Extension of the Thomas-Fermi approximation for trapped Bose-Einstein condensates with an arbitrary number of atoms

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By incorporating the zero-point energy contribution we derive simple and accurate extensions of the usual Thomas-Fermi (TF) expressions for the ground-state properties of trapped Bose-Einstein condensates that remain valid for an arbitrary number of atoms in the mean-field regime. Specifically, we obtain approximate analytical expressions for the ground-state properties of spherical, cigar-shaped, and disk-shaped condensates that reduce to the correct analytical formulas in both the TF and the perturbative regimes, and remain valid and accurate in between these two limiting cases. Mean-field quasi-1D and -2D condensates appear as simple particular cases of our formulation. The validity of our results is corroborated by an independent numerical computation based on the 3D Gross-Pitaevskii equation.

The experimental realization of Bose-Einstein condensates (BECs) of dilute atomic gases confined in optical and magnetic traps [1, 2, 3] has stimulated great activity in the characterization of these quantum systems. Of particular interest are the ground-state properties of trapped BECs with repulsive interatomic interactions [4]. These properties derive from the condensate wave function \( \psi(r) \) which, in the zero-temperature limit, satisfies the stationary Gross-Pitaevskii equation (GPE) [5]

\[
\left( -\frac{\hbar^2}{2m} \nabla^2 + V(r) + gN |\psi|^2 \right) \psi = \mu \psi, \quad (1)
\]

where \( N \) is the number of atoms, \( g = 4\pi\hbar^2a/m \) is the interaction strength, \( a \) is the s-wave scattering length, \( V(r) = \frac{1}{2}m(\omega_r^2 r^2 + \omega_z^2 z^2) \) is the harmonic potential of the confining trap, and \( \mu \) is the chemical potential.

Only in two limiting cases can Eq. (1) be solved analytically: in the Thomas-Fermi (TF) and perturbative regimes. When \( N \) is sufficiently large that \( \mu \gg \hbar \omega_r, \hbar \omega_z \), one enters the TF regime. In this case the kinetic energy can be neglected in comparison with the interaction energy and the GPE reduces to a simple algebraic equation. Useful analytical expressions can then be obtained for the condensate ground-state properties [4]. In the simple case of a spherical trap characterized by an oscillator length \( a_r = \sqrt{\hbar/m\omega} \), Eq. (1) leads in the TF limit to

\[
\frac{1}{2}m\omega_r^2 r^2 + gN |\psi(r)|^2 = \mu, \quad 0 \leq r \leq R \quad (2)
\]

where the condensate radius \( R = \sqrt{2\mu/\hbar \omega a_r} \) is determined from the condition \( |\psi(r)|^2 \geq 0 \), and the chemical potential \( \mu = \frac{1}{2} (15Na/a_r)^{2/5} \hbar \omega \) follows from the normalization of \( \psi(r) \).

In the opposite limit, when \( N \) is small enough that the interaction energy can be treated as a weak perturbation, one enters the (ideal gas) perturbative regime. In this case, to the lowest order, \( \psi(r) \) is given by the harmonic oscillator ground state, \( \psi(r) = (\pi a_r^2)^{-3/4} \exp(-r^2/2a_r^2) \), and the chemical potential satisfies

\[
(3/2)\hbar \omega + g\bar{n} = \mu \quad (3)
\]

where \( \bar{n} = N/(\sqrt{2}\pi a_r)^3 \) is the mean atom density. Away from these two limiting cases, in principle, one has to solve the GPE numerically. Very few theoretical works have addressed the question of looking for approximate analytical solutions valid in between the two analytically solvable regimes. The most relevant proposals are based on a variational trial wave function [6], or on the semiclassical limit of the Wigner phase-space distribution function of the condensate [7]. However, the practical usefulness of these approaches turns out to be somewhat limited in comparison with the simple TF approximation.

In this work we address the above question from a different point of view. We start from the usual TF approximation and modify it conveniently to account, in a simple manner, for the zero-point energy contribution. This enables us to derive simple and accurate extensions of the TF expressions that remain valid for an arbitrary number of atoms in the mean-field regime. Specifically, we obtain general analytical expressions for the ground-state properties of spherical, cigar-shaped, and disk-shaped condensates that reduce to the correct analytical formulas in both the TF and the perturbative regimes, and remain valid and accurate in between these two limiting cases.

We begin by considering a BEC in a spherical trap. In principle, we start from the TF relation of Eq. (2). However, since we intend to apply this equation to arbitrarily small condensates, we introduce a lower cutoff radius \( r_0 \), defined through \( \frac{1}{2}m\omega^2 r_0^2 = \frac{3}{2} \hbar \omega \), in order to be consistent with the fact that the contribution from the harmonic oscillator energy cannot be smaller than the zero-point energy. As for the small volume \( V_0 \sim a_r^3 \) corresponding to \( r \leq r_0 \), we do not aspire to get a precise knowledge of the wave function therein. Instead, we content ourselves with an effective condensate density \( \bar{n}_0 \) in that region. As we shall see, this is all that is needed to obtain very accurate
approximate formulas for most of the condensate ground-state properties. Thus we start from the ansatz

\[ \frac{1}{2} m \omega^2 r^2 + g N |\psi(r)|^2 = \mu, \quad r_0 < r \leq R \] (4a)

\[ \frac{3}{2} \hbar \omega + g \sqrt{6/\pi} \hat{n}_0 = \mu, \quad 0 \leq r \leq r_0 \] (4b)

with \( \psi(r) = 0 \) for \( r > R \). A renormalization constant \( \kappa^{-1} \equiv \sqrt{6/\pi} \) has been introduced in Eq. (4b) to guarantee the correct perturbative limit. In this limit \( \mu \to \frac{3}{2} \hbar \omega \) and \( R \to r_0 = \sqrt{3} a_r \). Under these circumstances, only Eq. (4b) contributes significantly to the chemical potential, and in this case \( \hat{n}_0 = N/V_0 \). This corresponds to a uniform spherical condensate, defined in the finite volume \( V_0 \). In order for this uniform density to produce the same chemical potential as the ground state of the harmonic oscillator over the volume of the entire space it is only necessary to renormalize the corresponding interaction strength by multiplying by \( \sqrt{6/\pi} \). Equations (4) also yield the correct result in the TF regime. This is mainly a consequence of the direct relation existing between the number of particles and the size of a trapped BEC. For large condensates, such that \( \mu \gg \hbar \omega \), one has \( R \gg r_0 \) and, as a result, the relative contribution from Eq. (4b) to the normalization integral that determines \( \mu \) becomes negligible. Since we have renounced an explicit expression for \( \psi(r) \) in \( V_0 \), in this respect, our approach cannot provide more information than the TF approach. Only when \( R \gg r_0 \) can we have a sufficiently precise knowledge of the wave function and, in this case, it coincides with the TF wave function.

The chemical potential follows from the normalization of \( \psi(r) \). After a straightforward calculation one obtains

\[ \frac{1}{15} \bar{R}^5 + \frac{\sqrt{3}}{2} (\kappa - 1) \bar{R}^3 - \frac{3\sqrt{3}}{2} \left( \kappa - \frac{3}{5} \right) = \frac{N}{a_r}, \] (5)

where \( \bar{R} \equiv R/a_r \), and \( \bar{\mu} = \frac{1}{\bar{R}} \bar{R}^2 \) is the chemical potential in units of \( \hbar \omega \). As Eq. (5) shows, the ground-state properties depend on the sole parameter \( \chi_0 \equiv N a_r/a_r \). When \( \chi_0 \gg 1 \) (TF limit) the above equation leads to

\[ \bar{\mu} = \frac{1}{5} (15 \chi_0)^{2/5}, \] as expected. The \( \chi_0 \ll 1 \) limit corresponds to the perturbative regime and, in this case, one obtains \( \bar{\mu} = 3/2 + \sqrt{2/\pi} \chi_0 \), which is nothing but the perturbative result (3). For arbitrary \( \chi_0 \), in principle one has to solve numerically the above quintic polynomial equation (which has only one physically meaningful real solution). This is a simple task that can be carried out with standard mathematical software packages. We have found, however, a rather accurate approximate solution. It can be shown that the expression

\[ \bar{R}^2 = 3 + \left( \frac{1}{(15 \chi_0)^{4/5}} + \frac{5}{2} + \frac{7}{2} \chi_0^{14/15} + 10 + \frac{\sqrt{\pi} / 2}{\chi_0} \right)^{-1} \] (6)

satisfies Eq. (5) with a residual error \( \leq 0.7\% \) for any \( \chi_0 \in (0, \infty) \). Figures (a) and (b) show, respectively, the predicted chemical potential, \( \bar{\mu} = \sqrt{2} R^2 \), and condensate radius, obtained from Eq. (6) (solid lines), along with the exact results obtained from the numerical solution of the 3D GPE (open circles). For the numerical calculation we have defined the radius through the condition \( |\psi(R)|^2 = 0.05 |\psi(0)|^2 \). With this definition, Eq. (6) reproduces the numerical \( R \) with a relative error smaller than 3% for any \( \chi_0 \). Most of the error, however, comes from the region where \( \chi_0 \gg 1 \) (TF limit) because in that region \( R \to R_{TF} \) and it rather satisfies \( |\psi(R)|^2 = 0 \). The accuracy with respect to the numerical \( \bar{\mu} \) is better than 0.5%.

A straightforward calculation yields the mean-field interaction energy per particle, \( \bar{\tau}_{\text{int}} \equiv \epsilon_{\text{int}}/\hbar \omega \equiv E_{\text{int}}/N \hbar \omega \),

\[ \bar{\tau}_{\text{int}} = \frac{1}{8 \sqrt{\pi}} \left[ \frac{8}{105} \bar{R}^7 + \sqrt{3} (\kappa - 1) \bar{R}^4 - 6 \sqrt{3} \left( \kappa - \frac{3}{5} \right) \right]. \] (7)

For \( \chi_0 \gg 1 \), one recovers the TF result, \( \epsilon_{\text{int}} = (2/7) \mu \). In the \( \chi_0 \ll 1 \) limit, using that \( \bar{R}^2 = 3 + 2 \sqrt{2/\pi} \chi_0 - (1/\pi)(1/9 + \sqrt{2/3 \pi}) \chi_0^2 + O(\chi_0^3) \) is a perturbative solution of Eq. (5), one obtains \( \epsilon_{\text{int}} = \chi_0 \hbar \omega / \sqrt{2 \pi} = g \mu / 2 \), which again is the correct result. Finally, the kinetic and potential energies can be readily obtained in terms of the previous results by using the exact relations (5)

\[ \epsilon_{\text{kin}} \equiv E_{\text{kin}}/N = \mu/2 - (7/4) E_{\text{int}}/N, \] (8a)

\[ \epsilon_{\text{pot}} \equiv E_{\text{pot}}/N = \mu/2 - (1/4) E_{\text{int}}/N. \] (8b)

In Fig. (a) we show the theoretical prediction for \( \bar{\tau}_{\text{int}}, \bar{\epsilon}_{\text{kin}}, \) and \( \bar{\epsilon}_{\text{pot}} \), obtained from Eqs. (6)–(8) (solid lines), along with the exact numerical results (open circles).
Next we consider a BEC confined in a cigar-shaped magnetic trap with oscillator lengths $a_{\perp} = \sqrt{\hbar/m\omega_{\perp}}$ and $a_z = \sqrt{\hbar/m\omega_z}$ and an aspect ratio $\lambda = \omega_z/\omega_{\perp} \ll 2$. We shall restrict ourselves to the mean-field regime, which requires $N\lambda a_{\perp}^2/\hbar^2 \gg 1$ [9, 10, 11]. As before, we start from the usual TF expression, which we assume to be valid up to a minimum radial distance $r_0 = \sqrt{2}a_{\perp}$, determined from the condition that the contribution from the radial harmonic oscillator energy should not be smaller than $\hbar\omega_{\perp}$. This defines an outer region $V_+ \equiv \{(r_{\perp}, z): r_{\perp}^2/R^2 + z^2/Z_{TF}^2 \leq 1 \land r_{\perp} > r_0\}$, which is nothing but the usual TF ellipsoidal density cloud, truncated at $r_{\perp} = r_0$. Note that unlike what happens with the condensate radius $R = \sqrt{2\mu/\hbar\omega_{\perp}}a_{\perp}$, which remains the same, now the axial condensate half-length $Z = \sqrt{2(\mu/\hbar\omega_{\perp} - 1)/a_z} \sqrt{\lambda}$ coincides with the TF value $Z_{TF}$ only in the limit $\mu/\hbar\omega_{\perp} \gg 1$. For large condensates, when $\mu \gg \hbar\omega_{\perp}$ (TF regime), this is the only region that contributes significantly. On the contrary, in the perturbative regime, as $\mu \rightarrow \hbar\omega_{\perp}$ most of the contribution comes from the inner cylinder $V_- \equiv \{(r_{\perp}, z): r_{\perp} \leq r_0 \land |z| \leq Z\}$. In this case, if $a \ll a_{\perp}$, the transverse dynamics becomes frozen in the radial ground state of the harmonic trap and the condensate wave function can be factorized as $\psi(r_{\perp}, z) = \phi(r_{\perp}) \phi(z)$, with $\phi(r_{\perp}) = (\pi a_{\perp}^2)^{-1/2} \exp(-r_{\perp}^2/2a_{\perp}^2)$. This corresponds to a mean-field quasi-1D condensate. Substituting then in Eq. (1) and integrating out the radial dynamics, one finds

$$
\hbar\omega_{\perp} + \frac{1}{2}m\omega_{\perp}^2r_{\perp}^2 + g_{1D}N|\phi(z)|^2 = \mu,
$$

where $g_{1D} = g/2\pi a_{\perp}^2$ [12], and we have used that $\mu \sim \hbar\omega_{\perp}$ to neglect the axial kinetic energy. Note that $g_{1D}$ can be conveniently rewritten as $g\bar{n}_2$ with $\bar{n}_2 = 1/\pi(r_0^2)^2$, indicating that one can account for the contribution from the radial ground state by using a uniform mean density per unit area normalized to unity in $V_-$. Guided by these simple ideas, we then propose the following ansatz:

$$
\frac{1}{2}m\omega_{\perp}^2r_{\perp}^2 + \frac{1}{2}m\omega_z^2z^2 + gN|\psi(r_{\perp}, z)|^2 = \mu, \quad r \in V_+ \\
\hbar\omega_{\perp} + \frac{1}{2}m\omega_{\perp}^2r_{\perp}^2 + gN\bar{n}_2|\phi(z)|^2 = \mu, \quad r \in V_- 
$$

with $\psi = 0$ elsewhere. The normalization of $\psi$ leads to

$$
\frac{1}{15}(\sqrt{\lambda}Z)^5 + \frac{1}{3}(\sqrt{\lambda}Z)^3 = N\lambda a_{\perp}/a_z,
$$

where $Z \equiv Z/a_z$ and $R \equiv R/a_{\perp}$. The chemical potential $\mu/\hbar\omega_{\perp}$ is given by $\mu = 1 + \frac{1}{2}(\sqrt{\lambda}Z)^2$. Now the relevant parameter determining the ground-state properties is $\chi_1 \equiv N\lambda a_{\perp}/a_z$. When $\chi_1 \gg 1$ (TF regime), Eq. (10) leads to $\mu = \frac{1}{2}(15\chi_1)^{2/5}$ and $Z = \lambda^{-1/2}(15\chi_1)^{1/5}$. When $\chi_1 \ll 1$ (mean-field quasi-1D regime), one obtains

$$
\bar{\mu} = \frac{1}{15}\chi_1 \left(\frac{1}{5}(\chi_1)^{2/5} + \frac{1}{3}(\sqrt{\lambda}Z)^3 \right)
$$

The mean-field interaction energy $\overline{\epsilon}_{\text{int}} \equiv \epsilon_{\text{int}}/\hbar\omega_{\perp}$ is

$$
\overline{\epsilon}_{\text{int}} = \frac{1}{15\chi_1} \left(\frac{1}{5}(\chi_1)^{2/5} + \frac{1}{3}(\sqrt{\lambda}Z)^3 \right).
$$

For $\chi_1 \gg 1$, Eq. (12) reduces to $\epsilon_{\text{int}} = (2/7)\mu$, while for $\chi_1 \ll 1$, it leads to $\epsilon_{\text{int}} = (2/5)(\mu - \hbar\omega_{\perp})$, which again are the correct analytical limits. As for the condensate density per unit length, $n_1(z) \equiv N \int 2\pi r_{\perp} dr_{\perp} |\psi(r_{\perp}, z)|^2$, after a straightforward calculation one finds

$$
n_1(z) = \frac{(\sqrt{\lambda}Z)^2}{4a} \left(1 - \frac{z^2}{Z^2}\right) + \frac{(\sqrt{\lambda}Z)^3}{16a} \left(1 - \frac{z^2}{Z^2}\right)^2
$$

The first term is the contribution from $V_-$ and thus it is the only one that contributes significantly in the $\chi_1 \ll 1$ limit. On the contrary, the second term, which is the contribution from $V_+$, gives the dominant contribution in the $\chi_1 \gg 1$ limit, in good agreement with previous results [11].

Figure 2 shows the theoretical predictions for the ground-state properties of arbitrary cigar-shaped condensates with $\lambda \ll 2$, obtained from Eqs. (8) and (11) (solid lines), along with exact numerical results (open circles).

Finally, we consider a BEC in a disk-shaped trap with $\lambda \gg 2$ and $a_z \gg a$. In this case, in the mean-field perturbative regime, which occurs when $\chi_2 \equiv Na/\lambda^2 a_z \ll 1$, the system reduces to a quasi-2D condensate satisfying
with \( g_{2D} = g/\sqrt{2\pi a_z} \) \[13\]. We then rewrite \( g_{2D} \) as \( g_{2D} = g\kappa_2^{-1}n_1 \), where \( n_1 = 1/2a_z \) is a uniform mean density per unit length and \( \kappa_2^{-1} \equiv \sqrt{2/\pi} \) is the appropriate renormalization factor, and propose the following ansatz:

\[
\frac{1}{2}m\omega_z^2 z^2 + \frac{1}{2}m\omega_{r\perp}^2 r_{\perp}^2 + gN|\psi(r_{\perp}, z)|^2 = \mu, \quad r \in V_+
\]

\[
\frac{1}{2}h\omega_z + \frac{1}{2}m\omega_{r\perp}^2 r_{\perp}^2 + g\kappa_2^{-1}N\bar{n}_1|\varphi(r_{\perp})|^2 = \mu, \quad r \in V_-
\]

with \( \psi = 0 \) elsewhere. In the above equations, \( V_+ \equiv \{(r_{\perp}, z) : r_{\perp}^2/R_{TF}^2 + z^2/Z^2 \leq 1 \land |z| > z_0\} \) and \( V_- \equiv \{(r_{\perp}, z) : r_{\perp} \leq R \land |z| \leq z_0\} \), where \( z_0 = a_z, R_{TF} = \sqrt{2\mu/h\omega_z}\sqrt{a_z}, R = \sqrt{2(\mu/h\omega_z - 1/2)\sqrt{a_z}} \), and \( Z = \sqrt{2\mu/h\omega_z}a_z \). More precisely, one expects \( \kappa_2^{-1} \rightarrow \sqrt{2/\pi} \) in the perturbative regime (\( \chi_2 \ll 1 \)), while \( \kappa_2^{-1} \rightarrow 1 \) in the TF regime (\( \chi_2 \gg 1 \)). The final results are not very sensitive to the specific functional form of \( \kappa_2^{-1} \). We thus propose one of the simplest possibilities:

\[
\kappa_2^{-1}(\chi_2) \equiv \sqrt{2/\pi} + \Theta(\chi_2 - 0.1) \times (1 - \sqrt{2/\pi}) \left(1 - \frac{R_{TF}(\chi_2 = 0.1)}{R_{TF}(\chi_2)}\right),
\]

where \( \Theta(x) \) is the Heaviside function and \( R_{TF}(\chi_2) = (15\chi_2)^{1/5}a_{\perp} \) is the TF radius. The normalization of \( \psi \) yields

\[
\frac{1}{15}Z^5 + \frac{1}{8}(\kappa_2 - 1)\frac{R^4}{\lambda^2} - \frac{R^2}{6\lambda} - \frac{1}{15} = \frac{Na}{\lambda^2 a_z^2},
\]

where \( Z \equiv Z/a_z, R \equiv R/a_{\perp} \), and \( Z^2 - R^2/\lambda = 1 \). The chemical potential is \( \mu = h\omega_z = 1/2(1 + R^2/\lambda) \).

For \( \chi_2 \gg 1 \) Eq. \([17]\) leads to the usual TF results, while for \( \chi_2 \ll 1 \) (mean-field quasi-2D regime), one obtains \( \mu = 1/2 + (2\sqrt{2/\pi}\chi_2)^{1/2} \) and \( R = \lambda^{1/2}(8\sqrt{2/\pi}\chi_2)^{1/4} \). An approximate solution that satisfies Eq. \([17]\) with a residual error less than 0.95% for any \( \chi_2 \in [0, \infty) \) is given by

\[
R_{\lambda} \equiv R/\sqrt{\lambda} = \left[(1/15\chi_2)^{8/5} + (\kappa_2/8\chi_2)^2\right]^{-1/8}.
\]

After some calculation one finds the following expressions for the mean-field interaction energy \( \bar{\epsilon}_{\text{int}} \equiv \epsilon_{\text{int}}/h\omega_z \) and the condensate density per unit area \( n_2(r_{\perp}) \):

\[
\bar{\epsilon}_{\text{int}} = \frac{1}{8\chi_2} \left( \frac{8Z^7}{105} + \frac{\xi}{6} - \frac{R_{\lambda}^4}{6} - \frac{R_{\lambda}^6}{15} - \frac{8}{105} \right)
\]

\[
n_2(r_{\perp}) = \frac{\xi [2\pi\lambda(r_{\perp}) - 1]}{4\pi a_a} + \frac{[2\pi\lambda(r_{\perp})]^{3/2} - 1}{6\pi a_a},
\]

where \( \xi \equiv (\kappa_2 - 1) \) and \( 2\pi\lambda(r_{\perp}) \equiv 1 + \frac{R_{\lambda}^2}{R^2} (1 - r_{\perp}^2/R^2) \).

In Fig. \[3\] we show the ground-state properties of arbitrary disk-shaped condensates with \( \lambda \gg 2 \), obtained from our analytical formulas [Eqs. \([8]\) and \([18]-[20]\)] (solid lines), along with exact numerical results (open circles).

In conclusion, modifying the usual TF approximation conveniently to account for the zero-point energy contribution, we have derived general analytical expressions for the ground-state properties of spherical, cigar-shaped, and disk-shaped condensates that reduce to the correct analytical formulas in both the TF and the mean-field perturbative regimes and remain valid and accurate in between these two limiting cases. Mean-field quasi-1D and -2D condensates appear as simple particular cases of our formulation.

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\[\text{FIG. 3: (Color online) Theoretical prediction for the ground-state properties of arbitrary disk-shaped condensates with } \lambda \gg 2 \text{ (solid lines). The open circles are exact numerical results obtained with } \lambda = 20. \text{ The dashed line is the TF prediction.}\]

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