Nonlinear dynamics of Bose-Einstein condensates by means of symbolic computations

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Abstract. The symbolic computations needed for the variational treatment of high-density Bose-Einstein condensates are described in detail. Two effectively one- and two-dimensional equations based on q-Gaussian functions are derived for the dynamics of cigar- and pancake-shaped condensates. The main result of our symbolic computations is that the variational recipe yields substantially different results for cigar- and pancake-shaped condensates, the variational equations for cigar-shaped condensates being considerable simpler than those for pancake-shaped condensates.

Keywords: Bose-Einstein condensates, q-Gaussian functions, symbolic computations

1 Introduction

The achievement of the first atomic Bose-Einstein condensate (BEC) in 1995 [1] marks the birth of a new research topic which draws from many distinct fields such as atomic and nuclear physics, condensed matter physics, nonlinear and quantum optics and, interestingly enough, even some selected chapters in symbolic and numerical computations. Along with their almost unprecedented experimental maneuverability, BECs are appealing to theoretical physicists due to a very accurate nonlinear partial differential equation, namely the Gross-Pitaevskii equation (GPE), which describes the $T = 0$ nonlinear dynamics of the condensate [2]. The numerical solution of the GPE is well documented by now [3,4,5,6,7,8], but most numerical recipes are time consuming and provide little immediate insight into the dynamics of the condensates, thought there is a long list of numerical and analytical investigations into the dynamics of quantum gases [9,10,11,12].

Variational methods have been extremely attractive in the BEC community because they provide straightforward analytical insight into the properties of the condensates. The most fashionable methods are those tailored around Gaussian functions, which are known to describe the bulk properties of the wave functions of dilute condensates [13], particularly the frequencies of the collective modes. While Gaussian functions are easy to work with they can not describe accurately the bulk properties of high-density (or, equivalently, highly interacting) condensates where more complex functions have to be considered. Two such functions, namely the S_n [14] and the q-Gaussian [15] functions, have the intriguing property of being able to describe both the low- and the high-density regime. The q-Gaussian functions, in particular, are known to recover analytically the hydrodynamic behavior of high-density condensates and we show here that they can be used to derive effectively one- and two-dimensional equations which describe cigar and pancake-shape condensates [15]. At a more general level, we show in this paper that computer algebra systems are ideally suited for variational investigations into the dynamics of BECs and offer almost immediate answers in regions where traditional paper and pencil calculations are extremely difficult.

2 Non-polynomial Schrödinger Equations

2.1 Cigar-shaped Condensates

The starting point of our investigation is the three-dimensional GPE

$$i\hbar\frac{\partial\psi\left(\mathbf{r},t\right)}{\partial t}=\left[-\frac{\hbar^2}{2m}\nabla^2+V\left(\mathbf{r}\right)+gN\left|\psi\left(\mathbf{r},t\right)\right|^2\right]\psi\left(\mathbf{r},t\right) \tag{1}$$

where $\hbar = h/2\pi$ is the reduced Planck constant, m is the mass of a boson, g measures the strength of the two-body interactions, N is the number of bosons and we consider the trapping potential

$$V\left(\mathbf{r}\right)=\frac{1}{2}m\omega_\perp^2r^2+\frac{1}{2}m\omega_z^2z^2, \tag{2}$$

with $\omega_z \ll \omega_r$, where ω_z (ω_r) represents the longitudinal (radial) frequency of the magnetic trap which confines the condensate. The associated Lagrangian density is given by

$$\begin{aligned}S\left[\psi\left(\mathbf{r},t\right)\right]=\int dtd\mathbf{r}\psi^*\left(\mathbf{r},t\right)&\left[i\hbar\frac{\partial}{\partial t}+\frac{\hbar^2}{2m}\nabla^2-V\left(\mathbf{r}\right)\right.\\&\left.-\frac{1}{2}gN\left|\psi\left(\mathbf{r},t\right)\right|^2\right]\psi\left(\mathbf{r},t\right),\end{aligned} \tag{3}$$

which we will compute analytically using the trial wave function $\psi\left(\mathbf{r},t\right) = \phi\left(r,t;a,q\right)f$ with

$$\phi\left(r,t;a,q\right)=c\left(1-r^2a\left(1-q\right)\right)^{1/(1-q)} \tag{4}$$

and a, q and f are functions of z and t. Imposing that the wave function is normalized to 1, that is $\int dr\left|\psi\right|^2=1$, we obtain

$$c = \sqrt{\frac{a\,(3-q)}{\pi}} \tag{5}$$

and after computing the $x - y$ integrals we have that the Lagrangian density (now only with respect to z) is given by

$$\begin{aligned} S\left[f\left(z,t\right)\right] = \int dtdz f^{*}\left(z,t\right) \Bigg[& i\hbar\frac{\partial}{\partial t} + \frac{\hbar}{2m}\frac{\partial^2}{\partial z^2} \\ & - \frac{gN\left|f\left(z,t\right)\right|^2}{2}\frac{a\left(q-3\right)^2}{\pi\left(5-q\right)} + \frac{\hbar^2}{2m}\frac{2a\left(q-3\right)}{1+q} \\ & - \frac{m\omega_\perp^2}{2}\frac{1}{2a\left(2-q\right)}\Bigg] f\left(z,t\right). \end{aligned} \tag{6}$$

Despite the unappealing form of the q-Gaussian function (which prohibits any immediate paper-and-pencil calculations) the Lagrangian density can be successfully computed analytically using MATHEMATICA's `Integrate` function. We have tried other computer algebra systems, namely Maple, Matlab and Python (with the SymPy library), and have found that, with the exception of Maple, no other program computed the integrals. We stress that despite their apparent difficulty the $x-y$ integrals yield very simple results (ratios of polynomials in q) which makes it straightforward to compute the *exact* Euler-Lagrange equations associated with $S\left[f\left(z,t\right)\right]$. The only requirement of the symbolic integrator is that $q \in [-1,1]$, because otherwise the q-Gaussian function develops two unphysical branches which make the norm of the wave function (and therefore the number of particles) to diverge. As the physically relevant density regime of the condensate is between $q = -1$ (which corresponds to the Thomas-Fermi limit) and $q = 1$ (which corresponds to the low-density limit), the aforementioned divergence is of no physical significance. The ease with which these computations are performed should be contrasted with the extremely restrictive analytical tractability of

$$S_n = \exp\left(-\sum_{k=1}^{n}\frac{x^{2k}}{k}\right) \tag{7}$$

for which one can not perform a simple norm such as $I_n = \int dx S_n^2(x)$ for $n \geq 3$, and already I_2 includes a confluent hypergeometric function.

The equation for $f^{*}(z,t)$ is given by

$$\begin{aligned} i\hbar\frac{\partial f\left(z,t\right)}{\partial t} = \Bigg[& -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial z^2} + gN\left|f\left(z,t\right)\right|^2\frac{a\left(q-3\right)^2}{\pi\left(5-q\right)} \\ & + \frac{\hbar^2}{m}\frac{a\left(3-q\right)}{1+q} + \frac{m\omega_\perp^2}{4a\left(2-q\right)}\Bigg] f\left(z,t\right), \end{aligned} \tag{8}$$

while the equations for a and q are given by

$$\frac{gN\left|f\left(z,t\right)\right|^{2}}{2\pi}\frac{\left(q-3\right)^{2}}{\left(5-q\right)}+\frac{\hbar^{2}}{m}\frac{\left(3-q\right)}{1+q}-\frac{m\omega_{\perp}^{2}}{4a^{2}\left(2-q\right)}=0 \tag{9}$$

and

$$\frac{gN\left|f\left(z,t\right)\right|^{2}}{2}\left(\frac{2a\left(q-3\right)}{\pi\left(5-q\right)}+\frac{a}{\pi}\frac{\left(q-3\right)^{2}}{\left(q-5\right)^{2}}\right)$$
$$-\frac{\hbar^{2}}{m}\left(\frac{a\left(3-q\right)}{\left(1+q\right)^{2}}+\frac{a}{1+q}\right)+\frac{m\omega_{\perp}^{2}}{4a\left(2-q\right)^{2}}=0. \tag{10}$$

The level of difficulty of these equations is similar to that of the equations derived by Salasnich *et al.* [16] for low-density condensates. With specific constraints for the coefficients all computer algebra systems mentioned above are able to provide analytic solutions for equations (9) and (10), but we find it more convenient to restrict the discussion to the high-density regime, that is $N \gg 1$, where the approximate solutions are given by

$$q\approx-1+3\left(\frac{2}{a_{s}\left|f\left(z,t\right)\right|^{2}N}\right)^{1/3} \tag{11}$$

and

$$a\approx\frac{m\omega_{\perp}}{8\hbar\sqrt{a_{s}\left|f\left(z,t\right)\right|^{2}N}}. \tag{12}$$

Using the above solutions we have the desired non-polynomial Schrödinger equation

$$i\hbar\frac{\partial f\left(z,t\right)}{\partial t}=\left\{-\frac{\hbar^{2}}{2m}\frac{\partial^{2}}{\partial z^{2}}+2\hbar\omega_{\perp}\left[\sqrt{a_{s}\left|f\left(z,t\right)\right|^{2}N}\right.\right.$$
$$\left.\left.-\frac{2^{1/3}}{3}\left(a_{s}\left|f\left(z,t\right)\right|^{2}N\right)^{1/6}\right]\right\}f\left(z,t\right) \tag{13}$$

which was originally introduced in [17] to model the emergence of Faraday waves in high-density cigar-shaped condensates. The main message conveyed by the above computations is that in the quasi one-dimensional case the q-Gaussian radial ansatz allows the *exact* calculation of the Euler-Lagrange equations which *i.*) can either be solved simultaneously by numerical means or *ii.*) one can use the approximate high-density regime solutions of equations (9) and (10) and solve numerically equation (13).

2.2 Pancake-shaped Condensates

For pancake-shaped condensates we apply the same variational treatment using the external potential

$$V(\mathbf{r}) = \frac{1}{2}m\omega_\perp^2 r^2 + \frac{1}{2}m\omega_z^2 z^2, \tag{14}$$

now with $\omega_z \gg \omega_r$, and decompose the wave function as $\psi(\mathbf{r},t) = \phi(z,t;w,q) f$ where

$$\phi(z,t;w,q) = c\left(1 - \frac{z^2(1-q)}{2w^2}\right)^{1/(1-q)} \tag{15}$$

and w, q and f are functions of r and t. As before, the wave function is normalized to 1, which yields the normalization constant

$$c = \left(\frac{1-q}{2}\right)^{1/4}\left(w\mathbf{B}\left(\frac{1}{2}, \frac{q-3}{q-1}\right)\right)^{1/2}. \tag{16}$$

Computing the Lagrangian density using the aforementioned ansatz we find

$$\begin{aligned} S[f(r,t)] = \int dtdr f^*(r,t) \Bigg[& i\hbar\frac{\partial}{\partial t} + \frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + \frac{\hbar^2}{2m}\frac{\partial^2}{\partial y^2} \\ & - \frac{mw^2\omega_\perp^2}{7-3q} - \frac{gN|f(r,t)|^2}{2} \cdot \frac{\sqrt{1-q}\mathbf{B}\left(\frac{1}{2}, \frac{q-5}{q-1}\right)}{w\sqrt{2}\mathbf{B}\left(\frac{1}{2}, \frac{q-3}{q-1}\right)^2} \\ & - \frac{\hbar^2}{m}\frac{U_2\left(\frac{1}{2}, 2, \frac{3}{2} - \frac{2}{q-1}, 1\right)}{w^2(3+q)} \Bigg] f(r,t). \end{aligned} \tag{17}$$

Unlike its cigar-shaped sibling, the above Lagrangian density includes both the Euler beta function and the confluent hypergeometric function U [18], which makes it very difficult to work with the exact Euler-Lagrange equation for an arbitrary value of q. One can, of course, derive the exact form of the Euler-Lagrange equations, but the numerous evaluations of the hypergeometric functions preclude simple numerical treatments. Following a detailed analysis of both the Euler beta function and the confluent hypergeometric function U [19], we have found that the Lagrangian density can be well approximated by

$$S[f(r,t)] \approx \int dtdr f^*(r,t) \left[i\hbar\frac{\partial}{\partial t} + \frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + \frac{\hbar^2}{2m}\frac{\partial^2}{\partial y^2} \right.$$

$$
-\frac{mw^2\omega_\perp^2}{7-3q}++\frac{\hbar^2}{2m}\frac{1}{w^2}\left(\frac{1}{4}-\frac{3}{2\,(q+1)}\right)
$$
$$
-\frac{gN\,|f\,(r,t)|^2}{2}\frac{a-b\,(q+1)}{w}\Bigg]\,f\,(r,t)\,, \tag{18}
$$

where a and b are two numerical constants. Using this approximation one can easily derive the Euler-Lagrange equations which lead to

$$
i\hbar\frac{\partial f\,(r,t)}{\partial t} = \Bigg[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial y^2}+\left(\frac{m}{8}\right)^{1/3}\left(\frac{5\,|f|^2\,ag\omega_\perp N}{2}\right)^{2/3}
$$
$$
+\,(3a-40b)\left(\frac{g\,|f|^2\,Nh^3\omega_\perp^4}{2}\right)^{2/9}\frac{m^{1/9}}{4\cdot a^{7/9}3^{1/3}5^{7/9}}\Bigg]\,f\,(r,t)\,.
$$

This is equation is not the exact two-dimensional counterpart of (13) due to the approximations used for the Euler beta and the hypergeometric functions.

3 Conclusions

We have investigated by variational means the dynamics of cigar- and pancake-shaped condensates and have derived effectively one- and two-dimensional equations using symbolic computations. Our main result is that the Euler-Lagrange equations obtained for a q-Gaussian ansatz are very sensitive to the geometry of the condensate. Cigar-shaped condensates, in particular, can be well described using relatively simple variational equations, while pancake-shaped condensates are described by more complex equations which involve the Euler beta function and the confluent hypergeometric function.

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References

1. Pethick, C.J., Smith, H.: Bose-Einstein Condensation in Dilute Gases. Cambridge University Press, Cambridge (2008)
2. Kevrekidis, P.G., Frantzeskakis, D.J., Carretero-González, R. (eds.): Emergent Nonlinear Phenomena in Bose-Einstein Condensates, Springer, New York (2008)
3. Adhikari, S.K.: Numerical study of the spherically symmetric Gross-Pitaevskii equation in two space dimensions. Phys. Rev. E 62, 2937 (2000)
4. Adhikari, S.K.: Numerical solution of the two-dimensional Gross–Pitaevskii equation for trapped interacting atoms. Phys. Lett. A 265, 91 (2000)

5. Adhikari, S.K., Muruganandam, P.: Bose-Einstein condensation dynamics from the numerical solution of the Gross-Pitaevskii equation. J. Phys. B: At. Mol. Opt. 35, 2831 (2002)
6. Adhikari, S.K., Muruganandam, P.: Bose–Einstein condensation dynamics in three dimensions by the pseudospectral and finite-difference methods. J. Phys. B: At. Mol. Opt. 36, 2501 (2003)
7. Muruganandam, P., Adhikari, S.K.: Fortran programs for the time-dependent Gross–Pitaevskii equation in a fully anisotropic trap. Comp. Phys. Comm. 180, 1888 (2009)
8. Vudragović, D. , Vidanović, I., Balaž, A., Muruganandam, P., Adhikari, S.K.: C programs for solving the time-dependent Gross–Pitaevskii equation in a fully anisotropic trap. Comp. Phys. Comm. 183, 2021 (2012)
9. Balaž, A., Nicolin, A.I., Faraday waves in binary nonmiscible Bose-Einstein condensates. Phys. Rev. A 85, 023613 (2012)
10. Vidanović, I., Balaž, A., Al-Jibbouri, H., Pelster, A.: Nonlinear Bose-Einstein-condensate dynamics induced by a harmonic modulation of the s-wave scattering length. Phys. Rev. A 84, 013618 (2011)
11. Balaž, A., Vidanović, I., Bogojević, A., Belić, A., Pelster, A.: Fast converging path integrals for time-dependent potentials: I. Recursive calculation of short-time expansion of the propagator. J. Stat. Mech. P03004 (2011)
12. Balaž, A., Vidanović, I., Bogojević, A., Belić, A., Pelster, A.: Fast converging path integrals for time-dependent potentials: II. Generalization to many-body systems and real-time formalism. J. Stat. Mech. P03005 (2011)
13. Pérez-García, V.M., Michinel, H., Cirac, J.I., Lewenstein, M., Zoller, P.: Low Energy Excitations of a Bose-Einstein Condensate: A Time-Dependent Variational Analysis. Phys. Rev. Lett. 77, 5320 (1996)
14. Keçeli, M., Ilday, F.Ö., Oktel, M.Ö. : Ansatz from nonlinear optics applied to trapped Bose-Einstein condensates. Phys. Rev. A 75, 035601 (2007)
15. Nicolin, A.I., Carretero-González, R. : Nonlinear dynamics of Bose-condensed gases by means of a q-Gaussian variational approach. Physica A 387, 6032 (2008)
16. Salasnich, L., Parola, A., Reatto, L.: Effective wave equations for the dynamics of cigar-shaped and disk-shaped Bose condensates. Phys. Rev. A 65 043614 (2002)
17. Nicolin, A.I., Raportaru, M.C.: Faraday waves in high-density cigar-shaped Bose-Einstein condensates. Physica A 389, 4663 (2010)
18. Wolfram, S.: The Mathematica book. Cambridge University Press, Cambridge (1999)
19. Nicolin, A.I. : Effective wave equation for the dynamics of high-density disk-shaped Bose-Einstein condensates. Rom. Rep. Phys. 61, 641 (2009)