Vortices in Atomic Bose-Einstein Condensates in the large gas parameter region

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Abstract

Most theoretical studies on Bose-Einstein condensates (BEC) in gases of alkali atoms confined in magnetic traps have been naturally conducted in the framework of the Gross-Pitaevskii (GP) equation[1]. The key point for the validity of this description is the dilute condition of these systems, i.e., the average distance between the atoms is much larger than the range of the atomic interaction. In this situation, the physics is dominated by two-body collisions, generally well described in terms of the s-wave scattering length a. The crucial parameter defining the condition of dilutness is the gas parameter $x(\mathbf{r}) = n(\mathbf{r})a^3$, where $n(\mathbf{r})$ is the local density of the system. For low values of the average gas parameter, $x_{av} \leq 10^{-3}$ the mean field Gross-Piatevskii equation does an excellent job (see Ref.[2] for an extended review). However, in the density ranges attained in recent experiments the local gas parameter may well exceed this value, exploiting the large variation of the scattering length in the vicinity of a Feshbach resonance[3,4].

Under these circunstances it is unavoidable to test the accuracy of the GP equation by performing microscopic calculations. We would like to imagine that the gas parameter has been driven to a region were one can still have a universal regime, i.e. that the specific shape of the potential is unimportant, and one can describe the system as a dilute system of hard-spheres, whose diameter coincides with the scattering length itself. However, the value of x is such that the calculation of the energy of the uniform hard-sphere Bose gas would require to take into account the second term in the low-density expansion[5] of the density energy:

$$\frac{E}{V} = \frac{2\pi n^2 a\hbar}{m}\left[1 + \frac{128}{15}\left(\frac{na^3}{\pi}\right)^{1/2} + \cdots\right], \tag{1}$$

where m is the mass of the hard-spheres. For the case of uniform systems, the validity of this expansion has been carefully studied both, using diffusion Monte Carlo[6] and Hyper-Netted-Chain techniques[7].

The energy functional associated with the GP theory is simply obtained in the local-density approximation (LDA) by keeping only the first term in the low-density expansion (1) :

$$E_{GP}[\Psi] = \int d\mathbf{r}\left[\frac{\hbar^2}{2m} \mid \nabla\Psi(r) \mid^2 + V_{trap}(\mathbf{r}) \mid \Psi \mid^2 + \frac{2\pi\hbar^2 a}{m} \mid \Psi \mid^4\right], \tag{2}$$

where

$$V_{trap}(\mathbf{r}) = \frac{1}{2}m(\omega_\perp^2 x^2 + \omega_\perp^2 y^2 + \omega_z^2 z^2) \tag{3}$$

is the confining potential defined by the two angular frequencies, $\omega_\perp$ and ω_z associated with

the external potential of the anisotropic trap. The wave function Ψ is normalized to the total number of particles which are assumed to be all in the condensate.

By performing a functional variation of $E_{GP}[\Psi]$ one finds the Euler-Lagrange equation, known as the GP equation,

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + V_{trap}(\mathbf{r}) + \frac{4\pi\hbar^2 a}{m} \mid \Psi \mid^2\right]\Psi = \mu\Psi, \tag{4}$$

where μ is the chemical potential. A logical step further, in the spirit of LDA, is to include into the energy functional (2) the next term of the low density expansion. Then, a similar functional variation process gives rise to a modified GP equation (MGP)[8]

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + V_{trap}(\mathbf{r}) + \frac{4\pi\hbar^2 a}{m} \mid \Psi \mid^2 \left(1 + \frac{32a^{3/2}}{3\pi^{1/2}} \mid \Psi \mid\right)\right]\Psi = \mu\Psi. \tag{5}$$

This modified GP equation has been used in Ref.[8] to estimate the corrections to the GP equation, in particular for the case of a deformed cylindrical trap using the scattering lengths corresponding to the first JILA experiments, which took advantage of the presence of a Feshbach resonance in collision of two ^{85}Rb atoms to tune their scattering length[3]. Also fully microscopic calculations using a hard-spheres interaction have been performed in the framework of Variational and Diffusion Monte Carlo methods[10–13].

In the present paper, we want to compare the results of the GP equations discussed above (Eqs.(4,5)) with Monte Carlo calculations for deformed traps under conditions $x > 10^{-3}$, where the validity of the GP equation is not clear. The study will be performed both for the ground state and also for excited states having a vortex line along the z-axis.

The starting point of the microscopic calculations is to define the Hamiltonian. For N trapped, interacting particles it is given by

$$H = -\frac{\hbar^2}{2m}\sum_{i=1}^{N}\nabla_i^2 + \sum_{i=1}^{N}V_{trap}(\mathbf{r}_i) + \sum_{i<j}^{N}V_{int}(\mid \mathbf{r}_i - \mathbf{r}_j \mid), \tag{6}$$

The pair interaction $V_{int}(\mid \mathbf{r}_i - \mathbf{r}_j \mid)$ is taken as a hard-core potential of diameter a, i.e., the scattering length.

The next step is to define a trial wave function,

$$\Psi_T(1, ..., N) = F(1, ..., N)\Psi_{MF}(1, ..., N) \tag{7}$$

where $F(1, ..., N)$ is a many-body correlation operator applied to the mean-field wave-function Ψ_{MF}. The advantage of using a correlated trial wave function lies in the fact

that non-perturbative effects, as the short-range repulsion for the hard-spheres, may be directly incorporated into the trial wave function. The simplest correlation operator has the Jastrow form[14],

$$F(1,...,N) = \prod_{i<j} f_j(r_{ij}). \tag{8}$$

In our variational calculations, we use a two-body correlation function which is the solution of the Schrödinger equation for a pair of particles at very low energy interacting via a hard-core potential of diameter a,

$$f(r) = \begin{cases} \left(1 - \frac{a}{r}\right) & r > a \\ 0 & r \leq a \ . \end{cases} \tag{9}$$

This type of correlation, besides being physically motivated, has been succesfully used in Ref.[10,11] to study both spherically symmmetric and deformed traps. These authors have also explored the quality of this correlation by comparing VMC results with this $f(r)$ and Difussion Monte Carlo calculations for the case of spherically symmetric traps[12].

The deformation of the trap is incorporated in the mean field wave function (Ψ_{MF}), which is taken as the product of N single particle wave functions

$$\varphi(\mathbf{r}) = A\lambda^{1/4} \exp\left[-\frac{1}{2}\alpha(x^2 + y^2 + \lambda z^2)\right], \tag{10}$$

where α is taken as the variational parameter of the calculation, and $A(\alpha)$ is a normalization constant. The parameter $\lambda = \omega_z/\omega_\perp$ is kept fixed and taken equal to the asymmetry of the trap. In this way, the mean-field wave function assumes to have all the particles in the condensate, which is described by the wave function φ (Eq. (10)).

The evaluation of the expectation value of the Hamiltonian with these correlated trial wave functions provides an upperbound to the ground state energy of the system

$$E_T = \frac{\langle \Psi_T \mid H \mid \Psi_T \rangle}{\langle \Psi_T \mid \Psi_T \rangle}. \tag{11}$$

The practical evaluation of the expectation value is performed by using the Metropolis Monte Carlo method of integration[15,16].

The energy results obtained with the Hamiltonian (Eq. (6)) can be directly compared with the output of the GP equations reported above (Eqs. (4,5)). However, one should keep in mind that the Monte Carlo calculation incorporates explicitly the interatomic correlations and therefore one could in principle find the natural orbits and extract the occupation of the

condensate[10]. In contrast, the Gross-Pitaevskii equations represent a mean-field description, with all the atoms in the condensate. When one takes as single-particle wave function φ the solution to the modified Gross-Pitaevskii (MGP) equation, addition correlations which take into account in the second order term of the low-density expansion of the energy (Eq. (1)) are incorporated to the density functional and, therefore, to the mean field wave function Ψ_{MF}.

For the comparison of the results obtained with the different GP equations and the variational Monte Carlo calculations, we consider a deformed trap with $\lambda = \omega_z/\omega_\perp = \sqrt{8}$, which was the experimental deformation of one of the first experiments concerning ^{87}Rb[17]. However, the scattering length is artificially changed to $a = 35a_{Rb}$, which was one of the values considered in Ref.[10] to study the correlation effects. The number of confined atoms is chosen to be 500 atoms, to keep the amount of computing time acceptable when using the Monte Carlo method . As usual, all the numerical results are given in units of the harmonic oscillator length $a_\perp = (\hbar/m\omega_\perp)^{1/2}$ and the harmonic oscillator energy $\hbar\omega_\perp$.

First we analyze the GP and the MGP results which are reported in Table I. For this scattering length, the corrections of the MGP to the chemical potential are of the order of 20%. The energy corrections are also relevant and it is interesting to study the different contributions to the energy: the kinetic energy,

$$E_{kin} = \frac{\hbar^2}{2m}\int d\mathbf{r} \mid \nabla\Psi(\mathbf{r}) \mid^2, \tag{12}$$

the harmonic oscillator energy associated to the presence of the trapping potential,

$$E_{HO} = \frac{m}{2}\int d\mathbf{r}(\omega_\perp^2(x^2+y^2)+\omega_z^2 z^2) \mid \Psi(\mathbf{r}) \mid^2, \tag{13}$$

and the interaction energies E_1 and E_2 given by

$$E_1 = \frac{2\pi\hbar^2 a}{m}\int d\mathbf{r} \mid \Psi(\mathbf{r}) \mid^2, \tag{14}$$

$$E_2 = \frac{2\pi\hbar^2 a}{m}\frac{128}{15}\left(\frac{a^3}{\pi}\right)^{1/2}\int d\mathbf{r} \mid \Psi(\mathbf{r}) \mid^5 . \tag{15}$$

The virial theorem is used to stablish a relation between the different contributions to the energy,

$$2E_{kin} - 2E_{HO} + 3E_1 + \frac{9}{2}E_2 = 0, \tag{16}$$

and serves as a proof of the numerical accuracy of the solution of the GP equations. Looking at the data it Table I, we see that this test is very well satisfied by all calculations.

Notice that the kinetic energy associated to the mean field descriptions is not negligible, indicating that the regime where the Thomas-Fermi approximation to the GP equation is valid has not been reached. In this limit, one has

$$\mu_{TF} = \frac{1}{2}(15\bar{a_s}N\lambda)^{2/5}\hbar\omega_\perp \tag{17}$$

where $\bar{a}_s = a_s/a_\perp^{HO}$ is the dimensionless scattering length, and the energy $E_{TF} = 5\mu_{TF}/7$. Therefore, in this approach, one gets $E_{TF} = 9.03$ and $\mu_{TF} = 12.64$, which do not agree with the values reported in Table I. However, they are close enough that one can use the peak value of the gas parameter calculated in the TF approximation,

$$x_{TF}^{pk} = \max_{\mathbf{r}} n(\mathbf{r})a^3 = \frac{1}{8\pi}(15\bar{a}_s N\lambda)^{2/5}\bar{a}_s^2, \tag{18}$$

to estimate the diluteness of the system. This calculation gives $x_{TF}^{pk} = 0.023$. At these rather large value of the diluteness paremeter, the expected size of the corrections brougth by the MGP equation to the GP results is in fact the one found in the present calculation. In addition, one expects that x is low enough that the MGP equation still provides a rather good description when compared with a microscopic calculation[6–8], as will be shown below.

The variational Monte Carlo results are also given in Table I. As expected, there is a very close agreement with the results provided by the MGP equation. Notice that in this approach, and using the Hamiltonian of Eq.6, the potential energy is zero, because the wave function is strictly zero inside the core. The total energy in this case is distributed between E_{HO} and the true kinetic energy. Actually the only energies that can be directly compared with the previous calculation are the total and the harmonic oscillator energies. (In the Monte Carlo calcuation, we have used the Pandharipande-Bethe prescription for the kinetic energy because it is well know that produces a kinetic energy with smaller variance.) In the minimization process we keep fixed the λ parameter in the single particle wavefunction Eq. (...), i.e., we assume that the deformation of the trap is transferred to the wavefunction, and vary only α. At the minimum, $\alpha = 0.7687$.

One can also explore the effects of the correlations in the density profiles, which are shown in Fig. 1 for the several approximationis used in this work. The repulsive character of the correction terms of the MGP equation translate in a decrease of the the value of the column density at the origin and an increase of the size of the condensate. Again, there is a much better agreement of the Monte Carlo profile with the MGP results than with the GP ones.

The good agreement between VMC and MGP is not a guarantee to conclude that they give a very good description of the system. However, as it was shown in Ref.[11] for the case of spherical traps, the improvements introduced in the wave function by a Difusion Montecarlo Calculation, i.e., obtaining the exact solution of the Hamiltonian, are rather small and the variational wave function (Eq. (10)) provides a very good description of the system. Therefore one can safely argue that the same will be true for deformed traps. For these values of the scattering length, or more precisely, of the diluteness parameter, the MGP equation is very useful to calculate the energy, chemical potential and the density profiles of the ground state of the system also for condensates with larger number of particles which would be computationally prohibitive for a Monte Carlo calculation.

Now we want to explore the situation for excited states and we consider .....

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	μ	E/N	E_{kin}/N	E_{HO}/N	E_{pot1}/N	E_{pot2}/N
GP	12.980	9.496836	0.39495	5.61911	3.4827765	–
MGP	15.453	11.06108	0.35353	6.94092	2.516691	1.249938
VMC		11.1169(24)				

TABLE I: Chemical potential and energies in the GP, MGP, VMC and DMC approximations without vortices. $a = 0.15155a_\perp$, $\lambda = \sqrt{8}$, $N = 500$.

	μ	E/N	E_{kin}/N	E_{HO}/N	E_{pot1}/N	E_{pot2}/N	E_{vor}/N
GP-1v	13.187	9.7835936	0.42508	5.74271	3.403871	–	0.21193
MGP-1v	15.623	11.305	0.37692	7.03774	2.482418	1.223280	0.18492
VMC-1v		11.3301(24)					

TABLE II: Chemical potential and energies in the GP, MGP, VMC and DMC approximations for the one-vortex state with the vortex line along the z-axis. $a = 0.15155a_\perp$, $\lambda = \sqrt{8}$, $N = 500$.

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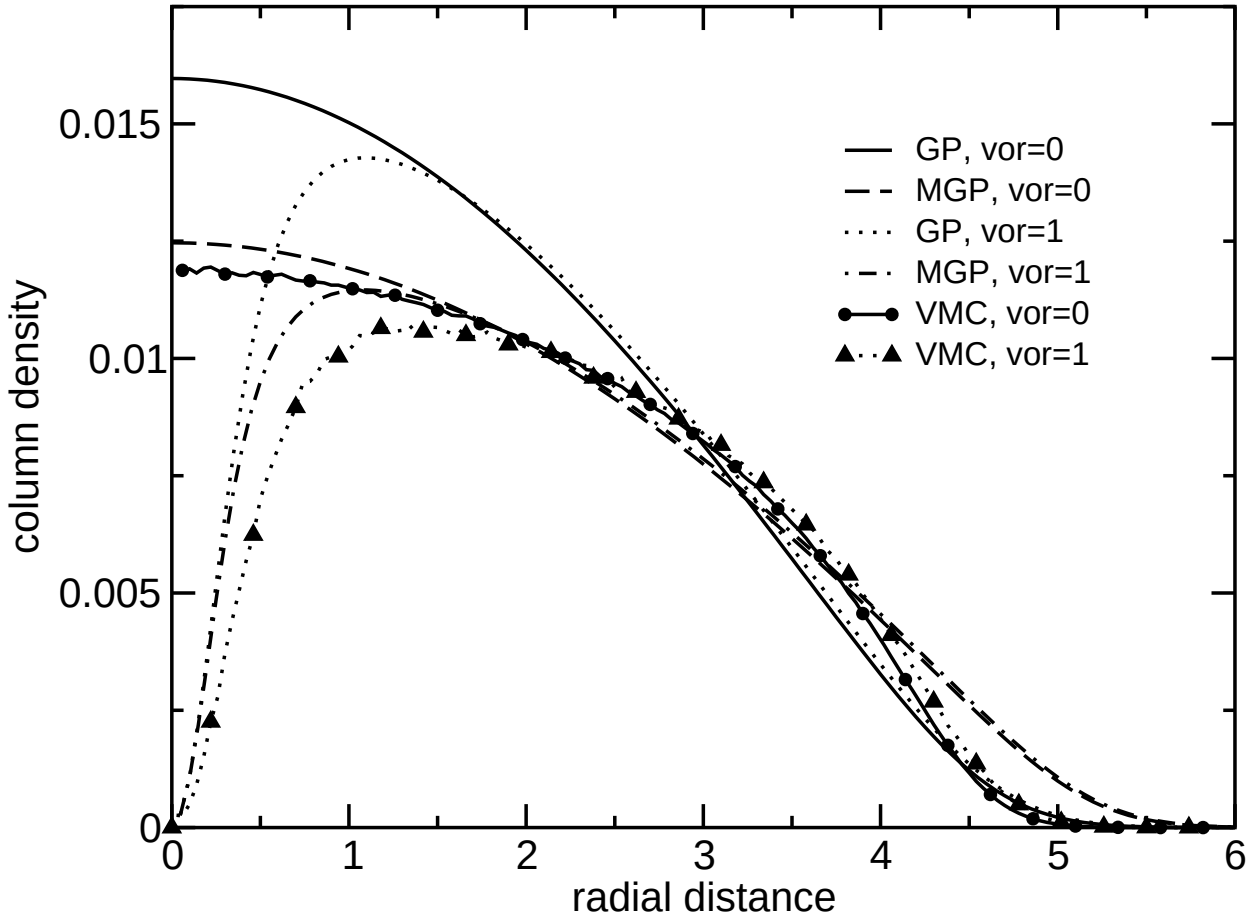

FIG. 1: Column density –*i.e.*, density $n(\mathbf{r})$ integrated along the z-axis– as a function of distance to this axis, for N=500, comparing GP (solid and dashed lines) and MGP (dotted and dash-dotted lines) results, with and without vortex, for $a = 35a_{Rb} = 0.15155a_{\perp}$. Also shown are the results a the variational Monte Carlo calculations (lines with symbols). The deformation and the oscillator lengths are as in Stringari's paper[17,18].