Ground-state properties of trapped Bose-Einstein condensates: Extension of the Thomas-Fermi approximation

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We derive general approximate formulas that provide with remarkable accuracy the ground-state properties of any mean-field scalar Bose-Einstein condensate with short-range repulsive interatomic interactions, confined in arbitrary cylindrically symmetric harmonic traps. Our formulation is even applicable for condensates containing a multiply quantized axisymmetric vortex. We have checked the validity of our formulas by numerically solving the three-dimensional Gross-Pitaevskii equation.

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I. INTRODUCTION

Since the experimental realization of the first dilute Bose-Einstein condensates (BECs) of trapped atomic gases [1–3] there has been great interest in the study of the physical properties of ultracold quantum gases [4]. Under the usual experimental conditions, these systems can be accurately described by the Gross-Pitaevskii equation (GPE) [5], a mean-field equation of motion governing the behavior of the condensate wave function $\psi(\mathbf{r})$. In the stationary case the GPE is given by the nonlinear Schrödinger equation

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

where μ is the chemical potential, N is the number of atoms, $g=4\pi\hbar^2 a/m$ is the interaction strength, determined by the s-wave scattering length a, and $V(\mathbf{r})$ is the trap potential.

In this work we shall concentrate in the usual case of condensates with repulsive interatomic interactions ($a>0$), confined in cylindrically symmetric harmonic traps, $V(\mathbf{r}) = \frac{1}{2}m(\omega_\perp^2 r_\perp^2 + \omega_z^2 z^2)$. To obtain the condensate ground-state properties one has to solve the nonlinear differential equation (1). No explicit analytical solutions are known, so that, in general, this has to be done numerically. However, solving numerically the three-dimensional (3D) GPE is a nontrivial computational task, especially for highly asymmetric trap geometries, where large basis or gridpoint sets can be required to guarantee convergence. Fortunately, approximate analytical solutions can be found in certain limiting cases. In the Thomas-Fermi (TF) regime, which essentially occurs for condensates with a large number of atoms, the kinetic energy can be neglected to a good approximation. In this case the GPE reduces to a simple algebraic equation and one can obtain explicit analytical expressions for the condensate ground-state properties [6]. This approximation, however, cannot reproduce correctly the decay of the wave function at the boundary of the atomic cloud, a region where the kinetic energy has a decisive influence. Corrections to the TF approximation have been proposed to account for the proper behavior of the density cloud at the condensate surface [7–9]. In the (ideal gas) perturbative regime, when the number of atoms in the condensate is sufficiently small, explicit analytical expressions can also be obtained by treating the interaction energy term in Eq. (1) as a weak perturbation.

Another approximation scheme that has proved to be useful in the characterization of dilute BECs is that based on variational techniques [6]. This approximation method has the additional interest that it can be equally applied to the study of the condensate dynamics [10,11]. By using appropriate variational trial wave functions, the ground-state properties of trapped Bose-condensed gases have been studied beyond the two analytically solvable regimes, for both isotropic [12] and highly anisotropic condensates [13]. For this purpose semiclassical approximations ($\hbar\to 0$) have also been considered [14,15]. These approximate methods can be applied to the study of vortex states as well [16–18].

Particular attention has been devoted to the physical properties of quasi-1D [19–23] and quasi-2D [24,25] condensates, systems so tightly confined in the radial or the axial dimension, respectively, that the corresponding dynamics is restricted to zero-point oscillations. In a previous work, by modifying the usual TF approximation conveniently, we derived very accurate approximate analytical expressions for the ground-state properties of trapped spherical, cigar-shaped, and disk-shaped condensates with an arbitrary number of atoms in the mean-field regime [26]. In this work we extend our previous results and derive general approximate formulas that provide with remarkable accuracy the ground-state properties of any mean-field scalar Bose-Einstein condensate with short-range repulsive interatomic interactions, confined in arbitrary cylindrically symmetric harmonic traps, and even containing a multiply quantized axisymmetric vortex.

II. MODEL

We consider a BEC with an axisymmetric vortex line of topological charge q, and confined in a harmonic trap characterized by oscillator lengths $a_\perp=\sqrt{\hbar/m\omega_\perp}$ and $a_z=\sqrt{\hbar/m\omega_z}$. The trap aspect ratio is given by $\lambda=\omega_z/\omega_\perp$. In this work we shall distinguish between ground and vortex states only through the value of the vortex charge. Accord-

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ingly, we shall refer to the lowest-energy state of the condensate compatible with an axisymmetric vortex of charge q as the ground state with a charge-q vortex. This terminology will permit us to make a unified treatment in which the actual ground state of the condensate is simply a particular case corresponding to $q=0$.

For condensates with a sufficiently small number of atoms the mean-field interaction energy can be treated as a weak perturbation. In this perturbative regime the condensate wave function that minimizes the energy functional is given, to the lowest order, by

$$\psi_q(r_\perp,z,\theta)=\exp(iq\theta)\varphi_q(r_\perp)\phi(z), \tag{2}$$

with

$$\varphi_q(r_\perp)=(\pi a_\perp^2|q|!)^{-1/2}(r_\perp/a_\perp)^{|q|}\exp(-r_\perp^2/2a_\perp^2), \tag{3}$$

$$\phi(z)=(\pi a_z^2)^{-1/4}\exp(-z^2/2a_z^2). \tag{4}$$

Using this result one obtains the following analytical expression for the chemical potential:

$$\mu=\frac{1}{2}\hbar\omega_z+(|q|+1)\hbar\omega_\perp+g\bar{n}, \tag{5}$$

where $\bar{n}=c_qN/(2\pi)^{3/2}a_\perp^2a_z$ is the mean atom density and the coefficient c_q is a function of the vortex charge that takes values in the interval [1,0) and accounts for the dilution effect that the centrifugal force associated with the vortex has on the condensate mean density

$$c_q=\frac{(2|q|)!}{2^{2|q|}(|q|!)^2}. \tag{6}$$

For $q=0$ one has $c_q=1$, and the usual results for the ground-state properties of a BEC in the perturbative regime are recovered. For a unit charge vortex the dilution coefficient takes the value $1/2$, and, in general, for $|q|\gg1$, it decreases slowly as $1/\sqrt{\pi|q|}$.

In the Thomas-Fermi regime, for condensates in the ground state ($q=0$) and with a sufficiently large number of atoms, one can neglect the kinetic energy in comparison with the interaction energy, and the stationary GPE leads to

$$\mu=\frac{1}{2}m\omega_z^2z^2+\frac{1}{2}m\omega_\perp^2r_\perp^2+gN|\psi(r_\perp,z)|^2. \tag{7}$$

In the presence of a vortex of charge $q\neq0$ the above equation is no longer a good approximation. In this case neglecting the kinetic energy amounts to neglecting the vortex itself. However, for a large N, the condensate density cloud outside the vortex core is still given, to a very good approximation, by the Thomas-Fermi profile. We thus shall assume the above TF expression to be valid up to a lower cutoff radius

$$r_\perp^0=\sqrt{2(|q|+1)}a_\perp, \tag{8}$$

determined from the condition that, in the presence of a vortex, the contribution from the radial harmonic oscillator energy cannot be smaller than $(|q|+1)\hbar\omega_\perp$, i.e.,

$$\frac{1}{2}m\omega_\perp^2(r_\perp^0)^2=(|q|+1)\hbar\omega_\perp. \tag{9}$$

Likewise, the contribution from the axial harmonic oscillator energy should not be smaller than the corresponding zero-point energy. To account for this fact we introduce a second cutoff z_0, defined through the condition

$$\frac{1}{2}m\omega_z^2z_0^2=\frac{1}{2}\hbar\omega_z, \tag{10}$$

which yields the axial cutoff

$$z_0=a_z. \tag{11}$$

This leads us to consider the TF expression (7) applicable in a volume V_3 that corresponds to the usual TF ellipsoidal density cloud truncated at both $r_\perp=r_\perp^0$ and $|z|=z_0$,

$$V_3\equiv\{(r_\perp,z):r_\perp^2/R_{\mathrm{TF}}^2+z^2/Z_{\mathrm{TF}}^2\leq1,\ r_\perp>r_\perp^0\wedge|z|>z_0\}. \tag{12}$$

In the above equation $R_{\mathrm{TF}}\equiv\sqrt{2\mu/\hbar\omega_\perp}a_\perp$ and $Z_{\mathrm{TF}}\equiv\sqrt{2\mu/\hbar\omega_z}a_z$ are the usual TF values for the condensate radius and axial half-length, respectively. In our approach, however, the condensate radius and axial half-length do not coincide with the above TF expressions. Because of the cutoffs we have introduced they are given instead by

$$R=\sqrt{2\mu/\hbar\omega_\perp-\lambda}a_\perp, \tag{13}$$

$$Z=\sqrt{2\mu/\hbar\omega_z-2(|q|+1)/\lambda}a_z. \tag{14}$$

However, when $\mu\gg(|q|+1)\hbar\omega_\perp$, then Z becomes indistinguishable from Z_{TF}. This is true, in particular, whenever $\lambda\gg2(|q|+1)$. Likewise, if $\mu\gg\frac{1}{2}\hbar\omega_z$, then $R\to R_{\mathrm{TF}}$.

More generally, for condensates with $\mu\gg(|q|+1)\hbar\omega_\perp$, which occurs whenever $\lambda\gg2(|q|+1)$, the relative contribution to the condensate properties coming from the region $r_\perp\leq r_\perp^0$ becomes negligible. The same occurs with the relative contribution from the region corresponding to $|z|\leq z_0$ when the chemical potential is much larger than the axial zero-point energy, which occurs whenever $\lambda\ll1$. It is then clear that when the number of atoms is sufficiently large that $\mu\gg(|q|+1)\hbar\omega_\perp+\frac{1}{2}\hbar\omega_z$ the dominant contribution comes from the V_3 volume introduced above.

Only for condensates with $\mu\simeq(|q|+1)\hbar\omega_\perp$ is the contribution from the region $r_\perp\leq r_\perp^0$ the most significant one. These are condensates with the transverse dynamics frozen in the lowest energy state compatible with a charge-q axisymmetric vortex. In this case the condensate wave function can be factorized as $\psi_q(r_\perp,z,\theta)=\exp(iq\theta)\varphi_q(r_\perp)\phi(z)$, with $\varphi_q(r_\perp)$ given by Eq. (3). After substituting this wave function in the stationary GPE, multiplying by ψ_q^*, and integrating over the radial dynamics, one obtains

$$\frac{1}{2}m\omega_z^2z^2+(|q|+1)\hbar\omega_\perp+g_{1\mathrm{D}}N|\phi(z)|^2=\mu, \tag{15}$$

where $g_{1\mathrm{D}}=c_qg/2\pi a_\perp^2$, and we have neglected the axial kinetic energy $\left(\sim\frac{1}{2}\hbar\omega_z\right)$ against $(|q|+1)\hbar\omega_\perp$. It is convenient to rewrite $g_{1\mathrm{D}}$ as $g\kappa_1^{-1}\bar{n}_2$, where $\bar{n}_2=1/\pi(r_\perp^0)^2=1/[2\pi a_\perp^2(|q|$

$+1)]$ is a uniform mean density per unit area normalized to unity in the region $r_\perp \leqslant r_\perp^0$, and

$$\kappa_1^{-1} \equiv (|q|+1)c_q \tag{16}$$

is the appropriate renormalization factor. The important point is that the effect of the vortex can be incorporated in an exact manner into a localized uniform mean density $\bar{n}_2$ with a renormalized interaction strength $g\kappa_1^{-1}$. We shall assume that, to a good approximation, this still remains true for condensates with an arbitrary chemical potential.

On the other hand, the contribution from the region $|z| \leqslant z_0$ is the most significant one only for condensates with $\mu \simeq \frac{1}{2}\hbar\omega_z$. In this case the axial dynamics is restricted to zero-point oscillations, and the wave function of such quasi-2D condensates can be written as $\psi_q(r_\perp, z, \theta) = \exp(iq\theta)\varphi(r_\perp)\phi(z)$, where now $\phi(z)$ is given by Eq. (4). Substituting into the stationary GPE and integrating out the axial dynamics one obtains

$$\frac{1}{2}\hbar\omega_z + \frac{1}{2}m\omega_\perp^2 r_\perp^2 + g_{2D}N|\varphi(r_\perp)|^2 = \mu, \tag{17}$$

where $g_{2D} = g/\sqrt{2\pi}a_z$, and now we have neglected the radial kinetic energy against the axial zero-point energy, which is a good approximation as long as $\mu \simeq \frac{1}{2}\hbar\omega_z$. As before, it is convenient to rewrite g_{2D} in terms of a uniform mean density per unit length normalized to unity in the volume $|z| \leqslant z_0$. To this end we introduce a renormalization factor $\kappa_2^{-1} \equiv \sqrt{2/\pi}$ and rewrite g_{2D} as $g\kappa_2^{-1}\bar{n}_1$ with $\bar{n}_1 = 1/2a_z$. This indicates that the contribution from the axial zero-point oscillations, which is the dominant contribution in these quasi-2D condensates, can be properly accounted for by simply introducing a localized uniform mean density per unit length with a renormalized interaction strength. Again, we shall assume this to be also valid for condensates with an arbitrary chemical potential. One finds, however, that somewhat more accurate results are obtained when one lets the renormalization factor κ_2^{-1} to approach unity in the TF regime [26]. Since the final results are little sensitive to the specific functional form of κ_2^{-1}, we propose one of the simplest possibilities [26]

$$\kappa_2^{-1}(\chi_2) \equiv \sqrt{2/\pi} + \Theta(\chi_2 - 0.1) \times (1 - \sqrt{2/\pi})\left(1 - \frac{R_{TF}(\chi_2 = 0.1)}{R_{TF}(\chi_2)}\right), \tag{18}$$

where $\Theta(x)$ is the step function, $\chi_2 \equiv Na/\lambda^2 a_z$, and $R_{TF}(\chi_2) = (15\chi_2)^{1/5}a_\perp$ is the TF radius.

Motivated by the above ideas and the fact that there exists a direct relation between the number of atoms and the size of a trapped BEC, we propose the following ansatz for the ground-state properties of any mean-field scalar Bose-Einstein condensate with an axisymmetric vortex of charge q, confined in an arbitrary axisymmetric harmonic trap:

$$\frac{1}{2}m\omega_z^2 z^2 + \frac{1}{2}m\omega_\perp^2 r_\perp^2 + gN|\psi(r_\perp, z)|^2 = \mu, \quad \mathbf{r} \in V_3,$$

$$\frac{1}{2}\hbar\omega_z + \frac{1}{2}m\omega_\perp^2 r_\perp^2 + g\kappa_2^{-1}N\bar{n}_1|\varphi(r_\perp)|^2 = \mu, \quad \mathbf{r} \in V_2,$$

$$\frac{1}{2}m\omega_z^2 z^2 + \alpha_q\hbar\omega_\perp + g\kappa_1^{-1}N\bar{n}_2|\phi(z)|^2 = \mu, \quad \mathbf{r} \in V_1,$$

$$\frac{1}{2}\hbar\omega_z + \alpha_q\hbar\omega_\perp + g\kappa_0^{-1}\bar{n}_0 = \mu, \quad \mathbf{r} \in V_0,$$

with $\psi = 0$ elsewhere. In the above equations $\alpha_q \equiv (|q|+1)$ and $\kappa_0 \equiv \kappa_1\kappa_2$, with κ_1 and κ_2 defined by Eqs. (16) and (18), respectively. As already seen, $\bar{n}_1 = 1/2a_z$ and $\bar{n}_2 = 1/2\pi a_\perp^2 \alpha_q$, whereas $\bar{n}_0$ is an effective mean density (per unit volume) localized in V_0 and defined in terms of μ through the above expressions. Note that κ_0^{-1} is exactly the renormalization constant required to make the latter of the above equations compatible with the other ones as well as with the perturbative result (5). The outer volume V_3 is defined by Eq. (12) while the remaining inner volumes are defined by

$$V_2 \equiv \{(r_\perp, z): r_\perp^0 < r_\perp \leqslant R \wedge |z| \leqslant z_0\},$$

$$V_1 \equiv \{(r_\perp, z): r_\perp \leqslant r_\perp^0 \wedge z_0 < |z| \leqslant Z\},$$

$$V_0 \equiv \{(r_\perp, z): r_\perp \leqslant r_\perp^0 \wedge |z| \leqslant z_0\}.$$

The ansatz we have just introduced represents a direct generalization of our previous proposal in Ref. [26] and extends the applicability of the approach to mean-field condensates confined in axisymmetric harmonic traps with an arbitrary geometry, and containing an axisymmetric vortex of charge q. As we shall see, in the appropriate limits the results obtained in the present work reduce to those previously obtained in Ref. [26].

From Eq. (14) the chemical potential can be written in terms of the dimensionless axial half-length $\bar{Z} \equiv Z/a_z$ as

$$\frac{\mu}{\hbar\omega_z} = \frac{1}{2}\bar{Z}^2 + \frac{1}{\lambda}(|q|+1). \tag{19}$$

As usual, the condition that the condensate contains N particles determines the precise value of μ. After a straightforward calculation one obtains

$$\frac{\chi_0}{\lambda^{5/3}} = \frac{1}{15}\bar{Z}^5 + \frac{\xi_1}{8}\bar{Z}^4 + \frac{\beta_q}{3\lambda}\bar{Z}^3 + \frac{1}{2}\left(\frac{\beta_q\xi_1}{\lambda} - \frac{\xi_3}{2}\right)\bar{Z}^2 - \frac{1}{2}\left(\frac{\beta_q\xi_3}{\lambda} - \frac{\xi_5}{4}\right), \tag{20}$$

where $\beta_q \equiv \kappa_1(|q|+1) = 1/c_q$, $\xi_n \equiv (\kappa_2 - 1/n)$ with $n = 1, 3, 5, \ldots$, and we have defined the dimensionless interaction parameter χ_0 as

$$\chi_0 \equiv Na/a_0, \tag{21}$$

with $a_0 \equiv (a_\perp^2 a_z)^{1/3}$ being the mean oscillator length. From Eqs. (13) and (14) one also finds the following expression for the condensate radius $\bar{R} \equiv R/a_\perp$:

$$\bar{R}^2 = \lambda(\bar{Z}^2 - 1) + 2(|q|+1). \tag{22}$$

The mean-field interaction energy per particle $\epsilon_{int} \equiv E_{int}/N$ is defined by $\epsilon_{int} = (1/2)\int g_r N|\psi(\mathbf{r})|^4 d^3\mathbf{r}$, where $N|\psi|^2$ represents the local density in each region and g_r de-

notes the corresponding renormalized interaction strength. After some calculation one obtains

$$\frac{\epsilon_{\rm int}}{\hbar\omega_z} = \frac{\lambda^{5/3}}{8\chi_0}\left[\frac{8}{105}\bar{Z}^7 + \frac{\xi_1}{6}\bar{Z}^6 + \frac{8\beta_q}{15\lambda}\bar{Z}^5 + \left(\frac{\beta_q\xi_1}{\lambda} - \frac{\xi_3}{2}\right)\bar{Z}^4 - 2\left(\frac{\beta_q\xi_3}{\lambda} - \frac{\xi_5}{4}\right)\bar{Z}^2 + \left(\frac{\beta_q\xi_5}{\lambda} - \frac{\xi_7}{6}\right)\right]. \quad (23)$$

Finally, the kinetic and potential energies can be readily obtained in terms of the previous results by using the *exact* relations [4]

$$\epsilon_{\rm kin} \equiv E_{\rm kin}/N = \mu/2 - (7/4)E_{\rm int}/N, \quad (24a)$$

$$\epsilon_{\rm pot} \equiv E_{\rm pot}/N = \mu/2 - (1/4)E_{\rm int}/N. \quad (24b)$$

Equations (19)–(24) provide the ground-state properties we are looking for. All that is needed is to solve the quintic polynomial equation (20). This is a general equation that provides the axial half-length $\bar{Z}$ of any mean-field scalar condensate as a function of only three parameters: the interaction parameter χ_0, the trap aspect ratio λ, and the vortex charge q. In certain particular cases it is possible to find useful approximate analytical solutions. However, in general, Eq. (20) has to be solved numerically. It is important to note that this is a trivial computational task that can be done immediately with the built-in capabilities of symbolic computational software packages such as MATHEMATICA or MATLAB. In fact, to obtain the roots of a polynomial one simply has to type in a single instruction and the answer is instantaneous.

III. LIMITING CASES

The above formulas simplify considerably in two limiting cases that, essentially, correspond to condensates confined in disk-shaped traps satisfying $\lambda \gg 2(|q|+1)$ and cigar-shaped traps satisfying $\lambda \ll 1$. We have already found these two limiting cases before. As mentioned above, in the first case the relative contribution to the condensate properties coming from the inner cylinder $r_\perp \leqslant r_\perp^0$ becomes negligible, while, in the second case, it is the relative contribution from the inner disk $|z| \leqslant z_0$ that becomes negligible. Under these circumstances we shall be able to find approximate analytical solutions of the polynomial equation (20).

A. Disk-shaped traps

Taking into account that $\beta_q/\lambda \leqslant (|q|+1)/\lambda$, it follows that in the limit $\lambda \gg 2(|q|+1)$ Eq. (20) reduces to

$$\chi_2 = \frac{1}{15}\bar{Z}^5 + \frac{\xi_1}{8}\bar{Z}^4 - \frac{\xi_3}{4}\bar{Z}^2 + \frac{\xi_5}{8}, \quad (25)$$

where $\chi_2 \equiv Na/\lambda^2 a_z$ is now the only relevant physical parameter. Using Eq. (22) one can easily see that for $q=0$ the above equation coincides exactly with that obtained previously in Ref. [26]. This is true in general (i.e., for any q) whenever $\lambda \gg 2(|q|+1)$. Under these circumstances the contribution of the vortex can be neglected to a good approximation and we can use the analytical solution found in Ref. [26]

$$\bar{Z}^2 = 1 + [(1/15\chi_2)^{8/5} + (\kappa_2/8\chi_2)^2]^{-1/4}. \quad (26)$$

From this result one immediately obtains the chemical potential using Eq. (19)

$$\frac{\mu}{\hbar\omega_z} = \frac{1}{2}\bar{Z}^2. \quad (27)$$

On the other hand, in the limit we are considering, the interaction energy (23) becomes

$$\frac{\epsilon_{\rm int}}{\hbar\omega_z} = \frac{1}{8\chi_2}\left(\frac{8}{105}\bar{Z}^7 + \frac{\xi_1}{6}\bar{Z}^6 - \frac{\xi_3}{2}\bar{Z}^4 + \frac{\xi_5}{2}\bar{Z}^2 - \frac{\xi_7}{6}\right). \quad (28)$$

As before, it is not hard to see that this equation is the same as that obtained previously in Ref. [26].

Another relevant physical quantity in the characterization of disk-shaped condensates is the condensate density per unit area, defined as $n_2(r_\perp) \equiv N\int dz|\psi(r_\perp,z)|^2$. Outside the vortex core $(r_\perp > r_\perp^0)$, which we are neglecting in this limit, a straightforward calculation leads to

$$n_2(r_\perp) = \frac{\xi_1[2\bar{\mu}_z(r_\perp)-1]}{4\pi a a_z} + \frac{[2\bar{\mu}_z(r_\perp)]^{3/2}-1}{6\pi a a_z}, \quad (29)$$

where $n_2(r_\perp > R) = 0$ and $\bar{\mu}_z(r_\perp) \equiv \mu_z(r_\perp)/\hbar\omega_z$ is given by

$$\bar{\mu}_z(r_\perp) \equiv \frac{1}{2} + \frac{1}{2}(\bar{R}/\sqrt{\lambda})^2\left(1 - \frac{r_\perp^2}{R^2}\right), \quad (30)$$

with $\bar{R}^2 \simeq \lambda(\bar{Z}^2-1)$ [Eq. (22)]. Again, this result coincides with that derived in Ref. [26]. In fact, in general, in the limit $\lambda \gg 2(|q|+1)$ the formalism proposed in the previous section becomes independent of both λ and q and reduces to that developed in Ref. [26].

It can be easily verified that $\mu_z(r_\perp)$ is nothing but the local chemical potential, defined as $\mu_z(r_\perp) = \mu - \frac{1}{2}m\omega_\perp^2 r_\perp^2$ [15]. Equation (29) is a cubic equation in $\bar{\mu}_z^{1/2}$ which has only one real solution. Solving this equation, after some algebra one finds the following expression for the local chemical potential as a function of the condensate density per unit area [27]:

$$\bar{\mu}_z(r_\perp) \equiv \frac{1}{8}[(\eta + \sqrt{\eta^2 - \xi_1^6})^{1/3} + (\eta - \sqrt{\eta^2 - \xi_1^6})^{1/3} - \xi_1]^2, \quad (31)$$

where $\eta = 4 + 6\xi_1 - \xi_1^3 + 24\pi a a_z n_2(r_\perp)$. In the TF regime ($\chi_2 \gg 1 \rightarrow a a_z n_2 \gg 1$), the above equation reduces to

$$\bar{\mu}_z(r_\perp) = [(3\pi/\sqrt{2})a a_z n_2(r_\perp)]^{2/3}, \quad (32)$$

which coincides with the expression that can be obtained directly from the 3D Gross-Pitaevskii equation in this regime. In the quasi-2D perturbative limit ($\chi_2 \ll 1 \rightarrow a a_z n_2 \ll 1$), Eq. (31) reduces to

$$\bar{\mu}_z(r_\perp) = 1/2 + 2\sqrt{2\pi} a a_z n_2(r_\perp). \tag{33}$$

This is again the correct result, as follows from the perturbative solution of the GPE in this limit.

Equations (29)–(31) permit us to derive a general formula for the (local) radial (first) sound velocity c_{2D} of a disk-shaped condensate, which is defined by

$$c_{2D}^2 = \frac{n_2}{m}\frac{\partial \mu_z}{\partial n_2}. \tag{34}$$

From Eq. (29) one immediately obtains

$$\frac{mc_{2D}^2}{\hbar\omega_z} = \frac{\frac{3}{2}\xi_1[2\bar{\mu}_z(r_\perp)-1] + [2\bar{\mu}_z(r_\perp)]^{3/2} - 1}{3\xi_1 + 3[2\bar{\mu}_z(r_\perp)]^{1/2}}. \tag{35}$$

This equation in the TF regime ($\chi_2 \gg 1$) reduces to

$$\frac{mc_{2D}^2}{\hbar\omega_z} = \frac{2}{3}\bar{\mu}_z(r_\perp) = \left(\frac{2\pi}{\sqrt{3}} a a_z n_2(r_\perp)\right)^{2/3}, \tag{36}$$

while in the quasi-2D perturbative regime ($\chi_2 \ll 1$), it reduces to

$$\frac{mc_{2D}^2}{\hbar\omega_z} = \bar{\mu}_z(r_\perp) - \frac{1}{2} = 2\sqrt{2\pi} a a_z n_2(r_\perp). \tag{37}$$

These are the correct limits as follows from the substitution of Eqs. (32) and (33) into Eq. (34). In fact, it is not hard to see that all the analytical formulas derived in this section reduce to the correct expressions in both the TF and the perturbative regimes [26].

For the particular case of a homogeneous disk-shaped condensate (no radial confinement and n_2 constant) the authors of Ref. [23] obtained an expression for the radial sound velocity that interpolates between the above two regimes. Such expression leads to the correct perturbative result and reproduces to a good approximation the TF result. Even though this expression is analytic, it is too complicated to be written in a useful compact way and the authors of Ref. [23] do not provide an explicit analytical formula in their work.

B. Cigar-shaped traps

In the $\lambda \ll 1$ limit Eq. (20) reduces to

$$\chi_1 = \frac{1}{15}(\sqrt{\lambda}\bar{Z})^5 + \frac{1}{3}\beta_q(\sqrt{\lambda}\bar{Z})^3, \tag{38}$$

with $\chi_1 \equiv \lambda N a/a_\perp$. In this limit the formalism becomes independent of λ and the vortex contribution enters in a rather simple way through the parameter

$$\beta_q = \frac{2^{2|q|}(|q|!)^2}{(2|q|)!}. \tag{39}$$

This fact will permit us to find an approximate analytical solution.

Given a polynomial equation $P(x)=\chi$, we define the residual error associated with the approximate solution x_ε as $[P(x_\varepsilon)-\chi]/\chi$ [26]. We have explicitly verified that the expression

$$\sqrt{\lambda}\bar{Z} = \left[\frac{1}{(15\chi_1)^{4/5} + \frac{1}{3}} + \frac{1}{57\chi_1 + 345} + \frac{1}{(3\chi_1/\beta_q)^{4/3}}\right]^{-1/4} \tag{40}$$

satisfies Eq. (38) with a residual error smaller than 3.2% for any $\chi_1 \in [0,\infty)$ and $0 \leqslant |q| \leqslant 10$. In fact, as seen in Ref. [26], in the absence of vortices ($q=0$) the above solution is somewhat more accurate and the error is less than 0.75%.

From Eq. (19) the chemical potential is given now by

$$\frac{\mu}{\hbar\omega_\perp} = (|q|+1) + \frac{1}{2}(\sqrt{\lambda}\bar{Z})^2. \tag{41}$$

In the $\lambda \ll 1$ limit the interaction energy becomes

$$\frac{\epsilon_{\rm int}}{\hbar\omega_\perp} = \frac{1}{15\chi_1}\left[\frac{1}{7}(\sqrt{\lambda}\bar{Z})^7 + \beta_q(\sqrt{\lambda}\bar{Z})^5\right]. \tag{42}$$

On the other hand, the condensate density per unit length, $n_1(z) \equiv N\int 2\pi r_\perp dr_\perp |\psi(r_\perp,z)|^2$, is

$$n_1(z) = \beta_q \frac{(\sqrt{\lambda}\bar{Z})^2}{4a}\left(1 - \frac{z^2}{Z^2}\right) + \frac{(\sqrt{\lambda}\bar{Z})^4}{16a}\left(1 - \frac{z^2}{Z^2}\right)^2 \tag{43}$$

with $n_1(z)=0$ for $|z|>Z$.

The local chemical potential, defined as $\mu_\perp(z) \equiv \mu - \frac{1}{2}m\omega_z^2 z^2$ [15], is given by

$$\frac{\mu_\perp(z)}{\hbar\omega_\perp} = (|q|+1) + \frac{1}{2}(\sqrt{\lambda}\bar{Z})^2\left(1 - \frac{z^2}{Z^2}\right). \tag{44}$$

The above analytical formulas generalize those obtained in Ref. [26] to the case of condensates containing an axisymmetric vortex. This is particularly interesting because, in this case, the usual TF approximation does not lead to explicit analytical formulas for the condensate properties. In the absence of vortices $\beta_q \to 1$ and one recovers the results of Ref. [26].

Substituting Eq. (44) into Eq. (43) and solving for $\bar{\mu}_\perp(z) \equiv \mu_\perp(z)/\hbar\omega_\perp$ one obtains the local chemical potential as a function of the condensate density per unit length

$$\bar{\mu}_\perp(z) = (|q|+1) + \sqrt{\beta_q^2 + 4a n_1(z)} - \beta_q. \tag{45}$$

This equation in the absence of vortices takes the simple form

$$\bar{\mu}_\perp(z) = \sqrt{1 + 4a n_1(z)}. \tag{46}$$

In the TF regime ($\chi_1 \gg 1 \to a n_1 \gg 1$) the above expression reduces to

$$\bar{\mu}_\perp(z) = 2\sqrt{a n_1(z)}, \tag{47}$$

which is the well-known result that can be obtained directly from the GPE in this regime [22]. In the mean-field quasi-1D limit ($\chi_1 \ll 1 \to a n_1 \ll 1$) Eq. (46) reads

$$\bar{\mu}_\perp(z) = 1 + 2a n_1(z). \tag{48}$$

This is again the correct result that follows from the perturbative solution of the GPE in this limit [22]. In fact, it can be

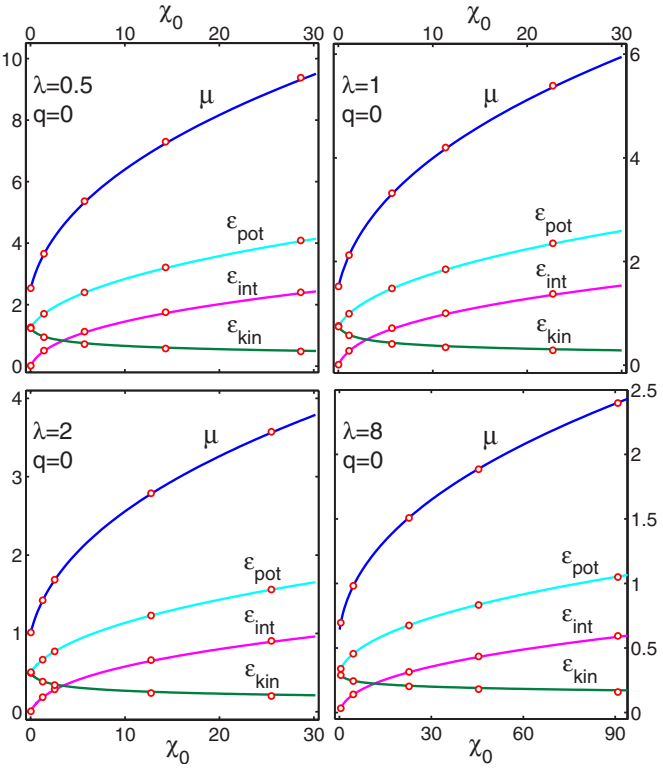

FIG. 1. (Color online) Theoretical prediction for the ground-state properties (in units of $\hbar\omega_z$) of arbitrary condensates with $q=0$ in different trap geometries λ (solid lines). The open circles are the exact numerical results.

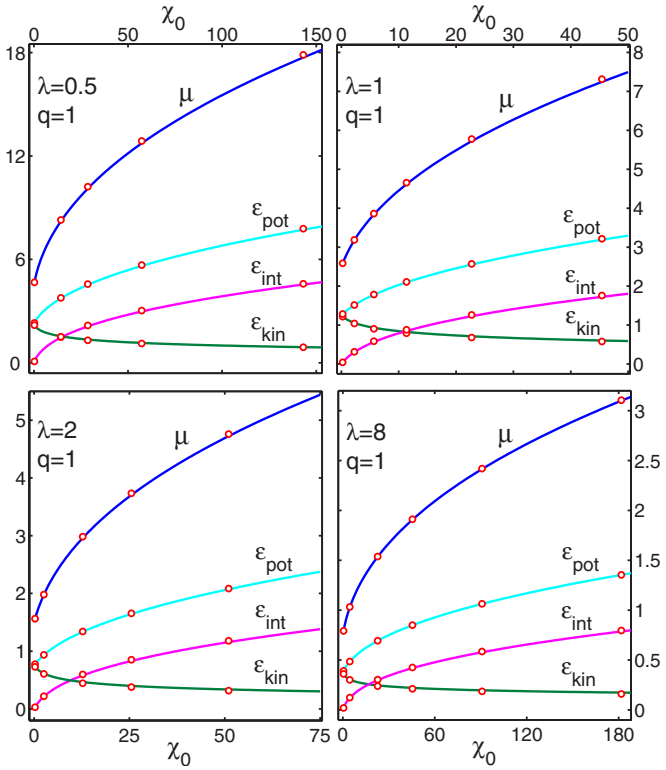

FIG. 2. (Color online) Theoretical prediction for the ground-state properties (in units of $\hbar\omega_z$) of arbitrary condensates with a $q=1$ vortex in different trap geometries λ (solid lines). The open circles are the exact numerical results.

easily verified that all the analytical formulas derived in this section have the correct limits in both the TF and the perturbative regimes [26].

From the above results one can derive a general formula for the (local) axial (first) sound velocity c_{1D} of a cigar-shaped condensate, defined by

$$c_{1D}^2 = \frac{n_1}{m}\frac{\partial \mu_\perp}{\partial n_1}. \tag{49}$$

Substitution of Eq. (45) in Eq. (49) leads to

$$\frac{mc_{1D}^2}{\hbar\omega_\perp} = \sqrt{\frac{4a^2 n_1^2(z)}{\beta_q^2 + 4an_1(z)}}. \tag{50}$$

In the absence of vortices and in the TF regime ($\beta_q=1$, $\chi_1 \gg 1$) the expression above reduces to

$$\frac{mc_{1D}^2}{\hbar\omega_\perp} = \sqrt{an_1(z)} = \frac{1}{2}\bar{\mu}_\perp(z). \tag{51}$$

This result is in agreement with the formula obtained by Zaremba for the sound velocity of a homogeneous cigar-shaped condensate in the TF regime [28].

In the quasi-1D mean field regime with no vortices ($\chi_1 \ll 1$, $\beta_q=1$) Eq. (50) reduces to

$$\frac{mc_{1D}^2}{\hbar\omega_\perp} = 2an_1(z) = \bar{\mu}_\perp(z) - 1, \tag{52}$$

which is also the correct result as follows from the substitution of Eq. (48) into Eq. (49).

For the particular case of a homogeneous cigar-shaped condensate (no axial confinement and n_1 constant) the authors of Ref. [23] have obtained an analytical expression for the axial sound velocity that reproduces correctly the perturbative result and, to a good approximation (with a relative error less than 3%), also the TF result, interpolating between these two regimes. This expression has been obtained using an approach different from that used here and, in fact, it exhibits a functional dependence on an_1 that is very different from that in Eq. (50). However, particularizing Eq. (50) for an axially homogeneous condensate one finds that, in this case, both expressions are in quantitative agreement within 3.75%.

IV. NUMERICAL RESULTS

To verify the predictions of our model we have numerically solved the stationary Gross-Pitaevskii equation (1) by using a pseudospectral method evolving in imaginary time. Figure 1 shows the ground-state properties of condensates with $q=0$ and an arbitrary number of particles (χ_0) in different trap geometries (λ). The open circles are exact numerical results obtained from the Gross-Pitaevskii equation. The

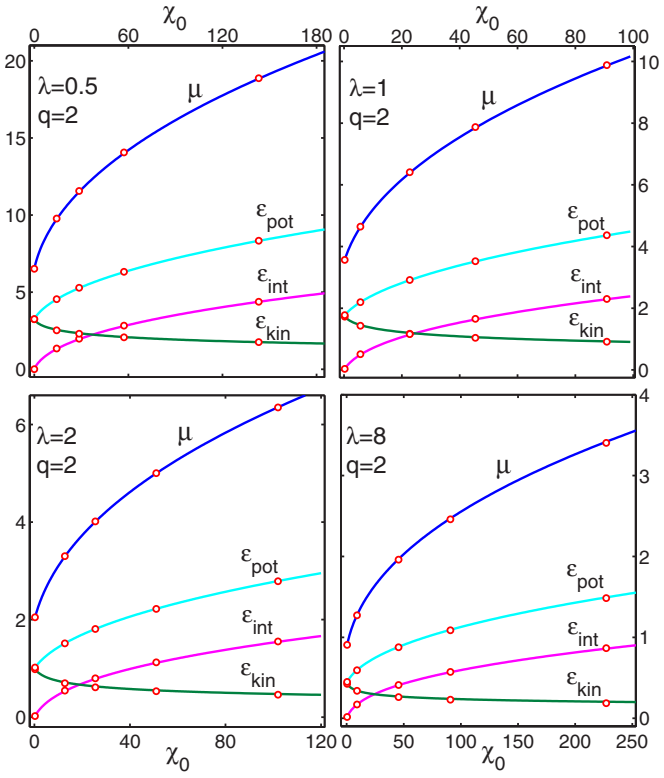

FIG. 3. (Color online) Same as Fig. 2 for arbitrary condensates with a $q=2$ vortex.

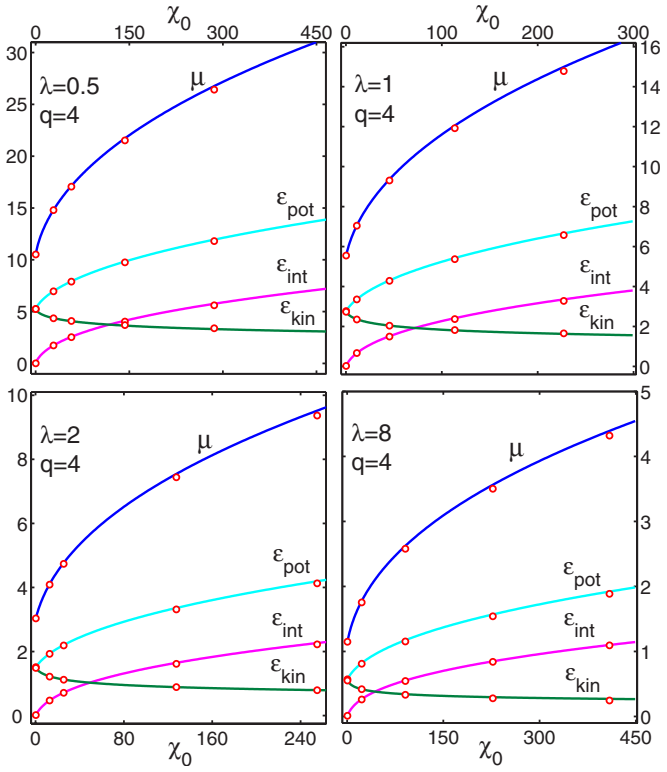

FIG. 4. (Color online) Same as Fig. 2 for arbitrary condensates with a $q=4$ vortex.

solid lines are the theoretical predictions (in units of $\hbar\omega_z$) obtained from Eqs. (19)–(24). We have solved the polynomial equation (20) by using a symbolic software package. As already said, this is a trivial computational task that only requires one to type in a single instruction.

As is evident from Fig. 1, the agreement is very good in all trap geometries (typically better than 1%). In particular, although our formalism is cylindrically symmetric it can describe accurately the properties of spherical condensates ($\lambda=1$). For trap anisotropies higher than those considered in Fig. 1 one can make use of the analytical solutions (26) and (40) found above. These cases will be examined below (Fig. 5).

In Figs. 2–4 we show the ground-state properties of condensates containing an axisymmetric vortex of charge $q=1$, 2, and 4, respectively. As before, the solid lines are the theoretical results obtained from Eqs. (19)–(24). These figures show that, regardless of the number of particles (χ_0) and trap geometry (λ), our model, despite its simplicity, can also reproduce very accurately the physical properties of condensates containing an axisymmetric vortex. This is remarkable because, rather crudely, we have incorporated the effect of the vortex into a uniform mean density $\bar{n}_2$ (with a renormalized interaction strength $g\kappa_1^{-1}$) localized in the inner cylinder $r_\perp \leqslant r_\perp^0$. In turn, the radius $r_\perp^0$ follows from Eq. (9), which cannot account for the effect of the mean-field interaction energy. However, for condensates of intermediate size, the interaction energy is no longer negligible in comparison with the kinetic energy. In fact, it plays an important role in determining the size of the vortex core, which decreases as N increases. Equation (9) cannot incorporate this correction, which is proportionally more important for a high q and an intermediate number of particles (for a sufficiently large N the overall contribution of the vortex becomes negligible). Thus, one expects the formulas above to be less accurate as q increases. This can be appreciated from Fig. 4, which shows that for condensates with a $q=4$ vortex and a χ_0 sufficiently large that $\epsilon_{\rm int} > \epsilon_{\rm kin}$ the theoretical predictions are slightly less accurate than those corresponding to a $q=1$ or a $q=2$ vortex.

Next, we consider the ground-state properties of condensates confined in disk-shaped traps satisfying $\lambda \gg 2(|q|+1)$ and cigar-shaped traps satisfying $\lambda \ll 1$. As already seen, in these limiting cases the theoretical results become independent of λ and can be directly obtained from explicit analytical formulas. In Fig. 5 we show the chemical potentials and interaction energies obtained from Eqs. (26)–(28) and (40)–(42), along with exact numerical results. The corresponding kinetic and potential energies follow immediately from Eqs. (24).

As Fig. 5(a) reflects, the chemical potential increases with the vortex charge, a consequence of the larger kinetic and potential energies associated with multiply quantized vortex states. However, as shown in Fig. 5(b), the opposite occurs with the mean interaction energy, which decreases as q increases because of the dilution effect that the centrifugal barrier produced by the vortex has on the mean condensate density. The small errors that can be appreciated in Fig. 5(b) are due, in part, to the fact that, for $q \neq 0$, the approximate solution (40) incorporates a residual error of order 2–3 %. The exact solution of the polynomial equation (38) leads to somewhat better results.

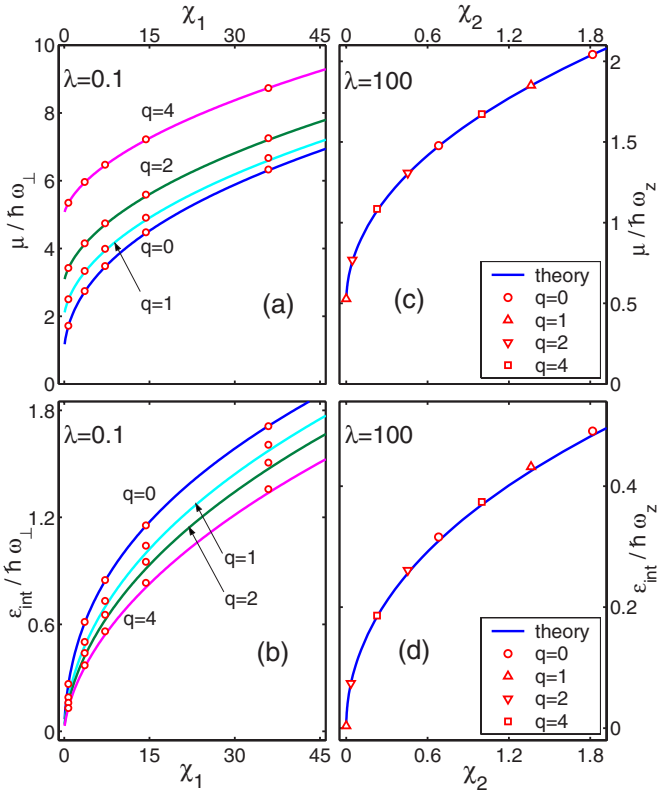

FIG. 5. (Color online) (a),(b): Theoretical prediction for the ground-state properties (in units of $\hbar\omega_\perp$) of arbitrary cigar-shaped condensates with $\lambda \ll 1$ and different vortex charges q (solid lines). The open circles are exact numerical results obtained with $\lambda = 0.1$. (c),(d) Theoretical prediction for the ground-state properties (in units of $\hbar\omega_z$) of arbitrary disk-shaped condensates with $\lambda \gg 2(|q|+1)$ and different vortex charges q (solid lines). The open symbols are exact numerical results obtained with $\lambda = 100$.

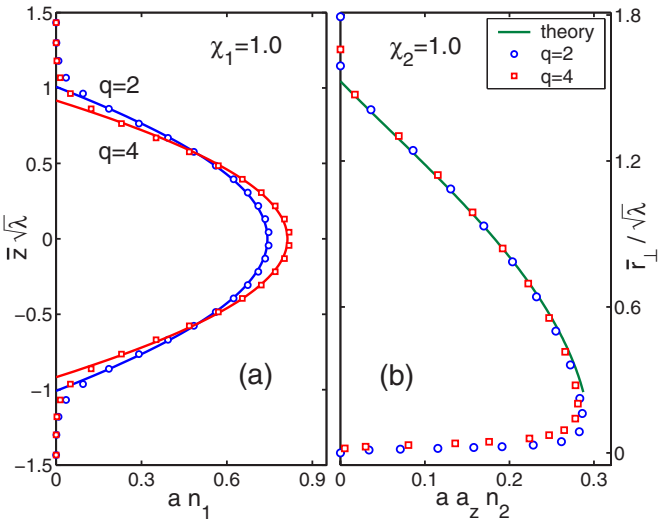

FIG. 6. (Color online) (a) Theoretical prediction for the condensate density per unit length $n_1(z)$ of arbitrary $\chi_1 = 1$ cigar-shaped condensates with $\lambda \ll 1$ and different vortex charges q (solid lines). The open symbols are exact numerical results obtained with $\lambda = 0.1$. (b) Theoretical prediction for the condensate density per unit area $n_2(r_\perp)$ of arbitrary $\chi_2 = 1$ disk-shaped condensates with $\lambda \gg 2(|q|+1)$ and different vortex charges q (solid line). The open symbols are exact numerical results obtained with $\lambda = 100$.

On the other hand, Figs. 5(c) and 5(d) reflect the fact that for highly asymmetric trap geometries satisfying $\lambda \gg 2(|q|+1)$ the vortex contribution to the condensate properties becomes negligible. Figure 6(a) shows the condensate density per unit length $n_1(z)$ of arbitrary cigar-shaped condensates with $\lambda \ll 1$ [obtained from our analytical formulas (40) and (43)], while Fig. 6(b) shows the condensate density per unit area $n_2(r_\perp)$ of arbitrary disk-shaped condensates with $\lambda \gg 2(|q|+1)$ [obtained from Eqs. (26) and (29)]. The good agreement between theoretical and exact results demonstrates that the formulas derived above are applicable for any trap geometry.

V. CONCLUSION

In a previous work we derived very accurate approximate analytical expressions for the ground-state properties of trapped spherical, cigar-shaped, and disk-shaped condensates with an arbitrary number of atoms in the mean-field regime [26]. In this work we have extended our previous proposal and have derived general approximate formulas that provide with remarkable accuracy the ground-state properties of any mean-field scalar Bose-Einstein condensate with short-range repulsive interatomic interactions, confined in arbitrary cylindrically symmetric harmonic traps, and even containing a multiply quantized axisymmetric vortex.

In the appropriate limits (corresponding to cigar-shaped and disk-shaped condensates) the ground-state properties follow from explicit analytical formulas that generalize those obtained in Ref. [26]. In the general case, however, one has to solve a quintic polynomial equation. In this regard, it is important to note that while solving the GP equation can be a complex computational problem (especially in highly asymmetric trap geometries), solving a polynomial equation is a trivial computational task. Using the built-in capabilities of symbolic software packages such as MATHEMATICA or MATLAB one obtains an instantaneous result after typing in a single instruction.

The model presented in this work is essentially a convenient approximation method motivated by two simple ideas: (i) There exists a direct relation between the number of particles and the size of a trapped BEC and (ii) the contribution from the harmonic oscillator energy to the chemical potential cannot be smaller than the zero-point energy. Applying these simple ideas one finds useful formulas of great generality that provide the condensate ground-state properties in terms of the correct physically relevant magnitudes. Moreover, even though no freely adjustable parameters are introduced, in all cases the formulas obtained reproduce simultaneously with a remarkable accuracy the condensate chemical potential and the interaction energy and, as a consequence, the kinetic and the potential energy as well. And this is true for mean-field condensates with any number of particles, confined in any axisymmetric harmonic trap, and even

containing an axisymmetric vortex. Finally, note that the results of this work are applicable in general to any nonlinear system characterized by the stationary nonlinear Schrödinger equation (1).

ACKNOWLEDGMENTS

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