On the Thomas-Fermi approximation in the bulk of trapped Bose-Einstein condensed gases

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Corrections to the Thomas-Fermi-type solution of the Gross-Pitaevskii equation are inevitable in order to get correctly the frequencies of the low lying modes out of the Bogolyubov equations. These corrections are important in the bulk, too, thus the failure of the Thomas-Fermi approximation is not confined to the surface. We discuss this effect quantitatively and consider similar phenomena of spin fluctuations in Bose-Einstein condensed gases in an optical trap.

Several properties of the recently much studied trapped Bose-Einstein condensed alkali metal vapors can be reasonably well explained in terms of the Gross-Pitaevskii equation and of the Hartree-Fock-Bogolyubov-Popov equations (for a review see [1]). These equations yield good approximations for the condensate shape and size, the chemical potential, the critical temperature and for the excitation frequencies. Note that they do not describe the damping of the collective excitations, as the Bogolyubov approximation neglects terms of the Hamiltonian that are of third and fourth order in the field operator (after having used the usual Bogolyubov prescription). Although themselves being approximations (even within the framework of nonrelativistic many body theory), they are usually subjects of further approximations to get solutions. This is not as if a numerical approach were so difficult, but rather to get a deeper understanding of the underlying physics and to clarify the significance of the involved mechanisms. The quantum hydrodynamical description introduced by Stringari [2] for trapped Bose gases has proven to be important in case of large particle numbers.

At large condensates, and for repulsive interaction (i.e., for $g > 0$, as in case of rubidium and sodium vapours) one can apply the Thomas-Fermi approximation for the solution of the Gross-Pitaevskii equation (1)

\[
\hat{\mathcal{L}} - g |\Phi_0(\vec{r})|^2 \Phi_0(\vec{r}) = 0
\]

where

\[
\hat{\mathcal{L}} = -\frac{\hbar^2}{2m} \Delta + V(\vec{r}) - \mu + 2g |\Phi_0(\vec{r})|^2 + 2g \langle \hat{\psi}^\dagger(\vec{r}) \hat{\psi}(\vec{r}) \rangle
\]

In the above equation $\Phi_0(\vec{r})$ stands for the 'condensate wavefunction', $V(\vec{r})$ denotes the trap potential, the average in the last term on then right hand side gives the density of the noncondensed atoms and $\mu$ is the chemical potential which is connected with the particle number and the temperature through $N = \int d^3 r \left[ |\Phi_0(\vec{r})|^2 + \langle \hat{\psi}^\dagger(\vec{r}) \hat{\psi}(\vec{r}) \rangle \right]$. In the following we shall consider such situations only where $\Phi_0(\vec{r})$ can be taken as real. The Thomas-Fermi approximation amounts to the omission of the kinetic term $-\frac{\hbar^2}{2m} \Delta \Phi_0(\vec{r})$. Thus one gets the equation

\[
g \left( \Phi_0^{TF}(\vec{r}) \right)^2 + 2g \langle \hat{\psi}^\dagger(\vec{r}) \hat{\psi}(\vec{r}) \rangle = \mu - V(\vec{r})
\]

Certainly, this equation cannot hold when $V(\vec{r}) > \mu$, as the left hand side of Eq. (3) cannot be negative. Actually it is well known that in the regime $V(\vec{r}) \lesssim \mu$ which defines approximately the surface of the condensate the Thomas-Fermi approximation breaks down, which becomes obvious if one inserts $\Phi_0^{TF}(\vec{r})$ into the neglected kinetic term. For a spherical condensate this surface layer is of width $\delta \approx \frac{1}{3} \left( \frac{\hbar^2}{m \omega} \right)^{2/3} r_{TF}$ where $r_{TF} = \frac{2m \omega}{\hbar^2}$ stands for the Thomas-Fermi radius of the condensate and $\omega$ is the trapping frequency. Note that $r_{TF} \propto N^{1/5}$ and $\delta \propto N^{-1/15} N^{-4/15} r_{TF}$. Surface corrections to the ground state energy have been thoroughly discussed and calculated [1], [3], [4]. From the point of view of the chemical potential and the condensate shape corrections to the Thomas-Fermi approximation are important only near the surface of the condensate. In contrast, from the point of view of the excitation frequencies corrections to the Thomas-Fermi approximation are inevitable in the bulk as well [5], [6]. First of all, recall that at low temperatures the lower excitation frequencies the Hartree-Fock Bogolyubov-Popov equations

\[
\hat{\mathcal{L}} u_j(\vec{r}) - g |\Phi_0(\vec{r})|^2 u_j(\vec{r}) = E_j u_j(\vec{r})
\]

\[
\hat{\mathcal{L}} v_j(\vec{r}) - g |\Phi_0(\vec{r})|^2 v_j(\vec{r}) = -E_j v_j(\vec{r})
\]

are rather well approximated by the solution of the equation
\[-\frac{g}{m} \nabla \left( (\Phi_0)^2 \nabla \varphi \right) = \omega^2 \varphi \]  

(5)

called hydrodynamic approximation. For cylindrically symmetric harmonic potential (which is relevant for the actual experimental situation) and by using the Thomas-Fermi expression \(\Phi_0\) at zero temperature, Eq. (5) has been solved analytically \([3, 4, 5]\) and the resulting \(\omega\) values agree reasonably with low temperature experimental data. Note that at zero temperature Eq. (5) is uncoupled from Eq. (4). When the radial trapping frequency \(\omega_r\) is smaller than the axial one \(\omega_z\) (disc-shaped condensate), the lowest nonzero eigenvalue is \(\omega = \omega_r\). Nevertheless, if one inserts the Thomas-Fermi expression for \(\Phi_0\) into the Hartree-Fock-Bogolyubov-Popov equation \(\Phi_j\), one obtains completely erroneous results, as we now explicitly show. Indeed, Eqs. (5), (6) imply

\[- \frac{\hbar^2}{2m} \Delta G_j = E_j F_j \]

(6)

\[- \frac{\hbar^2}{2m} \Delta F_j + 2g (\Phi_0)^2 F_j = E_j G_j \]

(7)

where \(G_j = u_j + v_j\) and \(F_j = u_j - v_j\). At low energies, i.e., when \(\hbar \omega \ll \mu \sim g (\Phi_0^2(0))^2\) the first term on the left hand side of Eq. (6) is much smaller than the second term, thus can be neglected. Therefore, instead of (7)

\[2g (\Phi_0)^2 F_j = E_j G_j \]

(8)

may be used. Eliminating \(G_j\) one gets

\[- \frac{\hbar^2}{2m} \Delta (\Phi_0)^2 F_j = E_j^2 F_j. \]

Introducing \(\tilde{\varphi} = \Phi_0^2 F_j\) and \(\tilde{\omega} = \frac{\hbar}{m}\) one finally arrives at

\[- \frac{g}{m} \Phi_0^2 \Delta \Phi_0^2 \tilde{\varphi} = \tilde{\omega}^2 \tilde{\varphi}. \]

(9)

This equation can be solved with the same techniques as Eq. (5), i.e., its validity is extended up to the surface of the condensate (as defined by the vanishing of \(\Phi_0^2\)) and then it is required that the solution does not diverge at the surface. Note that this induces the vanishing of the eigenfunction at the border, unlike in case of the hydrodynamical equation where the solution remains there nonzero. The first eigenvalue at zero temperature is \(\tilde{\omega} = \sqrt{\omega_r^2 + 2\omega_z^2}\). One may prove the inequality

\[- \int d^3\tilde{r} \tilde{\varphi} \Phi_0^2 \Delta (\tilde{\varphi} \Phi_0^2) \geq - \int d^3\tilde{r} \tilde{\varphi}^2 \Delta (\Phi_0^2)^2 \]

which readily implies that \(\tilde{\omega}^2 \geq \omega_r^2 + 2\omega_z^2\). Equality holds for the eigenfunction \(\tilde{\varphi} = \frac{1}{\sqrt{\Phi_0^2}}\). Comparing \(\tilde{\omega}\) with the experimentally confirmed result \(\omega = \omega_r\) the obvious conclusion is that Eq. (6) is not correct. We emphasize that the source of the error is the Thomas-Fermi approximation. Indeed, in Ref. [3] Eq. (6) has been derived from Eqs. (4) by using the full Gross-Pitaevskii equation (3). That derivation has been done for the zero temperature case and for low excitation energies. Taking into account the next correction to the Thomas-Fermi approximation, one can derive the correct equation \(\Phi_0^2\) even at finite temperatures. To this end, let us write \(\Phi_0 = \Phi_0^{TF} + \Phi_0^{(1)}\) where \(\Phi_0^{TF}\) satisfies Eq. (3) and \(\Phi_0^{(1)}\) is the correction term. We determine the latter perturbatively (assuming that we are sufficiently far from the surface), i.e., we insert the Ansatz above into Eq. (4) and keep the kinetic term \(-\hbar^2/2m \Delta \Phi_0^{(1)}\) while neglect \(-\hbar^2/2m \Delta \Phi_0^{(1)}\) and \((\Phi_0^{(1)})^2\). We get \(\Phi_0^{(1)} = \frac{\hbar^2}{2m} \Delta \Phi_0^{TF} + \frac{3\hbar^2}{2m} \Delta \Phi_0^{TF} \). Inserting these expressions into \(\Phi_0\) we get instead of Eqs. (3) and (4)

\[\left[ - \frac{\hbar^2}{2m} \Delta + \frac{\hbar^2}{2m} \Phi_0^{TF} \right] G_j = E_j F_j \]

(10)

\[\left[ - \frac{\hbar^2}{2m} \Delta + 2g (\Phi_0^{TF})^2 + \frac{3\hbar^2}{2m} \Phi_0^{TF} \right] F_j = E_j G_j \]

(11)

In Eq. (11) we apply the same approximation as in case of Eq. (9), namely, we keep only the dominant term \(2g (\Phi_0^{TF})^2 F_j\) on the left hand side, thus we arrive at Eq. (8) again. Comparing now Eq. (11) with Eq. (8) it is clearly seen that the additional term on the left hand side cannot be neglected. In fact, for low excitation energies the wavelength of the excitations is comparable to the condensate size, thus the kinetic energy term is of the same order of magnitude as the additional term on the left hand side of Eq. (8), as we show this below explicitly for \(T = 0\). Let us emphasize that this is true even deeply in the bulk, notwithstanding how small \(\Phi_0\) is compared to \(\Phi_0^{TF}\). Note that in case of the Gross-Pitaevskii equation the correction term \(\Phi_0^{(1)}\) should be compared to \(\Phi_0^{TF}\), and they become of the same order only in the surface region of the condensate. Unlike this, when adding the Bogolyubov equations to get Eq. (11), the lowest order terms (i.e., terms like \(2g (\Phi_0^{TF})^2 G_j\)) cancel exactly, and therefore the correction term \(\hbar^2 \Delta \Phi_0^{TF} / \Phi_0^{TF} G_j\) should be compared to the kinetic term \(\frac{\hbar^2}{2m} \Delta G_j\). Eqs. (10) and (11) lead readily to Eq. (3). Thus taking into account the first correction to the Thomas-Fermi approximation suffices to recover the hydrodynamic approximation, while without it one gets the wrong result. We want to investigate this question quantitatively. Having solved Eq. (3) at \(T = 0\) and using Eq. (11) one can calculate the terms on the left hand side of Eq. (11) separately. In case of \(\omega_z \gg \omega_r\) (disc-shaped condensate) we get for the ratio \(\frac{\hbar^2}{2m} \Delta G_j / \frac{\hbar^2}{2m} \Delta \Phi_0^{TF} G_j\) the expression

\[1 + \frac{2\omega^2}{\omega_r^2} \left[ 1 + \frac{1}{1 - \xi^2 (\xi^2 + 1)} + \frac{1}{1 - \xi^2 (1 - \eta^2)} \right]^{-1} \]

(12)

where \(\xi^2 = 1 - \omega^2 / \omega_r^2\) and \(\xi, \eta\) are the oblate spheroidal coordinates defined as \(\rho = \sqrt{x^2 + y^2} = \sqrt{\frac{2\omega}{m \omega_r^2} \sqrt{(\xi^2 + 1)(1 - \eta^2)}}, z = \frac{2\pi}{m \omega_r^2} \xi \eta\). For the lowest
excitation energies $\omega$ is of the same order of magnitude as $\omega_{t}$, therefore within the condensate the ratio of the two terms on the left hand side of Eq. (13) is of order unity.

As a further demonstration that the correction term describes an important bulk effect we exclude the surface region, hence we consider a situation when Eq. (3) holds for $\xi < \xi_{1} < \xi_{0} = \sqrt{1/\epsilon^{2} - 1}$, i.e., inside of the condensate, while Eq. (5) holds for $\xi_{1} < \xi < \xi_{0}$, i.e., near the surface. Note that the Thomas-Fermi surface is the ellipsoid $\xi = \xi_{0}$ and $\xi = \xi_{1}$ defines the ellipsoidal bordering surface between the regions of validity of Eqs. (3) and (5).

Then the correction to the eigenvalues of (3) comes from the bulk by construction. We calculate this correction by perturbation theory in first order, i.e., we consider Eq. (8) as the unperturbed one and the additional term

$$\frac{g}{m} \varphi_{0}^{TF} \Delta \varphi_{0}^{TF}$$

(13)
as a perturbation for $\xi < \xi_{1}$. The correction to the eigenvalues then has the form

$$\Delta \omega^{2} = -\frac{g}{m} \int_{0}^{\xi_{1}} d\xi \int_{-1}^{1} d\eta (\xi^{2} + \eta^{2}) \varphi^{2} \varphi_{0}^{TF} \Delta \varphi_{0}^{TF}$$

(14)

provided that the unperturbed eigenfunction $\varphi$ is normed by

$$\int_{0}^{\xi_{0}} d\xi \int_{-1}^{1} d\eta (\xi^{2} + \eta^{2}) \varphi^{2} = 1$$

(15)

In case of the lowest excitation frequency one gets

$$\Delta \omega^{2} = \frac{\omega^{2}_{t}}{12 \sqrt{1 - \epsilon^{2}}} \left\{ 3 \epsilon \xi_{1} (\xi_{1}^{2} + 1) \left( 5 - 4 \epsilon^{2} \right) - \epsilon^{2} (3 - 2 \epsilon^{2}) (\xi_{1}^{2} + 1) \right\} + 6 \frac{5 - 4 \epsilon^{2}}{\sqrt{1 - \epsilon^{2}}} \arctanh \left( \frac{\xi_{1}}{\xi_{0}} \right)$$

(16)

$$-3 \epsilon \xi_{1} (5 - 4 \epsilon^{2}) (\xi_{1}^{2} + 3) - 3 \epsilon^{2} (\xi_{1}^{2} + 1) \right\} \arctan \left( \frac{1}{\xi_{0}} \right)$$

Certainly, the validity of this expression is confined for small $\xi_{1}$ values only (i.e., perturbation deeply in the bulk). In this regime we get in case of $\omega^{2}_{t}/\omega^{2}_{z} = 1/8$ that $\sqrt{\omega^{2}_{t} + \Delta \omega^{2}} = \omega_{t} \approx 6.74 \omega_{t} \xi_{1}/\xi_{0}$. The linearity in $\xi_{1}$ means a proportionality to the volume. Note that the considered mode is just the Kohn mode whose frequency is known to be exactly the trapping frequency $\omega_{t}$.

The effect due to the correction term is a consequence of inhomogeneity (i.e., spatial dependence of $\varphi_{0}^{TF}$) which is induced by the presence of the trapping potential. In the Thomas-Fermi approximation the effect depends only on the external potential and the number of particles. Note that in case of a system contained in a box (with zero external potential inside) the Thomas-Fermi solution is uniform and the correction of the type discussed above is zero. In the extreme situation of a single particle, however, spatial dependence of the wave function can be a consequence of the boundary conditions, as it is in case of a particle in a box. Therefore, it is instructive to consider such a surface-induced inhomogeneity for a large number of particles. In case of a spherical box (with zero potential inside) we find that the boundary induces a correction to the uniform Thomas-Fermi wave function which is comparable with it near the surface and decays as $\exp(-kd)$ (where $k = 2 \sqrt{m \mu / \hbar}$) at a distance $d$ from the boundary. Thus, in the middle of the condensate the correction term is of order $\exp(-1/\epsilon)$, which is nonanalytic in the small parameter $\epsilon = \frac{1}{kr} = \frac{\sqrt{\pi R^{2}}}{3 \mu m N}$ ($R$ being the radius of the spherical box). It can be shown that one gets a similar nonanalytic boundary induced correction in case of smooth trapping potentials, too.

Let us add that most of the above observations also apply to the recently studied Bose condensates in optical traps where the Zeeman energy is much smaller than the interaction energy. Under such circumstances the total spin can freely rotate and new phenomena appear [12]. Among others, for the total spin $f = 1$ (as in case of $^{23}$Na and $^{87}$Rb) two types of ground states become possible. These are called ‘polar’ and ‘ferromagnetic’ and possess the form $\Phi_{0} \zeta$, where $\zeta$ is a normalized three component spinor. These ground states correspond to the spontaneous breaking of $U(1) \times S^{2}$ and $SO(3)$ symmetry, respectively. For simplicity, we consider a zero temperature situation. The substitute of the Gross-Pitaevskii equation is

$$\left[ -\frac{\hbar^{2}}{2m} \Delta + V(\vec{r}) - \mu + b \Phi_{0}^{2}(\vec{r}) \right] \Phi_{0}(\vec{r}) = 0$$

(17)

where $b = c_{0}$ for the polar ground state and $b = c_{0} + c_{2}$ for the ferromagnetic ground state. Note that $c_{0} = (g_{0} + 2g_{2})/3$ and $c_{2} = (g_{2} - g_{0})/3$ with $g_{0} = 4 \pi \hbar^{2} a_{0}/m$ and $g_{2} = 4 \pi \hbar^{2} a_{2}/2m$, where $a_{0}$ and $a_{2}$ are the s-wave scattering lengths in the total spin $F = 0$ and $F = 2$ channel, respectively. The polar ground state emerges if $c_{2} > 0$, while for $c_{2} < 0$ the ferromagnetic ground state becomes possible. Collective modes can be found in both the polar and the ferromagnetic ground state as solutions of the corresponding generalized Bogolyubov equations. They are the density modes in both the polar and ferromagnetic states and the spin wave mode in the polar state. The mathematical structure of the Bogolyubov equations is identical with the scalar case discussed above, therefore, all our previous considerations apply. In contrast, the equations, which are related to spin and quadrupolar spin fluctuations in the ferromagnetic phase have different structures. The modes have been found in the homogeneous system [8] and are determined in the presence of the external potential by the equations

$$\left[ -\frac{\hbar^{2}}{2m} \Delta + V(\vec{r}) - \mu + g_{2} \Phi_{0}^{2}(\vec{r}) \right] u_{j} = E_{j} u_{j}$$

(18)
for the spin and quadrupolar spin modes, respectively.

A combination of Eq. (18) with the Gross-Pitaevskii equation (17) shows that the bulk correction to the Thomas-Fermi approximation is important in this case, too. Taking this correction into account, we get for the spin fluctuations $\delta M_-$, $\Phi_0^{TF}$

$$\left[ \frac{\hbar^2}{2m} \nabla + V(\vec{r}) - \mu + (g_2 + 2|c_2|)\Phi_0^{2(\vec{r})} \right] u_j^- = E_j u_j^- (19)$$

This is similar to (but not identical with) the hydrodynamical equation (17). It is interesting to note that $\Phi_0^{TF}$ itself is a solution of the eigenvalue equation (18) with $E_j = 0$ (cf. Eq. (17)) which corresponds to the solution of Eq. (20) $\delta M_- = (\Phi_0^{TF})^2$ with $\omega_j = 0$. In case of quadrupolar spin fluctuations Eq. (19) is relevant. Inserting Eq. (17) the lowest order term $2|c_2| (\Phi_0^{TF})^2$ does not cancel, therefore one would think bulk corrections are negligible in this case, along with the kinetic energy of the mode in the bulk. For an extremely large condensate this is indeed the case for the lowest excitations. Nevertheless, the numerical value of $c_2$ in case of $^{87}$Rb (which is the only possible candidate for having a ferromagnetic ground state and $f = 1$ hyperfine spin) is $- (9 \pm 25) \times 10^{-2} g_2$, very small. Note that if $c_2$ is actually not negative, no ferromagnetic ground state is possible. The higher order terms (the kinetic term, for instance) can be estimated by $\frac{\hbar^2}{m} \omega^2 = \frac{\hbar^2 \omega^2}{4\pi}$, where $L$ is the major axis of the ellipsoidal condensate. On the other hand, $2|c_2| (\Phi_0^{TF})^2 \approx 2|c_2|\mu / g_2$. This will be larger than the other terms if

$$\sqrt{8|c_2| g_2} \approx 0.3 > \frac{\hbar \omega_c}{\mu} . \quad (21)$$

Here $\omega_c$ is the smallest trapping frequency. For $\omega_c = 20Hz$ we get $\hbar \omega_c / \mu = (10^4 / N)^{2/5}$, thus for $N > 2 \times 10^5$ Eq. (21) is satisfied. For larger particle numbers bulk corrections do not play a role for the lowest lying excitations. The kinetic term is also negligible, which looks rather paradoxical. The solution is that these excitations are confined to the vicinity of the Thomas-Fermi surface as noticed already by Ho [8]. For smaller particle numbers bulk corrections must be taken into account, and when the term $2|c_2|\Phi_0^2$ becomes negligible, the spectra of (18) and (19) coincide. Similarly to the case of spin fluctuations (cf. Eq. (20)) one can get the equation describing the quadrupolar spin waves in the bulk of the condensate as follows:

$$- \frac{\hbar}{2m} \nabla \left( \Phi_0^{TF} \right)^2 \nabla \left( \frac{\delta M_-^2}{(\Phi_0^{TF})^2} \right) + 2|c_2| \frac{\hbar}{\Phi_0^{TF}} \delta M_-^2 = \omega_j \delta M_-^2 \quad (22)$$

Here $\delta M_-^2 = 2\Phi_0^{TF} u_j^+$. It is interesting to look at the relative magnitude of the terms in the left hand side of Eq. (22). The second term is dominating if Eq. (21) holds. In any case its value in the lowest energy state (i.e. the gap for excitations confined to the bulk) can be estimated by using the Ansatz $u_j^+ = \frac{\hbar N}{\sqrt{\Phi_0^{TF}}}$. One obtains for the gap $\frac{\hbar N}{\sqrt{\Phi_0^{TF}}}$. As the derivation is independent of the form of the external potential, this result also applies in the homogeneous case. Then we get back the known result $2|c_2|\Phi_0^2$ for the gap [8]. Note that for a fixed harmonic external potential the gap increases with the particle number as $N^{2/5}$ (which is proportional to the average density and also to $\Phi_0^2$ in this case).

It is of worth noting that Eq. (22) is also the condition for the applicability of the hydrodynamic approximation in case of the spin fluctuations in the polar state. Due to the smallness of $c_2$ Eq. (22) is a more confining condition than the similar conditions in the scalar case and in the case of density fluctuations in the polar and ferromagnetic states. Namely, the condition for the latter ones is similar to (21), but $c_2$ should be replaced by $c_0$. This latter condition is also relevant to the applicability of Eqs. (21) and (22).

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