\) never becomes negative and there is a possibility of periodic \(\delta\)-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 that 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 generalised NLS and GP equations are equivalent. For the change of variables [17]

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

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

maps Eq.(2) to

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

and it is clear that for $Dn = 2$ the $\theta$ 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 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 only allows a self-similar solution of the type considered in this paper 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

$$\psi(x, t) \rightarrow h(t)^{-\frac{D}{2}} \exp \left( i h(t)^{\frac{4}{h(t)^2}} \right) \psi \left( \frac{x}{h(t)}, \frac{s(t)}{h(t)} \right). \quad (31)$$

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

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 which has an extremum, is effectively equivalent to a system describing a $D$-dimensional classical particle. This dynamical system generalises 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 generalised Gross-Pitaevskii Eq. (2) equation 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 delta function divergence at a finite time. We further showed, for $Dn \geq 2$ and $\kappa < 0$, that all spherically symmetric solutions with $E_{NLS} \leq 0$ collapse in a finite time to a $\delta$-function centered at the origin of the trap while we showed generally that even without such symmetry evolution may be to the $\delta$-function singularity. The ordinary Gross-Pitaevskii equation in 2 space dimensions and with $\kappa < 0, E_{NLS} = 0$, was shown to have periodic $\delta$-function collapses and subsequent revivals of the particle density.

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[16] Physically Eq. (25) must be a special solution related to the particular choice $\lambda = 0$. The normalisation of this solution is independent of the parameters and indeed one checks that $N$ must take the particular value $N = \frac{\pi}{2} \sqrt{\frac{3}{2|\kappa|}}$.

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