

Thomas-Fermi approximation to static vortex states in superfluid trapped atomic gases

M. Urban^{1,a}, P. Schuck^{1,2}, and X. Viñas³

¹ Institut de Physique Nucléaire, 91406 Orsay Cedex, France

² Laboratoire de Physique et Modélisation des Milieux Condensés, CNRS & Université Joseph Fourier, Maison des Magistères, B.P. 166, 38042 Grenoble Cedex 9, France

³ Departament d'Estructura i Constituents de la Matèria, Facultat de Física, Universitat de Barcelona, Diagonal 647, 08028 Barcelona, Spain

Received 28 November 2002 / Received in final form 10 April 2003

Published online 12 August 2003 – © EDP Sciences, Società Italiana di Fisica, Springer-Verlag 2003

Abstract. We revise the Thomas-Fermi approximation for describing vortex states in Bose condensates of magnetically trapped atoms. Our approach is based on considering the $\hbar \rightarrow 0$ limit rather than the $N \rightarrow \infty$ limit as Thomas-Fermi approximation in close analogy with the Fermi systems. Even for relatively small numbers of trapped particles we find good agreement between Gross-Pitaevskii and Thomas-Fermi calculations for the different contributions to the total energy of the atoms in the condensate. We also discuss the application of our approach to the description of vortex states in superfluid fermionic systems in the Ginzburg-Landau regime.

PACS. 03.65.Sq Semiclassical theories and applications – 03.75.Lm Tunneling, Josephson effect, Bose-Einstein condensates in periodic potentials, solitons, vortices and topological excitations

1 Introduction

The discovery of Bose-Einstein condensation in trapped alkali-metal gases at ultra-low temperature [1–3] has developed a huge amount of experimental and theoretical investigations. The experimental conditions are such that the atomic gas is at very low density and that the interactions can be parametrized in terms of a scattering length a . In this situation a mean-field description through the Gross-Pitaevskii equation (GPE) [4,5] is able to give, at least at low temperature, a precise description of the atomic condensates and their dynamics [6–9].

One important question concerns the superfluid character of the Bose condensates. Among other properties, the existence of quantum vortices is a signal of the superfluidity. The possibility of trapped quantized vortices was one of the primary motivations of the GP theory [4,5] and some amount of theoretical work about this topic has been developed during the last years [6,7,9–12]. The experimental evidence of such quantized vortices has recently been verified [13,14].

Since the number N of atoms involved in the condensate is generally large, it is natural to think that the Thomas-Fermi (TF) approach can be applied extensively in some aspects of the Bose-Einstein condensation

in traps. This TF limit is usually identified with the limit of number of atoms N going to infinity rather than to be interpreted as the $\hbar \rightarrow 0$ limit as it happens in the case of Fermi statistics. Recently, the TF approximation for the ground state of Bose-Einstein condensates of magnetically trapped atoms has been discussed as the $\hbar \rightarrow 0$ limit [15]. From this point of view the TF kinetic energy, which is dropped in the $N \rightarrow \infty$ limit of the ground-state calculation, can be obtained for any number of particles. In this $\hbar \rightarrow 0$ limit, a good agreement between the GP and TF kinetic energies is found even for low and intermediate number of particles. With the interpretation of the TF approach as the $\hbar \rightarrow 0$ limit, it is also possible to perform semiclassical TF calculations for the ground state of Bose-Einstein condensates of atoms with negative scattering length (⁷Li atoms) and to compute the excitation energy of collective monopole and quadrupole oscillations where the kinetic energy of the ground state of the condensate plays a crucial role [15].

The TF limit considered as $N \rightarrow \infty$ limit has also been applied to the description of vortex states [10,11,16,17]. In this case it is assumed that the radial and axial kinetic energies can be neglected, and only the rotational kinetic energy is retained [16]. This approximation, however, gives a bad description of the vortex-core region. A better description of this region in the limit of large N can be achieved by splitting the condensate wave function into

^a e-mail: urban@ipno.in2p3.fr

a product of a slowly-varying envelope, which is obtained by completely neglecting the kinetic energy, times the solution of the GPE describing a vortex in homogeneous matter [18]. In contrast to these large- N methods, in this paper, we will again consider the TF approximation as the $\hbar \rightarrow 0$ limit in order to describe the vortex state semiclassically. In addition to the formal aspects, this approach has the practical advantages mentioned above, *i.e.*, that one can calculate the kinetic energy, that it can therefore be used also in the attractive case, and that it works well also in the case of relatively few particles.

The experimental and theoretical achievements in Bose-Einstein condensation have also triggered the investigation of trapped Fermi gases at very low temperatures [19–21]. One of the most important goals of the experiments is to reach the BCS transition to the superfluid phase, associated with the appearance of a macroscopic order parameter of strongly correlated Cooper pairs in dilute gases of trapped fermionic atoms. Several theoretical studies about this topic have recently been developed [22, 23]. In the case where the critical temperature is much higher than the spacing between the levels in the trap, the macroscopic order parameter can be obtained through the Ginzburg-Landau equation (GLE) [24], which is formally equivalent to the GPE. In a recent publication [25] also vortex states were discussed within the framework of the GLE. As a second application of our TF approach we will briefly discuss vortex states in a superfluid gas of trapped fermionic atoms. Due to the analogy between the GPE and the GLE our semiclassical approach can immediately be transferred to this problem.

The paper is organized as follows: in the second section we establish the TF theory projected on states of defined z -component of the angular momentum and apply it to describe vortex states of a non-interacting Bose condensate. In the third section we include the interaction among the atoms in the trap and compare our semiclassical prediction with the results obtained from the quantal solution of the GPE for several typical examples. The fourth section is devoted to the discussion of vortex states in superfluid trapped Fermi systems. Our conclusions are laid out in the last section.

2 The Thomas-Fermi approximation to static vortex states

We start by considering states having a vortex line along the z -axis and all the atoms flowing around it with quantized circulation. The order parameter can be written in the form [6, 11]

$$\Phi(\mathbf{r}) = \phi(r_{\perp}, z) e^{i\kappa\varphi}, \quad (1)$$

where r_{\perp} and z are the radial and axial coordinates, φ is the angle around the z -axis, κ is an integer, and $\phi(r_{\perp}, z) = \sqrt{\rho(r_{\perp}, z)}$, $\rho(r_{\perp}, z)$ being the density. The vortex state has a tangential velocity $v = \hbar\kappa/(mr_{\perp})$ where κ is the quantum of circulation, and the angular momentum along the z -axis

is $N\hbar\kappa$. The function $\phi(r_{\perp}, z)$ is obtained as the solution of the following non-linear Schrödinger equation

$$\left[-\frac{\hbar^2}{2m} \left(\frac{\partial^2}{\partial r_{\perp}^2} + \frac{1}{r_{\perp}} \frac{\partial}{\partial r_{\perp}} + \frac{\partial^2}{\partial z^2} \right) + \frac{\hbar^2 \kappa^2}{2mr_{\perp}^2} + V_{\text{ext}}(r_{\perp}, z) + g\phi^2(r_{\perp}, z) \right] \phi(r_{\perp}, z) = \mu \phi(r_{\perp}, z), \quad (2)$$

which is the GPE for the static vortex state problem. In equation (2), V_{ext} is an external potential which for simplicity we have considered to be a spherical harmonic oscillator (HO) with frequency ω ,

$$V_{\text{ext}}(\mathbf{r}) = \frac{1}{2}m\omega^2(r_{\perp}^2 + z^2). \quad (3)$$

The coupling constant is given by $g = 4\pi\hbar^2 a/m$ with m the atomic mass and a the s -wave scattering length.

For the remaining part of this section, we will concentrate on the non-interacting case, *i.e.*, $V(\mathbf{r}) = V_{\text{ext}}(\mathbf{r})$. The effect of interactions will be considered in the next section. For non-interacting particles one recovers the case of a stationary Schrödinger equation for the harmonic oscillator potential, which is solved by

$$\Phi_{\kappa}(\mathbf{r}) = \sqrt{\frac{N}{\pi^{3/2} \kappa! a_{\text{HO}}^3}} \left(\frac{r_{\perp}}{a_{\text{HO}}} \right)^{\kappa} e^{-(r_{\perp}^2 + z^2)/(2a_{\text{HO}}^2)} e^{i\kappa\varphi} \quad (4)$$

with the HO length a_{HO} defined by $a_{\text{HO}} = \sqrt{\hbar/(m\omega)}$. The corresponding energy eigenvalue is given by

$$\mu = \left(\frac{3}{2} + \kappa \right) \hbar\omega. \quad (5)$$

To derive the TF approximation to the quantal solution of the non-interacting vortex state (4), we start from the complete set of eigenfunctions of $\hat{\mathbf{p}}^2$, \hat{p}_z and \hat{L}_z

$$\langle \mathbf{r} | k_z, k_{\perp}, \kappa \rangle = J_{\kappa}(k_{\perp} r_{\perp}) e^{i\kappa\varphi} e^{ik_z z}, \quad (6)$$

which are normalized to

$$\int d^3r \langle \mathbf{r} | k_z, k_{\perp}, \kappa \rangle \langle k'_z, k'_{\perp}, \kappa' | \mathbf{r} \rangle = \frac{4\pi^2}{k_{\perp}} \delta(k_{\perp} - k'_{\perp}) \delta(k_z - k'_z) \delta_{\kappa\kappa'}. \quad (7)$$

At lowest order in \hbar (*i.e.*, at TF level), the corresponding single-particle propagator [26] can be written as

$$C^{\beta}(\mathbf{r}, \mathbf{r}') = \langle \mathbf{r} | e^{-\beta\hat{H}} | \mathbf{r}' \rangle \approx \sum_{\kappa} \int \frac{dk_z dk_{\perp}}{4\pi^2} k_{\perp} J_{\kappa}(k_{\perp} r_{\perp}) J_{\kappa}(k_{\perp} r'_{\perp}) e^{i\kappa(\varphi - \varphi')} \times e^{ik_z(z - z')} e^{-\beta[V(\mathbf{R}) + \hbar^2(k_{\perp}^2 + k_z^2)/(2m)]}, \quad (8)$$

where $\mathbf{R} = (\mathbf{r} + \mathbf{r}')/2$. Equation (8) has been obtained under the assumption that all the gradients of the potential

can be neglected, which is the usual hypothesis of the TF theory. From now on we restrict ourselves to some given value of κ . The spectral density matrix is easily obtained as the inverse Laplace transform of the propagator [26]:

$$g_{\kappa}^{\mu}(\mathbf{r}, \mathbf{r}') = \mathcal{L}_{\beta \rightarrow \mu}^{-1} C_{\kappa}^{\beta}(\mathbf{r}, \mathbf{r}') \\ = \int \frac{dk_z dk_{\perp}}{4\pi^2} k_{\perp} J_{\kappa}(k_{\perp} r_{\perp}) J_{\kappa}(k_{\perp} r'_{\perp}) e^{ik_z(z-z')} \\ \times e^{ik_z(z-z')} \delta\left(\mu - V(\mathbf{R}) - \frac{\hbar^2(k_{\perp}^2 + k_z^2)}{2m}\right). \quad (9)$$

Its local part, $g_{\kappa}^{\mu}(\mathbf{r}) \equiv g_{\kappa}^{\mu}(\mathbf{r}, \mathbf{r})$, is proportional to the density of the Bose condensate. After performing the k_{\perp} integral we obtain for the density

$$\rho_{\kappa}(\mathbf{r}) = N c_{\kappa} g_{\kappa}^{\mu}(\mathbf{r}) \\ = \frac{mN c_{\kappa}}{2\pi^2 \hbar^2} \int_0^{k_0(\mathbf{r})} dk_z J_{\kappa}^2\left(\sqrt{k_0^2(\mathbf{r}) - k_z^2} r_{\perp}\right) \theta[\mu - V(\mathbf{r})], \quad (10)$$

where

$$k_0(\mathbf{r}) = \frac{\sqrt{2m[\mu - V(\mathbf{r})]}}{\hbar}, \quad (11)$$

and c_{κ} is the normalization constant.

As it is done for the ground state [15], c_{κ} is determined by imposing that (10) be normalized to N . Thus c_{κ} is just the inverse of the level density $g_{\kappa}(\mu)$:

$$\frac{1}{c_{\kappa}} = g_{\kappa}(\mu) = \int d^3r g_{\kappa}^{\mu}(\mathbf{r}). \quad (12)$$

The other quantity entering in the density of the Bose condensate, equation (10), is the chemical potential μ which corresponds to the lowest eigenvalue of the GPE. In order to determine the chemical potential μ , a requantization of the TF approximation is necessary [15]. The need for a requantization of the TF theory for individual states has been recognized in reference [27] and our procedure of requantization clearly follows what is proposed there. The standard semiclassical quantization procedure is given by the Wentzel-Kramers-Brillouin (WKB) method. However, in order to have a more explicit formula, we apply here the simplified method described in reference [15], which becomes exact in the three dimensional HO case. Thus for the non-interacting case we fix the chemical potential to be equal to the GPE eigenvalue, equation (5).

To proceed further it is useful to write the Bessel function in equation (10) as a power series [28]:

$$J_{\kappa}(x) = \sum_{i=0}^{\infty} \frac{(-1)^i}{i!(\kappa+i)!} \left(\frac{x}{2}\right)^{\kappa+2i}. \quad (13)$$

Using this result, performing the remaining k_z integral, and remembering the identity

$$\sum_{i_1, i_2=0}^{\infty} \binom{\kappa+j}{i_1} \binom{\kappa+j}{i_2} \delta_{j, i_1+i_2} = \binom{2\kappa+2j}{j}, \quad (14)$$

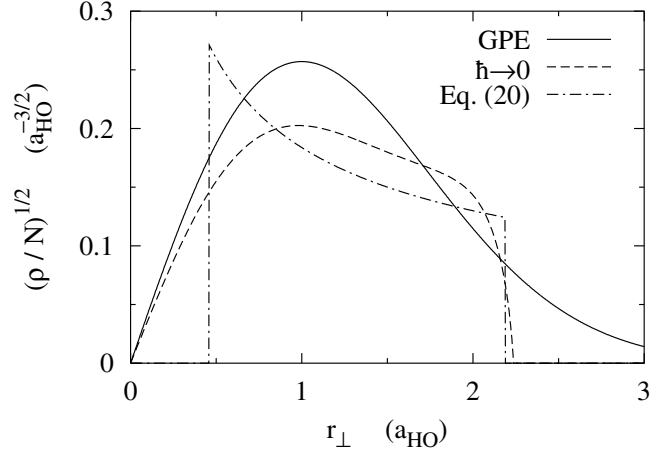


Fig. 1. Square root of the normalized TF ($\hbar \rightarrow 0$) density and quantal wave function (GPE) for a non-interacting Bose condensate with $\kappa = 1$ as a function of r_{\perp} for $z = 0$. The third curve corresponds to equation (20). Wave function and radius are given in HO units ($a_{\text{HO}}^{-3/2}$ and a_{HO} , respectively).

we obtain the following expression for the local spectral density:

$$g_{\kappa}^{\mu}(\mathbf{r}) = \frac{mk_0(\mathbf{r})}{2\pi^2 \hbar^2} \\ \times \sum_{j=0}^{\infty} \frac{(-1)^j [k_0(\mathbf{r}) r_{\perp}]^{2\kappa+2j}}{j!(2\kappa+j)!(2\kappa+2j+1)} \theta[\mu - V(\mathbf{r})]. \quad (15)$$

For the non-interacting harmonic oscillator the integral in equation (12) can be evaluated analytically, with the result

$$\frac{1}{c_{\kappa}} = \frac{1}{\hbar\omega} \sum_{j=0}^{\infty} \frac{(-1)^j [\mu/(\hbar\omega)]^{2\kappa+2j+2}}{j!(2\kappa+j)!(2\kappa+2j+1)(2\kappa+2j+2)}. \quad (16)$$

Figure 1 displays the square root of the normalized TF density (10) for $\kappa = 1$ along the r_{\perp} coordinate for $z = 0$, where HO units have been used. In the same figure the quantal wave function which describes the $\kappa = 1$ vortex state [see Eq. (4)] is also plotted. As it can be seen from equation (15), for $r_{\perp} \rightarrow 0$ the semiclassical TF density goes to zero in the same way as the quantum mechanical result, *i.e.*, $\rho_{\kappa}(\mathbf{r}) \propto r_{\perp}^{2\kappa}$. At the classical turning point [$V(\mathbf{r}) = \mu$] the TF density goes to zero as $\rho_{\kappa} \propto [k_0(\mathbf{r})]^{1+2\kappa}$. Thus the turning point will be changed by the interaction only *via* the change of the chemical potential μ .

The reader unfamiliar with the Thomas-Fermi approach may be worried about the locally relatively strong deviations of the semiclassical density from its quantal (GPE) counterpart. In this respect it should be remembered that the TF densities must be considered in the sense of distributions [26] [see *e.g.* the step function in Eq. (10)] and, therefore, they only make sense when used under integrals to calculate expectation values of “slowly varying” operators. In fact, the \hbar corrections to the density (not considered here) still deviate much more

strongly from the true quantal densities, since they contain a square-root singularity at the classical turning point. Nonetheless these \hbar corrections, when used under integrals, improve the results for cases where the gradients of the potential are not too strong [29]. It has been found in the past [15,26] that when used in this way the TF approach (eventually with inclusion of \hbar corrections) can yield very accurate results for expectation values. The relation of the TF approach with \hbar^2 corrections to the WKB approach has been discussed in reference [27].

The TF kinetic energy density can also be derived from the spectral density matrix (9) as

$$\begin{aligned}\tau_\kappa(\mathbf{R}) &= \left(-\frac{\hbar^2}{2m} \nabla_{\mathbf{r}}^2 g_\kappa^\mu(\mathbf{r}, \mathbf{r}') \right)_{\mathbf{r}, \mathbf{r}' \rightarrow \mathbf{R}} \\ &= \frac{\hbar^2}{2m} \int \frac{dk_z dk_\perp}{4\pi^2} k_\perp (k_\perp^2 + k_z^2) J_\kappa^2(k_\perp R_\perp) \\ &\quad \times \delta\left(\mu - V(\mathbf{R}) - \frac{\hbar^2}{2m} (k_\perp^2 + k_z^2)\right) \\ &= [\mu - V(\mathbf{R})] g_\kappa^\mu(\mathbf{R}).\end{aligned}\quad (17)$$

Using equations (10, 17) it can easily be checked that the expectation values of the kinetic and potential energies fulfill the virial theorem as it is expected in the TF approach [30]. Thus due to our choice of the chemical potential μ (5), our semiclassical TF approximation to the vortex state in the non-interacting case exactly reproduces the quantal expectation values of the kinetic and potential energies in spite of the aspect of the semiclassical density profile as compared with the quantal one.

It is easy to see that with the HO potential the argument of the Bessel function entering in the density cannot become large:

$$k_\perp r_\perp \leq k_0(\mathbf{r})|\mathbf{r}| \leq \frac{\mu}{\hbar\omega} = \frac{3}{2} + \kappa. \quad (18)$$

For example, in the case $\kappa = 1$ the argument becomes at most $5/2$, and already the first four terms of the expansion (13) give an accuracy better than 0.5%. In the case $\kappa = 0$, the result of reference [15] is recovered if one takes only the first term of the expansion in the TF density, equation (10).

For completeness we note that in the literature also a different approach for projecting the semiclassical density matrix onto good angular momentum L^2 and L_z can be found [31]. Repeating the steps described there for the projection onto good L_z only (*i.e.*, essentially using asymptotic expansions for the Bessel functions) one finds the following expression for the Wigner transform of the spectral density matrix:

$$g_\kappa^\mu(\mathbf{R}, \mathbf{p}) = \hbar \delta(H^{\text{cl}} - \mu) \delta(L_z^{\text{cl}} - \hbar\kappa) \quad (19)$$

with $H^{\text{cl}} = \mathbf{p}^2/(2m) + V(\mathbf{R})$ and $\mathbf{L}^{\text{cl}} = \mathbf{R} \times \mathbf{p}$. From this formula the density is easily obtained by integration over \mathbf{p} :

$$\rho_\kappa(\mathbf{R}) = \frac{mNc_\kappa}{4\pi^2\hbar^2R_\perp} \theta\left(\mu - V(\mathbf{R}) - \frac{\hbar^2\kappa^2}{2mR_\perp^2}\right). \quad (20)$$

The constant c_κ is determined by the normalization condition, which for the non-interacting case results in $c_\kappa = 2\hbar^2\omega^2/(\mu - \kappa\hbar\omega) = 4\hbar\omega/3$. The density profile corresponding to equation (20) is also shown in Figure 1. From this figure it is evident that equation (20) makes sense only as a distribution for the calculation of expectation values and not for the calculation of local quantities like the density itself. However, since the density given by equation (20) does not at all depend on the shape of the potential (except for the determination of the turning points), this form seems difficult to be used for a self-consistent calculation in the interacting case. Let us note that again the virial theorem is fulfilled and expectation values of operators can be obtained very accurately [31,32].

3 The interacting case

Let us now discuss the TF approximation to the quantal solution of the GPE (2). Of course the semiclassical formalism described in the previous section can still be applied provided that the potential $V(\mathbf{r})$ in the interacting case is given by

$$V(\mathbf{r}) = V_{\text{ext}}(\mathbf{r}) + g\rho(\mathbf{r}). \quad (21)$$

As it was mentioned before, the TF density corresponding to the vortex state (10) depends on two independent constants to be determined: the normalization c_κ and the chemical potential μ . In the interacting case, and following the same strategy as in reference [15], we determine c_κ and μ by imposing that the TF density be normalized to the number of particles N in the Bose condensate and that the integrated level density

$$\begin{aligned}N_\kappa^I(\mu) &= \int d^3r \int_0^\mu d\mu' g_\kappa^{\mu'}(\mathbf{r}) \\ &= \int d^3r \theta[\mu - V(\mathbf{r})] \frac{k_0^3(\mathbf{r})}{2\pi^2} \\ &\quad \times \sum_{j=0}^{\infty} \frac{(-1)^j [k_0(\mathbf{r})r_\perp]^{2\kappa+2j}}{j!(2\kappa+j)!(2\kappa+2j+1)(2\kappa+2j+3)}\end{aligned}\quad (22)$$

become equal to that of the non-interacting HO, which for $\mu = (3/2 + \kappa)\hbar\omega$ is given by

$$N_\kappa^{\text{HO}} = \sum_{j=1}^{\infty} \frac{(-1)^j (2\kappa+2j)! (3/2 + \kappa)^{2\kappa+2j+3}}{j!(2\kappa+j)!(2\kappa+2j+3)!}. \quad (23)$$

The strategy for the self-consistent solution in the interacting case is now very simple. Instead of starting with a fixed particle number N , it is convenient to choose some value for Nc_κ . Then we choose some initial value for μ . For given Nc_κ and μ we solve equation (15) for $g_\kappa^\mu(\mathbf{r})$, which is non-linear since also the right-hand side depends on $g_\kappa^\mu(\mathbf{r})$ through

$$k_0(\mathbf{r}) = \frac{\sqrt{2m[\mu - V_{\text{ext}}(\mathbf{r}) - gNc_\kappa g_\kappa^\mu(\mathbf{r})]}}{\hbar}. \quad (24)$$

Then the integral (22) is evaluated and the result is compared with the corresponding result for the non-interacting harmonic oscillator, equation (23). If the level number is too small ($N_\kappa^I < N_\kappa^{\text{HO}}$), μ is increased, otherwise ($N_\kappa^I > N_\kappa^{\text{HO}}$) μ is decreased. This procedure is iterated until $N_\kappa^I = N_\kappa^{\text{HO}}$. Finally the particle number is obtained by evaluating the integral

$$N = \int d^3r \rho(\mathbf{r}) = N c_\kappa \int d^3r g_\kappa^\mu(\mathbf{r}). \quad (25)$$

Before comparing the results obtained within our TF approach to the results from solving the GPE numerically, let us briefly discuss two approximation methods which have been developed for the case of large N . The first one, known as the TF limit in the literature and discussed, *e.g.*, in references [10,11,16,17], is obtained by dropping the kinetic energy part e_{kin} coming from the radial and axial motion and retaining only the rotational part e_{rot} of the total kinetic energy, *i.e.*, only derivatives with respect to φ in equation (2). Under this assumption it is easily obtained that the $N \rightarrow \infty$ limit of the density of the vortex state reads

$$\rho(\mathbf{r}) = \frac{1}{g} \left(\mu - \frac{\hbar^2 \kappa^2}{2m r_\perp^2} - \frac{1}{2} m \omega^2 (r_\perp^2 + z^2) \right). \quad (26)$$

In this limit the density vanishes inside of $r_{\perp, \text{min}}$ and outside of $r_{\perp, \text{max}}$, defined by the zeros of equation (26). The chemical potential μ is obtained through the particle-number condition. The formula (26) has the advantage that it represents an analytic expression for $\rho(\mathbf{r})$, but it is clear that the result $\rho = 0$ inside a vortex core with radius $r_{\perp, \text{min}}$ is not realistic. We will call hitherto formula (26) the $N \rightarrow \infty$ TF limit.

The second approximation method, known as the “method of matched asymptotics” (MA), was introduced in reference [33] to describe the dynamics of vortices, and used in reference [34] to calculate the energy of a static vortex. We will follow here the simplified derivation for the case of a straight vortex given in reference [18]. First let us briefly review the description of a vortex state in a system with $V_{\text{ext}} = 0$. In this case it is useful to define the asymptotic density $\rho_0 = \mu/g$ and the healing length $\xi_0 = \hbar/\sqrt{2m\rho_0 g}$ [10], and to write the condensate wave function in the form

$$\phi(r_\perp) = \sqrt{\rho_0} f_\kappa \left(\frac{r_\perp}{\xi_0} \right) = \sqrt{\frac{\mu}{g}} f_\kappa \left(\frac{\sqrt{2m\mu}}{\hbar} r_\perp \right). \quad (27)$$

Inserting this expression into the GPE (2) with $V_{\text{ext}} = 0$, one obtains the following differential equation for the function f_κ :

$$-\frac{1}{x} f'_\kappa(x) - f''_\kappa(x) + \frac{\kappa^2}{x^2} f_\kappa(x) + f_\kappa^3(x) = f_\kappa(x). \quad (28)$$

With the boundary conditions (for $\kappa \geq 1$)

$$f_\kappa(0) = 0 \quad \text{and} \quad \lim_{x \rightarrow \infty} f_\kappa(x) = 1 \quad (29)$$

this differential equation can be solved numerically [10,35]. Now we turn to the case of a trapped system. In the limit of large N it is clear that the external potential V_{ext} can be regarded as constant on the length scale ξ_0 corresponding to the size of the vortex core. (More precisely, the condition which has to be fulfilled reads $Na/a_{\text{HO}} \gg 1$, as it is the case for the $N \rightarrow \infty$ TF approach.) Thus we obtain an approximate description of the trapped system by replacing the chemical potential μ by a local chemical potential $\mu - V_{\text{ext}}(\mathbf{r})$. Inside the classically allowed region [$V_{\text{ext}}(\mathbf{r}) < \mu$] the order parameter then takes the form

$$\phi(\mathbf{r}) = \sqrt{\frac{\mu - V_{\text{ext}}(\mathbf{r})}{g}} f_\kappa \left(\frac{\sqrt{2m[\mu - V_{\text{ext}}(\mathbf{r})]}}{\hbar} r_\perp \right). \quad (30)$$

As before, the chemical potential μ is determined by the particle-number condition.

Note that in the region far away from the vortex core, *i.e.*, for $r_\perp \gg \xi_0$, one can expand $f_\kappa(x)$ in powers of $1/x$. Using equations (28, 29), one obtains

$$f_\kappa(x) = 1 - \frac{\kappa^2}{2x^2} - \frac{\kappa^2(8 + \kappa^2)}{8x^4} - \dots \approx \sqrt{1 - \frac{\kappa^2}{x^2}}. \quad (31)$$

Inserting this into equation (30) one immediately recovers equation (26). However, this shows that equation (26) is not valid for $r_\perp \lesssim \xi_0$, *i.e.*, inside the vortex core. Another difference between equation (30) and equation (26) concerns the behavior of the wave function at the outer classical turning point. In contrast to the usual $N \rightarrow \infty$ TF limit, the kinetic energy corresponding to the wave function (30) is not diverging, since the square-root $\sqrt{\mu - V_{\text{ext}}}$ in equation (30) is multiplied by the function f_κ , which is proportional to $(\mu - V_{\text{ext}})^{\kappa/2}$ near the classical turning point. Nevertheless it is not reasonable to use equation (30) to calculate the kinetic energy near the turning point, since the decrease of the function f_κ is just indicating that the local healing length $\xi(\mathbf{r}) = \hbar/\sqrt{2m(\mu - V_{\text{ext}})}$ becomes large and that the approximation breaks down.

Now we proceed to a detailed numerical comparison of the ($\hbar \rightarrow 0$) TF predictions with the exact quantal values obtained from the GPE, equation (2). For our numerical application we consider ^{87}Rb atoms in a spherical trap represented by a HO potential with length $a_{\text{HO}} = 0.791 \mu\text{m}$ [9]. The s -wave scattering length is taken as $a = 100 a_0$ [6] where a_0 is the Bohr radius. Table 1 collects the chemical potential (μ), the total (e_{tot}), HO (e_{HO}), self-interaction (e_{self}), and kinetic energies per particle for vortex states of condensates with 100, 10^4 , and 10^6 atoms in the trap. The kinetic energy is split into the rotational part (e_{rot}) and in the one corresponding to the radial and axial motion (e_{kin}). The numerical values displayed in Table 1 show that our ($\hbar \rightarrow 0$) TF approach reproduces very well the quantal eigenvalue (μ) as well as the total energy per particle (e_{tot}) even for a small number of particles such as 100. The agreement between the quantal and TF values improves when the number of particles in the condensate increases, as it is expected. The HO and

Table 1. Chemical potential (μ) and energy per particle (e_{tot}) and its different contributions in $\hbar\omega$ units: harmonic oscillator energy (e_{HO}), interaction energy (e_{self}), and kinetic energy split into its rotational (e_{rot}) and radial and axial (e_{kin}) parts. The parameters chosen correspond to a single-quantized vortex ($\kappa = 1$) in a spherical trap ($a_{\text{HO}} = 0.791 \mu\text{m}$) containing 100, 10^4 , and 10^6 ^{87}Rb atoms (scattering length $a = 100 a_0$). The results obtained from the GPE are compared with the results from the ($\hbar \rightarrow 0$) TF approach and from two approximation methods for large N : the so-called $N \rightarrow \infty$ TF method, equation (26), and the method of matched asymptotics (MA), equation (30). Note that e_{kin} is neglected in the $N \rightarrow \infty$ TF limit and not accessible within the matched-asymptotic approach.

N		μ	e_{tot}	e_{HO}	e_{self}	e_{rot}	e_{kin}
10^2	GPE	2.74	2.62	1.34	0.12	0.480	0.686
	$\hbar \rightarrow 0$	2.72	2.61	1.33	0.10	0.501	0.673
	$N \rightarrow \infty$	1.88	1.59	0.87	0.29	0.438	0
	MA	1.86	—	0.84	0.23	0.689	—
10^4	GPE	8.40	6.30	3.67	2.10	0.271	0.255
	$\hbar \rightarrow 0$	8.28	6.19	3.62	2.09	0.350	0.130
	$N \rightarrow \infty$	8.19	5.99	3.54	2.19	0.253	0
	MA	8.23	—	3.57	2.17	0.272	—
10^6	GPE	50.18	35.93	21.53	14.26	0.087	0.059
	$\hbar \rightarrow 0$	50.13	35.86	21.50	14.27	0.116	-0.024
	$N \rightarrow \infty$	50.14	35.86	21.50	14.28	0.083	0
	MA	50.14	—	21.50	14.27	0.086	—

the self-interaction contributions to the total energy are also well reproduced by our semiclassical approach. For very large numbers of particles ($N = 10^6$) the quantal results are also well reproduced by the $N \rightarrow \infty$ TF limit, equation (26), because the neglected contribution (*i.e.*, the kinetic energy due to the radial and axial motion e_{kin}) is very small. However, it should be pointed out that the key assumption of this $N \rightarrow \infty$ limit is not fulfilled, because the kinetic energy of the radial and axial motion is still of the same order as the rotational energy, as can be seen from the quantal results (GPE) listed in Table 1. In fact, even in the limit $N \rightarrow \infty$ the ratio $e_{\text{kin}}/e_{\text{rot}}$ does not go to zero (see Appendix). The method of matched asymptotics, equation (30), gives better results than the $N \rightarrow \infty$ TF limit, equation (26), except in the case of small numbers of particles ($N = 100$), where both large- N methods fail.

Concerning the kinetic energy some comments are in order. First of all, we want to point out that the $N \rightarrow \infty$ theory neglects (and in fact cannot access [15]) the contributions coming from the radial and axial motion, so they are not listed in Table 1. For a small number of atoms, such as 100, our $\hbar \rightarrow 0$ limit is able to reproduce reasonably well both, e_{rot} and e_{kin} contributions to the total kinetic energy per particle. When the number of the atoms in the trap grows, the total kinetic energy per particle decreases and the agreement between the quantal result and the TF prediction worsens for this quantity. This situation is also found in the ground-state case discussed in reference [15] where the (small) quantal and TF kinetic energies can differ by a factor two for a large number of particles (see Tab. II of Ref. [15]). The reason for these disagreements between the quantal and TF kinetic energies for large number of atoms in the condensate lies in the fact that in this case the kinetic energy is dominated by quantal corrections that are non-analytical in \hbar

and consequently cannot be reproduced in a pure TF approximation [15]. A detailed comparison shows that the ($\hbar \rightarrow 0$) TF theory systematically overestimates the rotational part and underestimates the axial and radial parts of the kinetic energy, the latter even becoming negative for very large numbers of particles, although the total kinetic energy remains always positive. The reason for this behavior is that the TF density is too high inside the vortex core, as will be discussed below.

It should be pointed out that, as happens for the non-interacting case, the virial theorem, which for the interacting case reads [6]

$$2(e_{\text{kin}} + e_{\text{rot}}) - 2e_{\text{HO}} + 3e_{\text{self}} = 0, \quad (32)$$

is also fulfilled in our TF approach to vortex states for a Bose condensate in a spherical trap.

Figures 2–4 display the normalized order parameter for 100, 10^4 , and 10^6 atoms of ^{87}Rb in the trap along the radial axis r_{\perp} for $z = 0$. The dashed line corresponds to the ($\hbar \rightarrow 0$) TF limit. For comparison we show the corresponding order parameter obtained from the quantal solution of the GPE (2) (solid line), which is obtained through imaginary time step techniques [6], and the order parameter obtained from the method of matched asymptotics, equation (30) (dashed-dotted lines). Looking at the shape of the semiclassical ($\hbar \rightarrow 0$) compared with the quantal order parameter one can see that the agreement increases with the number of particles in the condensate, as it happens in the TF approximation for the ground state. The effect of the self-interaction that progressively modifies the density profile of the condensate in the vortex state with respect to the non-interacting case is also followed by our semiclassical TF densities. Only inside the vortex core ($r_{\perp} \approx 0$) the agreement worsens with increasing number of particles.

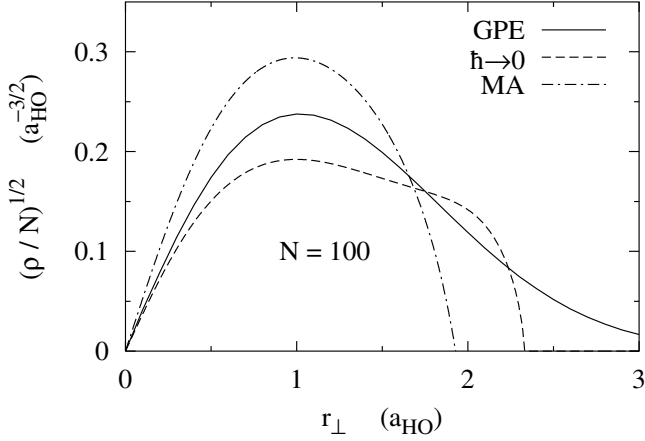


Fig. 2. Normalized order parameter obtained from the GPE, from the ($\hbar \rightarrow 0$) TF limit, and from the approximation of matched asymptotics (MA) for large N [Eq. (30)], of an interacting Bose condensate of 100 ^{87}Rb atoms in a spherical trap with $a_{\text{HO}} = 0.791 \mu\text{m}$ in a vortex state with $\kappa = 1$ as a function of r_{\perp} for $z = 0$ in HO units.

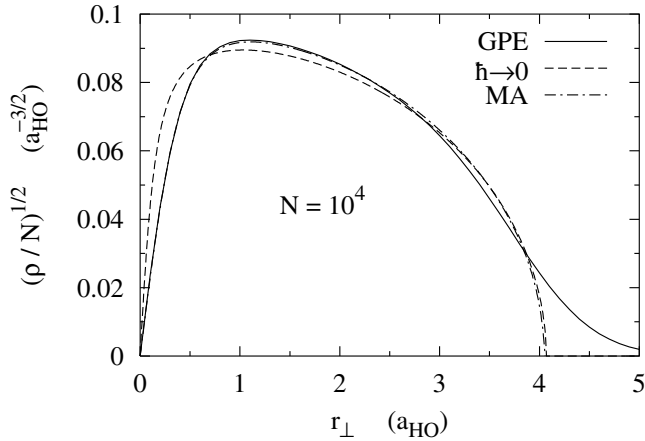


Fig. 3. Same as Figure 2, but for 10^4 atoms in the trap.

This can easily be understood by looking at the corresponding self-consistent potentials shown in Figure 5. The main assumption of our semiclassical TF theory is that gradients of the potential can be neglected. This assumption becomes more and more justified with increasing number of particles, except in the vicinity of the z -axis ($r_{\perp} \approx 0$), where the self consistent potential rises rapidly from zero to $\approx \mu$. For the case of moderate numbers of particles, the semiclassical description of the vortex core could be improved by considering higher \hbar corrections to the TF solution, which take into account the gradients of the potential. However, we should remember that the \hbar or gradient expansion is an asymptotic series which can only work as long as the gradients of the potential are not too strong, even though the theory often works quite far beyond its limits (see Ref. [29]). For very steep potentials only a partial resummation of the \hbar series like in WKB, to account for the nonanalytical behavior in \hbar , can help. This will further be discussed in Appendix.

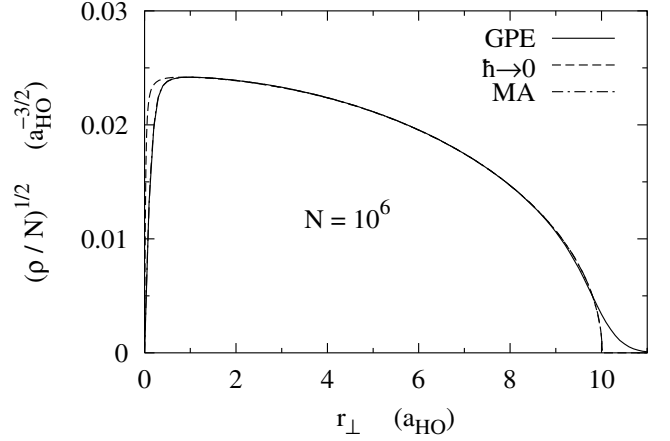


Fig. 4. Same as Figure 2, but for 10^6 atoms in the trap.

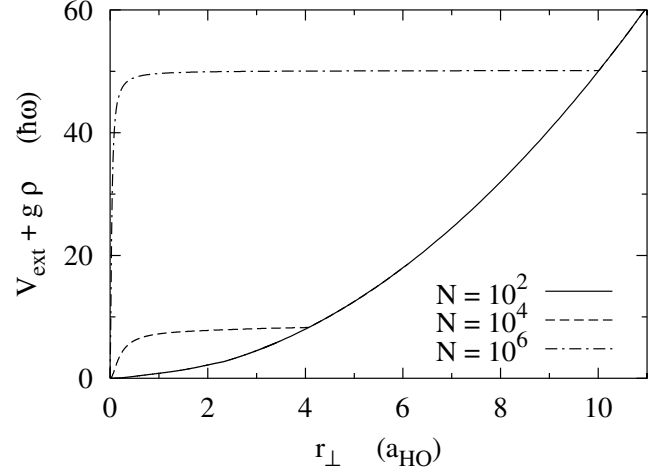


Fig. 5. Self-consistent potentials in units of $\hbar\omega$ as a function of r_{\perp} in units of a_{HO} obtained in our ($\hbar \rightarrow 0$) TF approach corresponding to the density profiles shown in Figures 2–4.

As can be seen in Figures 3 and 4, for large numbers of particles the density profiles obtained from equation (30) follow remarkably well the quantal profile except near the classical turning point where the approach breaks down.

Comparing the so-called $N \rightarrow \infty$ TF approach [Eq. (26)] with the $\hbar \rightarrow 0$ TF approach proposed in this work, one can see from Table 1 that our TF method reproduces better the different quantal contributions to the energy of the vortex state for small ($N = 100$) and moderate ($N = 10^4$) numbers of particles in the condensate while, for large numbers both limits ($\hbar \rightarrow 0$ and $N \rightarrow \infty$) coincide. Concerning the density profiles, the difference is obvious: in our approach the density profile goes like $\sqrt{\rho} \propto r_{\perp}^{\kappa}$ as in the quantal case, whereas in the $N \rightarrow \infty$ TF limit there is a small $\rho = 0$ region determined by the inner turning point $r_{\perp, \text{min}}$. It should be mentioned that within the improved (matched asymptotics) $N \rightarrow \infty$ approximation [Eq. (30)], the density profile also goes like $\sqrt{\rho} \propto r_{\perp}^{\kappa}$, and contrary to our $\hbar \rightarrow 0$ approach it is capable to reproduce the density profile in the vortex core in the case of large N . However, this method has nothing to

do with the semiclassical asymptotic \hbar expansion considered here.

Finally it should also be pointed out that our TF limit is able to deal with vortices in the attractive case (negative scattering length). In this case the kinetic energy is crucial and the large- N limit is not well-defined. The same is true for the description of the ground state (*i.e.*, no vortex), as shown in reference [15]. There the $\hbar \rightarrow 0$ approach has been used in the repulsive as well as in the attractive case, whereas the $N \rightarrow \infty$ approximations (the so-called $N \rightarrow \infty$ TF limit as well as the method of matched asymptotics) can be applied only in the repulsive case.

4 Application to vortices in superfluid trapped fermionic gases

In this section we will describe how our TF approach can also be used for the description of vortices in superfluid fermionic systems. This is possible since at least for a certain range of temperatures, the so-called Ginzburg-Landau regime, the order parameter $\Delta(\mathbf{r})$ is described by an equation which has exactly the same form as the GPE (2). As derived in reference [24], for temperatures T near the critical temperature T_c and for low trapping frequencies ω ($\hbar\omega \ll k_B T_c$) the Ginzburg-Landau equation (GLE) reads

$$\left[-K^2 R_{\text{TF}}^2 \nabla^2 + \frac{1+2\lambda}{2\lambda} \frac{\mathbf{r}^2}{R_{\text{TF}}^2} - \ln \frac{T_c^{(0)}}{T} \right] \Delta(\mathbf{r}) + \frac{7\zeta(3)}{8\pi^2} \left| \frac{\Delta(\mathbf{r})}{k_B T} \right|^2 \Delta(\mathbf{r}) = 0, \quad (33)$$

with the definitions $K = \sqrt{7\zeta(3)/(48\pi^2)} \hbar\omega/(k_B T)$, $\lambda = 2k_F a/\pi$, and $R_{\text{TF}} = \hbar k_F/(m\omega)$, where k_F denotes the local Fermi momentum at the center of the trap. The temperature $T_c^{(0)}$ is the critical temperature of a homogeneous system having the same density as the trapped system has at the center. It is given by $T_c^{(0)} = (8e^{-2}\gamma/\pi)\epsilon_F e^{-1/\lambda}$ [36], with $\gamma \approx 1.781$ and $\epsilon_F = \hbar^2 k_F^2/(2m)$.

It is convenient to rewrite equation (33) in terms of dimensionless quantities. To that end we define

$$\tilde{\mathbf{r}} = \left(\frac{1}{K} \right)^{1/2} \left(1 + \frac{1}{2\lambda} \right)^{1/4} \frac{\mathbf{r}}{R_{\text{TF}}}, \quad (34)$$

$$\tilde{g} = \frac{7\zeta(3)}{16\pi^2} \frac{1}{K} \left(\frac{2\lambda}{1+2\lambda} \right)^{1/2}, \quad (35)$$

$$\tilde{\mu} = \frac{1}{2K} \left(\frac{2\lambda}{1+2\lambda} \right)^{1/2} \ln \frac{T_c^{(0)}}{T}, \quad (36)$$

$$\tilde{\Phi} = \frac{\Delta}{k_B T}. \quad (37)$$

With these definitions, equation (33) becomes

$$\left(-\frac{1}{2} \tilde{\nabla}^2 + \frac{1}{2} \tilde{\mathbf{r}}^2 + \tilde{g} |\tilde{\Phi}(\tilde{\mathbf{r}})|^2 \right) \tilde{\Phi}(\tilde{\mathbf{r}}) = \tilde{\mu} \tilde{\Phi}(\tilde{\mathbf{r}}), \quad (38)$$

which is the same as the GPE rewritten in HO units, *i.e.*, with the replacements $\mathbf{r}/a_{\text{HO}} \rightarrow \tilde{\mathbf{r}}$, $g/(\hbar\omega a_{\text{HO}}^3) \rightarrow \tilde{g}$, and $\phi a_{\text{HO}}^{3/2} \rightarrow \tilde{\Phi}$.

However, there is one important difference between the GPE describing the Bose-Einstein condensate and the GLE describing the order parameter $\Delta(\mathbf{r})$ of a superfluid Fermi system. In a Bose-Einstein condensate, the particle number N , *i.e.*, the norm of $\tilde{\Phi}$, is fixed, and the chemical potential $\tilde{\mu}$ has to be determined from the GPE (38). For the GLE the situation is reversed: the chemical potential $\tilde{\mu}$ is fixed by the temperature T and other parameters [Eq. (36)], whereas the normalization of $\tilde{\Phi}$, *i.e.*, the magnitude of the gap Δ , has to be determined from equation (38).

The lowest possible value of $\tilde{\mu}$, for which a solution of the GLE (38) can be found, corresponds to the case that the normalization N goes to zero, such that the nonlinear term can be neglected. In this case equation (38) reduces to the Schrödinger equation of the non-interacting harmonic oscillator with the lowest eigenvalue $\tilde{\mu}_{\text{min}} = 3/2$. This gives an upper limit for $T/T_c^{(0)}$, which was used in reference [24] to estimate the critical temperature T_c of the trapped Fermi system.

In this article we are interested in vortex states, *i.e.*, in solutions of the form (1). In the framework of the GL theory, vortex states of superfluid Fermi systems are discussed in reference [25], where the GLE (38) is solved for a two-dimensional geometry, *i.e.*, $\phi(r_\perp, z) \equiv \phi(r_\perp)$, corresponding to a trap with an extremely elongated potential. In two dimensions the lowest possible value of $\tilde{\mu}$, for which vortex solutions can be found, is given by $\mu_{\text{min}}^{2d} = 1 + \kappa$. However, as in our discussion of vortex states in Bose-Einstein condensates, we will consider the spherical case, in which the maximum temperature for the existence of vortex states is determined by $\tilde{\mu}_{\text{min}} = 3/2 + \kappa$.

Since the GLE is identical with the GPE, it is obvious that our TF approach described in the previous sections can immediately be applied also to the GLE. Only the iteration procedure for the self-consistent solution is somewhat different, since now $\tilde{\mu}$ is given instead of N . We start with some guess for N_{c_κ} and calculate the integrated level density, equation (22). Now, if $N_\kappa^I < N_\kappa^{\text{HO}}$, the value of N_{c_κ} is increased, otherwise it is decreased. This procedure is iterated until $N_\kappa^I = N_\kappa^{\text{HO}}$. Due to this quantization rule it is clear that Δ goes to zero when the temperature approaches the critical temperature corresponding to $\tilde{\mu} = 3/2 + \kappa$.

We are now going to compare the results of our TF approach with the fully quantal solution of equation (38). The parameters used for our calculations are taken from reference [22], *i.e.*, we consider $N_{\text{Li}} = 573\,000$ ${}^6\text{Li}$ atoms (scattering length $a = -2160 a_0$) in a trap with $\omega = 2\pi \times 144$ Hz. The self-consistent mean-field potential of the cloud has been neglected in the derivation of the GLE (33) in reference [24], but we take it into account in an approximate way by replacing the external trapping frequency ω by a higher one, $\omega_{\text{eff}} = 2\pi \times 170$ Hz, as it has been done, *e.g.*, in reference [23]. The parameters R_{TF} and $T_c^{(0)}$ are obtained from $\epsilon_F = (3N_{\text{Li}})^{1/3} \hbar\omega_{\text{eff}}$

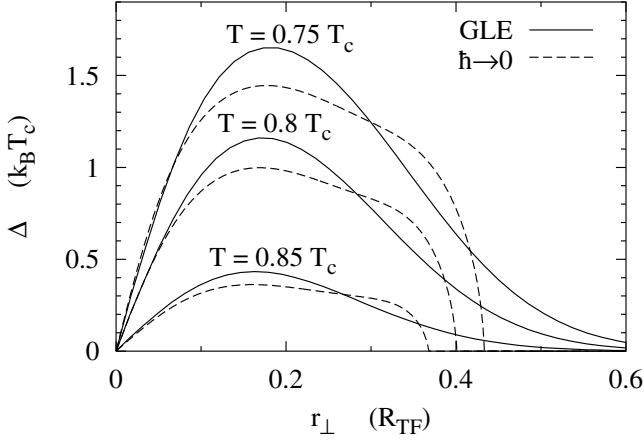


Fig. 6. Order parameter Δ of a superfluid trapped Fermi gas in a vortex state with $\kappa = 1$ as a function of r_{\perp} for $z = 0$. The parameters were chosen corresponding to 573 000 ${}^6\text{Li}$ atoms in a spherical trap with $\omega = 2\pi \times 144$ Hz. The order parameter Δ is given in units of $k_B T_c$ ($T_c = 31.2$ nK), the radius r_{\perp} in units of R_{TF} ($R_{\text{TF}} = 48.7$ μm). Solid lines result from the numerical solution of the GLE (33), whereas the dashed lines are obtained within the ($\hbar \rightarrow 0$) TF approach. The three pairs of curves correspond to three different temperatures (from bottom to top: $0.85T_c$, $0.8T_c$, and $0.75T_c$).

and the relations given below equation (33), with the result $R_{\text{TF}} = 48.7$ μm and $T_c^{(0)} = 36.7$ nK. The temperature corresponding to $\tilde{\mu} = 3/2$, *i.e.*, the critical temperature of the trapped system, is $T_c = 31.2$ nK.

In Figure 6 we show the order parameter Δ obtained from the numerical solution of equation (33) (solid lines). For the parameters listed above, the lowest temperature for which vortex states can exist, *i.e.*, the temperature for which $\tilde{\mu} = 5/2$, is approximately $0.86T_c$. Therefore we display the order parameter only for temperatures below this value, namely for $T/T_c = 0.85$, 0.8 , and 0.75 . For $T/T_c = 0.85$ the order parameter is still very small, and it increases rapidly as the temperature decreases. As can be seen in Figure 6, in all three cases the “amplitude” of the order parameter and the position of the maximum are well reproduced by our TF approximation. Note that also the vortex core is well described.

As already stated, our TF solution has to be interpreted in terms of distributions, and then the agreement is even better than it seems from Figure 6 if one looks at integrated quantities. As an example we consider the normalization $N = \int d^3\tilde{r} |\tilde{\phi}(\tilde{\mathbf{r}})|^2$. For the three temperatures mentioned above, the normalizations obtained from the numerical solution of the GLE and those corresponding to our TF approximation are in good agreement, as shown in Table 2. As a more meaningful example for an integrated quantity let us look at the GL free energy F_{GL} . The explicit expression for the functional $F_{\text{GL}}[\Delta]$ is given in reference [24]. Following this reference, we retain only the leading terms in the small quantities K , \mathbf{r}/R_{TF} , $\ln(T_c^{(0)}/T)$, and $\Delta/(k_B T_c)$. Then, after integration by parts, the GL

Table 2. Normalization N of the order parameter and GL free energy F_{GL} for the parameters used in Figure 6, obtained from the numerical solution of the GLE and from our ($\hbar \rightarrow 0$) TF approximation.

T/T_c		N	F_{GL} (μK)
0.85	GLE	2.12	-0.0079
	$\hbar \rightarrow 0$	2.37	-0.0088
0.8	GLE	16.37	-0.391
	$\hbar \rightarrow 0$	18.41	-0.440
0.75	GLE	34.18	-1.44
	$\hbar \rightarrow 0$	38.20	-1.61

free energy functional becomes

$$F_{\text{GL}}[\Delta] = \frac{mk_F}{2\pi^2\hbar^2} \int d^3r \left\{ -K^2 R_{\text{TF}}^2 \Delta^* \nabla^2 \Delta + \left[\left(\frac{1}{2\lambda} + 1 \right) \frac{\mathbf{r}^2}{R_{\text{TF}}^2} - \ln \frac{T_c^{(0)}}{T} \right] |\Delta|^2 + \frac{7\zeta(3)}{16\pi^2} \frac{1}{(k_B T)^2} |\Delta|^4 \right\}. \quad (39)$$

In the TF approach, the first term ($\propto \Delta^* \nabla^2 \Delta$) cannot be obtained directly from the TF approximation for $\Delta(\mathbf{r})$, but it rather has to be calculated analogous to the kinetic energy density in equation (17). As a consequence, most of the terms cancel, as it is the case if $\Delta(\mathbf{r})$ is the exact solution of the GLE (33), and only the last term ($\propto |\Delta|^4$) survives, but with negative sign. Thus, for the TF approximation as well as for the exact solution of the GLE, we can write in terms of the dimensionless variables defined above

$$F_{\text{GL}} = \frac{4\epsilon_F^2 (k_B T)^2}{\pi^2 (\hbar\omega)^3} K^{5/2} \left(\frac{2\lambda}{1+2\lambda} \right)^{1/4} \int d^3\tilde{r} \left(-\frac{\tilde{g}}{2} |\tilde{\phi}|^4 \right). \quad (40)$$

Results for F_{GL} obtained from the numerical solution of equation (33) and from the TF solution are listed in Table 2. The agreement is as good as for the normalizations N . In fact, the deviations are mainly due to the different normalizations, *i.e.*, the ratio F_{GL}/N obtained from the TF approximation is very close to the exact one.

To conclude this section, we stress that in the range of validity of the GLE the “chemical potential” $\tilde{\mu}$ must not become large. This is the reason for the rather small normalizations of the order parameter and results in a shape of the order parameter as a function of \mathbf{r} which resembles very much the shape of a non-interacting HO wave function. Under these conditions it is clear that the $N \rightarrow \infty$ limit cannot be used as an approximate solution of the GLE, as has also been noted in reference [25].

5 Summary and conclusions

Using the semiclassical Thomas-Fermi approximation understood as $\hbar \rightarrow 0$ limit rather than $N \rightarrow \infty$ limit,

we have studied the vortex states of a Bose condensate of atoms confined in a spherical magnetic trap.

We started analyzing the vortex states in a non-interacting trapped Bose gas. Due to the symmetry of the problem, we have obtained first the Thomas-Fermi density projected on states of defined L_z . In this non-interacting case the density is normalized by adjusting the normalization constant c_κ , and the chemical potential μ is fixed, according to the WKB quantization rule, to the quantal eigenvalue of the quantum state.

In the interacting case the normalization constant and the chemical potential are fixed to normalize the Thomas-Fermi density to the number of particles and that the integrated level density become equal to that of the non-interacting case. For particle numbers where the kinetic energy coming from the radial and axial motion is a non-negligible part of the total kinetic energy, our Thomas-Fermi approach, understood as $\hbar \rightarrow 0$ limit, yields very satisfying results as compared with the corresponding quantal values. For a very large number of particles in the condensate, the small Thomas-Fermi kinetic energy, obtained in our approach, is smaller than the quantal kinetic energy, which, for large number of particles, is also dominated by quantal corrections as it happens for the ground state [15].

The vortex state density profiles obtained in our Thomas-Fermi approximation reproduce quite well the quantal ones, especially for a very large number of particles. However, inside the vortex core our Thomas-Fermi densities are too high. Also near the classical turning point our TF densities locally fail because at this point the density is completely dominated by quantal contributions which are non-analytical in \hbar and which cannot be reproduced by semiclassical approximations of the TF type. However, it shall be kept in mind that the semiclassical density has to be understood as distribution very efficient for describing expectation values rather than local quantities such as the density profile. In this sense we see that the quantities presented in Table 1 are much more accurate than one would expect from an inspection of the local densities shown in Figures 2–4.

The approach is also well suited for the description of vortex states of superfluid trapped fermionic systems in the GL regime, where the various approximations developed for large N cannot be used at all. It should be mentioned that the conditions for the validity of the GLE imply that the parameters of the equivalent GPE always correspond to a rather small number of particles. In this case the normalization of the order parameter (see Tab. 2) and the position of the maximum are well reproduced by the $\hbar \rightarrow 0$ limit as compared with numerical solutions of the GLE. Also the vortex-core region is well described in this case.

We are indebted to A. Polls for supplying us the GP code and to him, M. Guilleumas, and S. Stringari for useful comments. One of us (M.U.) acknowledges support by the Alexander von Humboldt foundation (Germany) as a Feodor-Lynen fellow. X.V. acknowledges financial support from DGI and FEDER

(Spain) under grant BFM2002-01868, from DGR (Catalonia) under grant 2001SGR-00064, and from the CICYT-IN2P3 collaboration.

Appendix: Large- N limit for vortex states

In order to discuss the large- N limit for vortex states more thoroughly, we start from equation (30), which, as shown in Figure 4, becomes very accurate in the limit of large N . Let us look at the different contributions to the kinetic energy, e_{rot} and e_{kin} . In the infinite system, the energies per unit length, dE_{rot}/dz and dE_{kin}/dz can easily be obtained from the numerical solution for f_κ . Since dE_{rot}/dz diverges logarithmically, the corresponding integral has to be cut off at some radius R [35]. For $\kappa = 1$ the results read ($R \gg \xi_0$):

$$\frac{dE_{\text{rot}}}{dz} = \frac{\pi \hbar^2 \rho_0}{m} \left(\ln \frac{R}{\xi_0} - 0.40 \right), \quad (41)$$

$$\frac{dE_{\text{kin}}}{dz} = 0.28 \frac{\pi \hbar^2 \rho_0}{m}. \quad (42)$$

In complete analogy to the derivation of the total energy of a vortex in a trapped system in reference [37], one can use these results to obtain explicit expressions for the rotational and radial kinetic energies of a vortex, e_{rot} and $e_{\text{kin}}^{\text{core}}$, which for a spherical trapping potential read

$$e_{\text{rot}} = \frac{1}{N} \frac{4\pi\rho_0}{3} \frac{\hbar^2}{m} r_{\text{max}} \left(\ln \frac{r_{\text{max}}}{\xi_0} - 1.18 \right), \quad (43)$$

$$e_{\text{kin}}^{\text{core}} = 0.28 \frac{1}{N} \frac{4\pi\rho_0}{3} \frac{\hbar^2}{m} r_{\text{max}}. \quad (44)$$

Here $r_{\text{max}} = \sqrt{2\mu/(m\omega^2)}$ is the radius of the condensate. However, the kinetic energy has also another contribution $e_{\text{kin}}^{\text{trap}}$ due to the finite size of the trapped system. Since outside the vortex core the shape of the condensate is almost not changed, we assume that for this contribution the relation derived in reference [38] for the case without vortex, remains valid:

$$e_{\text{kin}}^{\text{trap}} = \frac{5}{2} \frac{\hbar^2}{mr_{\text{max}}^2} \left(\ln \frac{r_{\text{max}}}{a_{\text{HO}}} - 0.26 \right). \quad (45)$$

Since the volume of the vortex core is negligible in the limit $N \rightarrow \infty$, μ depends on N in the same way as in the large- N limit for the ground state,

$$\mu = \frac{\hbar\omega}{2} \left(\frac{15Na}{a_{\text{HO}}} \right)^{2/5}. \quad (46)$$

Using this, we finally obtain

$$e_{\text{rot}} = \hbar\omega \left(\frac{a_{\text{HO}}}{15Na} \right)^{2/5} \left(\ln \frac{15Na}{a_{\text{HO}}} - 2.95 \right), \quad (47)$$

$$e_{\text{kin}} = \hbar\omega \left(\frac{a_{\text{HO}}}{15Na} \right)^{2/5} \left(\frac{1}{2} \ln \frac{15Na}{a_{\text{HO}}} - 0.51 \right). \quad (48)$$

From these equations we conclude that the ratio $e_{\text{kin}}/e_{\text{rot}}$ does not go to zero, but approaches $1/2$ for $N \rightarrow \infty$.

Hence, neglecting the radial and axial parts of the kinetic energy, but retaining the rotational part, as it is done in the literature [10, 11, 16, 17], is not justified and does not correspond to the proper $N \rightarrow \infty$ limit. Instead, the correct large- N limit is given by equation (30), except at the surface of the condensate. The latter can be approximated, *e.g.*, by the exact solution of the GPE for a linear potential, as it has been done in reference [38] in order to derive equation (45), and also in reference [37].

It should, however, be noted that equations (30, 45) correspond to a partial resummation to all orders in \hbar as demonstrates the nonanalytical dependence on \hbar of these quantities. Such resummation techniques, also encountered in the WKB approximation, are necessary whenever the asymptotic Wigner-Kirkwood \hbar expansion breaks down. This is always the case when the gradients of the potential start to diverge like in the vortex core for $N \rightarrow \infty$, see Figure 5.

References

- M.H. Anderson, J.R. Ensher, M.R. Matthews, C.E. Wieman, E.A. Cornell, *Science* **269**, 198 (1995)
- K.B. Davis, M.-O. Mewes, M.R. Andrews, N.J. van Druten, D.S. Durfee, D.M. Kurn, W. Ketterle, *Phys. Rev. Lett.* **75**, 3969 (1995)
- C.C. Bradley, C.A. Sackett, J.J. Tollett, R.G. Hulet, *Phys. Rev. Lett.* **75**, 1687 (1995)
- L.P. Pitaevskii, *Zh. Eksp. Theor. Phys.* **40**, 646 (1961) [*Sov. Phys. JETP* **13**, 451 (1972)]
- E.P. Gross, *Nuovo Cim.* **20**, 454 (1961); *J. Math. Phys.* **4**, 195 (1963)
- F. Dalfovo, S. Stringari, *Phys. Rev. A* **53**, 2477 (1996)
- F. Dalfovo, L.P. Pitaevskii, S. Stringari, *J. Res. Natl. Inst. Stand. Technol.* **101**, 537 (1996)
- A.S. Parkins, D.F. Walls, *Phys. Rep.* **303**, 1 (1998)
- F. Dalfovo, S. Giorgini, L.P. Pitaevskii, S. Stringari, *Rev. Mod. Phys.* **71**, 463 (1999)
- A.L. Fetter, A.A. Svidzinsky, *J. Phys. Cond. Matt.* **13**, R135 (2001)
- D.S. Rokhsar, *Phys. Rev. Lett.* **79**, 2164 (1997)
- M. Guilleumas, R. Graham, *Phys. Rev. A* **64**, 033607 (2001)
- M.R. Matthews, B.P. Anderson, P.C. Haljan, D.S. Hall, C.E. Wieman, E.A. Cornell, *Phys. Rev. Lett.* **83**, 2498 (1999); B.P. Anderson, P.C. Haljan, C.E. Wieman, E.A. Cornell, *Phys. Rev. Lett.* **85**, 2857 (2000)
- K.W. Madison, F. Chevy, W. Wohlleben, J. Dalibard, *Phys. Rev. Lett.* **84**, 806 (2000); *J. Mod. Opt.* **47**, 2715 (2000)
- P. Schuck, X. Viñas, *Phys. Rev. A* **61**, 043603 (2000)
- Tin-Lun Ho, V.B. Shenoy, *Phys. Rev. Lett.* **77**, 3276 (1996)
- S. Sinha, *Phys. Rev. A* **55**, 4325 (1997)
- M. Modugno, L. Pricoupenko, Y. Castin, *Eur. Phys. J. D* **22**, 235 (2003)
- B. DeMarco, D.S. Jin, *Science* **285**, 1703 (1999)
- A.G. Truscott, K.E. Strecker, W.I. McAlexander, G.B. Partridge, R.G. Hulet, *Science* **291**, 2570 (2001)
- F. Schreck, L. Khaykovich, K.L. Corwin, G. Ferrari, T. Bourdel, J. Cubizolles, C. Salomon, *Phys. Rev. Lett.* **87**, 080403 (2001)
- M. Houbiers, R. Ferwerda, H.T.C. Stoof, W.I. McAlexander, C.A. Sackett, R.G. Hulet, *Phys. Rev. A* **56**, 4864 (1997)
- M. Farine, P. Schuck, X. Viñas, *Phys. Rev. A* **62**, 013608 (2000)
- M.A. Baranov, D.S. Petrov, *Phys. Rev. A* **58**, R801 (1998)
- M. Rodriguez, G.-S. Paraoanu, P. Törmä, *Phys. Rev. Lett.* **87**, 100402 (2001)
- P. Ring, P. Schuck, *The Nuclear Many-Body Problem* (Springer, New York, 1980)
- H. Krivine, M. Casas, J. Martorell, *Ann. Phys. (N.Y.)* **200**, 304 (1990)
- M. Abramowitz, I.A. Stegun, *Handbook of Mathematical Functions* (Dover, New York, 1965)
- M. Centelles, X. Viñas, M. Durand, P. Schuck, D. Von-Eiff, *Ann. Phys. (N.Y.)* **266**, 207 (1998)
- B.G. Englert, *Semiclassical Theory of Atoms*, Lecture Notes in Physics **300** (Springer, Berlin, 1988)
- R.W. Hasse, *Ann. Univ. M. Curie-Sklodowska (Lublin, Poland) XL/XLI* (1985/1986), p. 191; *Nucl. Phys. A* **467**, 407 (1987)
- X. Viñas, P. Schuck, M. Farine, M. Centelles, *Phys. Rev. C* **67**, 054307 (2003)
- A. Svidzinsky, A. Fetter, *Phys. Rev. A* **62**, 063617 (2000)
- A. Aftalion, T. Riviere, *Phys. Rev. A* **64**, 043611 (2001)
- V.L. Ginzburg, L.P. Pitaevskii, *Zh. Eksp. Theor. Fiz.* **34** (1958), 1240 [*Sov. Phys. JETP* **7**, 858 (1958)]
- C.A.R. Sá de Melo, M. Randeria, J.R. Engelbrecht, *Phys. Rev. Lett.* **71**, 3202 (1993)
- E. Lundh, C.J. Pethick, H. Smith, *Phys. Rev. A* **55**, 2126 (1997)
- F. Dalfovo, L. Pitaevskii, S. Stringari, *Phys. Rev. A* **54**, 4213 (1996)