Excited stationary states of trapped Bose-Einstein condensates

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We investigate the excited stationary states of Bose-Einstein condensates trapped in harmonic potentials. We derive simple analytical approximations of the first few eigenstates of the associated time-independent one-dimensional Gross-Pitaevskii equation and their energies. Our results are excited state generalizations of the Thomas-Fermi approximation of the ground state.

As opposed to traditional studies of liquid helium, the recent experimental work on Bose-Einstein condensation centers on inhomogeneous mesoscopic systems. However, such systems are highly nonlinear and no exact analytical expressions for the wavefunctions and associate energies are yet known. In order to understand the behavior of Bose-Einstein condensates (BEC) it would be beneficial to have at least simple approximate expressions for the condensate wave functions. These could be used to study the qualitative behavior of the condensate and, given the approximate expressions are precise enough, might even be useful for the determination of overlap factors between different wave functions, spectra and other quantities of interest. Yukalov et al. have investigated this problem using a perturbation method. Also, Kivshar et al. recently highlighted the connection between this problem and that of dark solitons and gave numerical solutions to the first few excited stationary states. In this communication we derive simple analytical approximations to the stationary states \( \Phi_n \) \( (n = 0, 1, 2, \ldots) \) of the one-dimensional Gross-Pitaevskii equation for a BEC confined in a harmonic trap:\[\begin{align*}
\left(-\frac{\partial^2}{\partial z^2} + \lambda^2 z^2 + \frac{Q}{2} |\Phi_n(z)|^2 - 2\varepsilon_n\right) \Phi_n(z) = 0.
\end{align*}\] (1)

Here \( z \) is the longitudinal trap coordinate, the aspect ratio, \( \lambda = \omega_z/\omega \ll 1 \), is given by the ratio of the longitudinal trap frequency \( \omega_z \) to the transversal trap frequency \( \omega \), \( \lambda \) formally is the effective spring constant of the 1-dimensional problem. \( \lambda \) is assumed to be much smaller than unity in order to yield a cigar-shaped condensate which can be modeled by a 1-dimensional problem. \( Q/2 = 4\pi aN/\omega_0 \) is the effective non-linearity for the interaction of the \( N \) trapped atoms with mass \( m \) and scattering length \( a \) in the trap with an effective diameter \( a_0 = \sqrt{\hbar/(m\omega)} \).

The states \( \Phi_n \) are normalized to unity, but, owing to the non-linearity of the Gross-Pitaevskii-equation, they do not form an orthogonal set, generally \( \langle \Phi_n | \Phi_m \rangle \neq 0 \).

It is convenient to rescale the Gross-Pitaevskii-equation to make the coefficients of the kinetic and the non-linear term equal to unity. Using the rescaling \( Y_n = \Phi_n \frac{1}{2} \sqrt{Q/\varepsilon_0} \) and \( x = z\sqrt{2\varepsilon_0} \), Eq. (1) becomes:

\[\begin{align*}
\left(-\frac{\partial^2}{\partial x^2} + \lambda^2 x^2 + |Y_n(x)|^2 - \epsilon_n\right) Y_n(x) = 0.
\end{align*}\] (2)

The advantage of this scaling is that the solutions are parameterized solely by \( \lambda \). The energy eigenvalue \( \epsilon_n = \varepsilon_n/\varepsilon_0 \) is now scaled in units of the Thomas-Fermi energy \( \varepsilon_0 = (3^{2/3}/8) \cdot (Q\lambda)^{2/3} \) of the lowest stationary state and the spring constant is expressed in terms of \( \lambda^2 = (\omega_z/\omega)^2 = (512/9) \cdot \varepsilon_0/Q^2 \). Our choice of rescaling results in the normalization \( \langle \Phi_n | \Phi_n \rangle = 1 = \frac{4 \sqrt{\pi}}{\sqrt{2\lambda}} \langle Y_n | Y_n \rangle \) which can be written as:

\[\begin{align*}
\langle Y_n | Y_n \rangle = \frac{4}{\lambda^3}.
\end{align*}\] (3)

The Thomas-Fermi approximation of \( Y_0 \) entirely neglects the contribution from the kinetic energy term and yields the standard approximate solution \( Y_0(z) \) of (3):

\[\begin{align*}
Y_0(z) = \sqrt{1 - \lambda^2 x^2}, \text{ for } |x| < X_0 = 1/\lambda
\end{align*}\] (4)

and \( Y_0(x) = 0 \) otherwise, as illustrated in Fig. [4].

FIG. 1. Plot of the parabolic trap potential, the standard Thomas-Fermi solution for the condensate state \( Y_0 \) (dashed line) and the corresponding exact numerical solution (solid line). The value of the nonlinearity is \( \lambda = 1/30 \). Both solutions have been displaced vertically by their respective energy values and share the same arbitrary vertical scaling.
To generalize the Thomas-Fermi approach to excited stationary states, $Y_n$ for $n > 0$, we need to include the kinetic energy term. Our approach to deriving a solution is based on a piecewise ansatz which is motivated as follows. Over small regions about some fixed point $x = x'$ the potential energy term $\lambda^2 x^2$ can be considered slowly varying compared to the other terms in Eq. (2). The local solution about $x'$ is then given approximately by the solution of the nonlinear Schrödinger equation

$$\left(-\frac{\partial^2}{\partial x^2} + |Y_n(x)|^2 - \epsilon_n'\right) Y_n(x) = 0, \quad (5)$$

where $\epsilon_n' = \epsilon_n - \lambda^2 x^2$. This equation is well known in soliton theory; the solutions with finite amplitude are given by the Jacobi-sine function ‘sn’:

$$\sqrt{\epsilon_n'} A \ 	ext{sn} \left(\sqrt{\epsilon_n'}(1 - A^2/2)(x - a), \frac{A}{\sqrt{2 - A^2}}\right), \quad (6)$$

where $a$ is an arbitrary displacement along the $x$ axis and $0 < A \leq 1$. The wavelength of the function in (6) is given by

$$\lambda = \frac{4}{\sqrt{\epsilon_n'(1 - A^2/2)}} \times K\left(\frac{A}{\sqrt{2 - A^2}}\right), \quad (7)$$

where $K$ is a complete elliptic integral of the first kind [1]. Imagine joining the solutions for two different values of $x'$ smoothly at some intermediate point along the $x$ axis. As an example, let this intermediate point be a zero of the two solutions. The slope of (6) at a zero is given by $\epsilon_n' A \sqrt{1 - A^2/2}$ and so a smooth join requires the value of $A$ to be larger for the solution with the larger value of $|x'|$ to compensate for the smaller value of $\epsilon_n' = \epsilon_n - \lambda^2 x^2$. Repeating this smooth joining of solutions for successive pairs of $x'$ values along the $x$ axis leads to a set of piecewise solutions for which the value of $A$ increases with $|x'|$. At the critical value $A = 1$ the wavelength becomes infinite and the solution of Eq. (6) is given by the corresponding limit of (6) namely

$$\sqrt{\epsilon_n} \tan\left(\sqrt{\epsilon_n'/2}(x - a)\right). \quad (8)$$

This piecewise analysis implies that the general finite-amplitude solution of Eq. (2) will be oscillatory near the origin and change to a tanh-like function some distance away. Moreover, the tanh function in (6) is relatively flat for $|x - a|$ significantly different from zero, and so (6) is approximated well by just the prefactor $\sqrt{\epsilon_n} = \sqrt{\epsilon_n - \lambda^2 x^2}$. We note that this prefactor is the Thomas-Fermi solution (3) in terms of the local variable $x'$.

We can reduce the number of piecewise segments needed in our ansatz using energy considerations [2]. The potential energy and its variation are smallest in the center of the trap and to a good approximation we can neglect the trap potential in this region. This amounts to replacing $\epsilon_n'$ with $\epsilon_n$ and holding $A$ constant in our oscillatory solution (6) to give an oscillating function $Y_{osc}$ which has a fixed wavelength and amplitude. Further away from the center of the trap the potential energy increases at the expense of the kinetic energy to the extent that the later becomes negligible. The wave function is then well described by the conventional Thomas-Fermi solution $\sqrt{\epsilon_n - \lambda^2 x^2}$. Thus, replacing $x'$ with $x$ in the prefactor $\sqrt{\epsilon_n - \lambda^2 x^2}$ of (6) yields a function $Y_{tf}$ which provides a transition between $Y_{osc}$ and the Thomas-Fermi solution. We will call $Y_{tf}$ the “tail function” as it gives the shape of the condensate in its outer regions.

Our ansatz is to match these two segments $Y_{osc}$ and $Y_{tf}$ smoothly at points $x = \pm T_n$ which lie symmetrically about the origin. In analogy to Eq. (6) we also set $Y_n(x) = 0$ for $|x| > X = \sqrt{\epsilon_n}/\lambda$ where $X$ is the half-width of the condensate in the Thomas-Fermi approximation. Thus our ansatz is given by

$$Y_n(x) = \begin{cases} 
Y_{osc}(x), & |x| \leq T_n \\
Y_{tf}(x), & T_n < |x| \leq X \\
0, & X < |x| 
\end{cases} \quad (9)$$

where

$$Y_{osc}(x) = \sqrt{\epsilon_n} A \times \text{sn} \left(\sqrt{\epsilon_n(1 - A^2/2)}(x - T_n), \frac{A}{\sqrt{2 - A^2}}\right),$$

$$Y_{tf}(x) = \left(\frac{x}{|x|}\right)^n \sqrt{\epsilon_n - \lambda^2 x^2} \times \tanh \left(\sqrt{\epsilon_n - \lambda^2 T_n^2}/2(|x| - T_n)\right).$$

The points $x = \pm T_n$, where the solution switches between the oscillatory part and the tail function is given by $T_n = (n - 1) A/4$. The forms of $T_n$ and $Y_{osc}(x)$ ensure that $Y_n(x)$ is either symmetric or antisymmetric for $n$ even or odd.

The parameters $A$, $T_n$ and $\epsilon_n$ are determined by the requirements that the two segments match smoothly and that the solution is normalized according to Eq. (4). The first requirement is satisfied when the gradients, $\frac{\partial}{\partial x} Y_{osc}|_{x=T_n}$ and $\frac{\partial}{\partial x} Y_{tf}|_{x=T_n}$ are equal, i.e. when

$$\epsilon_n A \sqrt{1 - A^2/2} = (\epsilon_n - \lambda^2 T_n^2)/\sqrt{2}. \quad (10)$$

For notational simplicity we concentrate on the second excited state $Y_2$, i.e. $n = 2$. The expression for $T_2$ can be approximated by $T_2 \approx 2/\epsilon_2 \text{arctanh}(\sqrt{1 + A^2}/2) \approx 2/\epsilon_2 \cdot \ln(2/\sqrt{1 - A})$. This can be used to solve Eq. (10) for $A \approx 1 - \lambda \epsilon_2 W(8\epsilon_2/\lambda)/2$ where $W$ is the Lambert function defined by $W \exp(W) = x$. This, in turn, can be approximated to give $A \approx 1 - \lambda \epsilon_2 \ln(8\epsilon_2/\lambda)/2$ and therefore $T_2 \approx -\ln(\lambda \epsilon_2 \ln(8\epsilon_2/\lambda)/8)/\sqrt{2\epsilon_2}$. Thus we now have a simple expression for $T_2$ in terms of $\epsilon_2$. 
The second requirement, i.e. that $Y_2(x)$ be normalized according to Eq. (3), determines the value of $\epsilon_2$. The contribution from the oscillatory part of the wave function is

$$\langle Y_{osc}|Y_{osc}\rangle = 2 \left[ \sqrt{2} \arctanh(\sqrt{(1 + A^2)/2}) \right. \left. - \sqrt{(1 + A^2)/\epsilon_2}\right]$$

and the contribution from the tails is approximately

$$\langle Y_{tf}|Y_{tf}\rangle \approx 2 \int_{-T}^{X} dx \left[ \lambda^2 (T^2 - x^2) + (\epsilon_n - \lambda^2 T^2) \tanh^2(\sqrt{(\epsilon_n - \lambda^2 x^2)/2}) \right]. \quad (11)$$

We use $\tanh(\sqrt{\epsilon_n x}) \approx 1$ to find a simplified expression for (11). Inserting the above expression for $A$ and $T$ into $\langle Y_2|Y_2\rangle = 4/(3\lambda)$, treating $\lambda$ and $\delta_2 = \epsilon_2 - \epsilon_0$ as small expansion parameters and performing a somewhat tedious calculation using an expansion in $\delta_2$ followed by an expansion in $\lambda$ finally yields $\epsilon_2 \approx 1 + 2\sqrt{2}\lambda$.

The derivation for the general case $n = 1, 2, 3, \ldots$ is very similar. We find that

$$\epsilon_n \approx 1 + n\sqrt{2}\lambda, \quad (12)$$

$$A \approx 1 - \lambda \epsilon_n \ln(8\epsilon_n/\lambda)/2, \quad (13)$$

and

$$T_n \approx (1-n) \ln(\lambda \epsilon_n \ln(8\epsilon_n/\lambda)/8)/\sqrt{2\epsilon_n}. \quad (14)$$

Eq. (3) together with Eqs. (12-14) are the main results of this communication and give our analytical approximations of the stationary states of a harmonically trapped condensate. We note, however, that the greater the value of $n$, the more stringent the requirements on the aspect ratio $\lambda$ to be small.

We should expect, and do obtain, best results for low order $n$ because in this case the above approximations are least critical. In a more detailed paper [5] we will present a self-consistency argument to justify our approach. Figs. 2-4 compare our analytical and the exact (numerically determined) wave functions for low-order excited states and illustrate the increasing deviation from the fixed wavelength approximation for more highly excited states. As in the Thomas-Fermi solution in Fig. 1, the omission of the kinetic energy for the outer regions of the condensate leads to the artificial truncation at the outer edge $x = X$ of the wave functions rather than a Gaussian tail. Also Fig. 3 shows that the fixed wavelength approximation of Eq. (3) for the oscillatory segment of the solution breaks down for high excitation numbers. Interestingly we have found that the overlap between the numerical and the analytical solutions to $Y_4$ is higher for larger values of $\lambda$ (e.g. $\lambda = 1/20$). We believe this is a consequence of the fixed wavelength approximation, we will explore this point elsewhere.
These excited stationary states may soon be realized experimentally. Various possibilities to generate excited states have been discussed in the literature. Moreover, Burger et al. recently produced a slowly-moving dark soliton using the ‘phase imprinting method’. It should be possible with a slight modification of their experiment to generate the first excited state $Y_1(x)$ as a stationary dark soliton. The generation of higher excited states should also be possible in a similar manner.

In conclusion, we have derived simple, approximate analytic expressions of the excited stationary solutions of the 1-dimensional Gross-Pitaevskii equation using an ansatz based on piecewise solutions. Our analytic solutions agree very well with numerical solutions for a sufficiently small aspect ratio. Generalizations of the approach presented here should be rather straightforward, for example, one can introduce a coordinate dependent wavelength of the oscillatory part of the solution rather than using the fixed wavelength approximation. Further details will be explored elsewhere.

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