Time-Dependent Variational Approach to Bose-Einstein Condensation

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Abstract

We discuss the mean-field approximation for a trapped weakly-interacting Bose-Einstein condensate (BEC) and its connection with the exact many-body problem by deriving the Gross-Pitaevskii action of the condensate. The mechanics of the BEC in a harmonic potential is studied by using a variational approach with time-dependent Gaussian trial wave-functions. In particular, we analyze the static configurations, the stability and the collective oscillations for both ground-state and vortices.

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I. INTRODUCTION

Few years ago, the Bose-Einstein condensation has been observed with alkali-metal vapors confined in magnetic traps at very low temperatures.[1–3] By now, the total number of groups that have achived Bose-Einstein condensation is over a dozen. The confining potential is accurately described by a harmonic trap, and theoretical studies of the Bose-Einstein condensate (BEC) in harmonic traps have been performed for the ground state, elementary excitations and vortices (for a review see Ref. 4).

In the first part of this paper, we discuss the time-dependent Gross-Pitaevskii (GP) equation,[5,6] which describes the macroscopic wave-function of a weakly-interacting Bose condensate at zero temperature. We deduce the GP action and the GP equation by imposing the least action principle to the quantum many-body action of the system within the mean-field approximation.[7] Such approach is mathematically equivalent to the field theory one, but it avoids the tricky issues related with spontaneous symmetry breaking.

The rest of the paper is devoted to the study of BEC by using Gaussian trial wave-functions to minimize the GP action. Minimizing the GP action with a Gaussian trial function makes it possible to obtain approximate solutions for the condensate wave function, which can be treated, to a large extent, analytically. This method has been used by several authors to study the BEC static properties and the dynamics near the ground-state.[8–14] Here we extend its application also to vortex states. The presence of vortex states is a signature of the macroscopic phase coherence of the system. Moreover, vortices are important to characterize the superfluid properties of Bose systems.[7]

II. VARIATIONAL PRINCIPLE AND MEAN-FIELD APPROXIMATION

Let us consider a N-body quantum system with Hamiltonian $\hat{H}$. The exact time-dependent Schrödinger equation can be obtained by imposing the quantum least action principle to the action

$$S = \int dt < \psi(t)| i\hbar \frac{\partial}{\partial t} - \hat{H} |\psi(t) > , \quad (1)$$

where ψ is the many-body wave-function of the system and

$$< \psi(t)|\hat{A}|\psi(t) >= \int \ d^3\mathbf{r}_1 ... d^3\mathbf{r}_N \ \psi^*(\mathbf{r}_1, ..., \mathbf{r}_N, t) \hat{A} \psi(\mathbf{r}_1, ..., \mathbf{r}_N, t) , \quad (2)$$

for any quantum operator $\hat{A}$. Looking for stationary points of S with respect to variation of the conjugate wave-function ψ^* gives

$$i\hbar \frac{\partial}{\partial t} \psi = \hat{H} \psi , \quad (3)$$

which is the many-body time-dependent Schrödinger equation.

As is well known, except for integrable systems, it is impossible to obtain the exact solution of the many-body Schrödinger equation and some approximation must be used.

In the mean-field approximation the total wave-function is assumed to be composed of independent particles, i.e. it can be written as a product of single-particle wave-functions ϕ_j. In the case of identical fermions, ψ must be antisymmetrized.[7] By looking for stationary action with respect to variation of a particular single-particle conjugate wave-function ϕ_j^* one finds a time-dependent Hartree-Fock equation for each ϕ_j:

$$i\hbar \frac{\partial}{\partial t} \phi_j = \frac{\delta}{\delta \phi_j^*} < \psi|\hat{H}|\psi >= \hat{h} \phi_j , \quad (4)$$

where $\hat{h}$ is a one-body operator. In general, the one-body operator $\hat{h}$ is nonlinear. Thus the Hartree-Fock equations are non-linear integro-differential equations. Note that for alkali-metal vapors, which are quite diluite, the independent-particle approximation gives reliable results.[4] Obviously, it is possible to go beyond the independent-particle approximation by including correlations in the many-body wave-function.[8] This is particularly useful to reproduce the properties of the superfluid ^{4}He, that is a strongly interacting system.[9,10]

III. GROSS-PITAEVSKII ACTION

In this section we discuss the zero-temperature mean-field approximation for a system of trapped weakly-interacting bosons in the same quantum state, i.e. a Bose-Einstein condensate.[7] In this case the Hartree-Fock equations reduce to only one equation, the Gross-Pitaevskii equation,[5,6] which describes the dynamics of the condensate. As previously discussed, this equation is intensively studied because of the recent experimental achievement of Bose-Einstein condensation for atomic gasses in magnetic traps at very low temperatures.[1−3]

The Hamiltonian operator of a system of N identical bosons of mass m is given by

$$\hat{H} = \sum_{i=1}^{N} \Big(-\frac{\hbar^2}{2m}\nabla_i^2 + V_0(\mathbf{r}_i)\Big) + \frac{1}{2}\sum_{ij=1}^{N} V(\mathbf{r}_i, \mathbf{r}_j) \; , \tag{5}$$

where $V_0(\mathbf{r})$ is an external potential and $V(\mathbf{r}, \mathbf{r}')$ is the interaction potential. In the mean-field approximation the totally symmetric many-particle wave-function of the Bose-Einstein condensate reads

$$\psi(\mathbf{r}_1, ..., \mathbf{r}_N, t) = \phi(\mathbf{r}_1, t) \; ... \; \phi(\mathbf{r}_N, t) \; , \tag{6}$$

where $\phi(\mathbf{r}, t)$ is the single-particle wave-function. Note that such factorization of the total wave-function is exact in the case of a non-interacting condensate. The quantum action of the system is then simply given by

$$S_{GP} = N \int dt < \phi(t)| i\hbar \frac{\partial}{\partial t} - \hat{h}_s |\phi(t) > \; , \tag{7}$$

where

$$\hat{h}_s = -\frac{\hbar^2}{2m}\nabla^2 + V_0(\mathbf{r}) + \frac{1}{2}(N-1)\int d^3\mathbf{r}' |\phi(\mathbf{r}')|^2 V(\mathbf{r}, \mathbf{r}') \; . \tag{8}$$

We call S_{GP} the Gross-Pitaevskii (GP) action of the Bose condensate. By using the quantum least action principle we get the Euler-Lagrange equation

$$i\hbar \frac{\partial}{\partial t}\phi(\mathbf{r}, t) = \Big[-\frac{\hbar^2}{2m}\nabla^2 + V_0(\mathbf{r}) + (N-1)\int d^3\mathbf{r}' V(\mathbf{r}, \mathbf{r}') |\phi(\mathbf{r}', t)|^2 \Big] \phi(\mathbf{r}, t) \; , \tag{9}$$

which is an integro-differential nonlinear Schrödinger equation. Such equation and the effect of a finite-range interaction have been analyzed only by few authors (see, for example, Ref. 14-16). In fact, at low energies, it is possible to substitute the true interaction with a pseudo-potential[7]

$$V(\mathbf{r},\mathbf{r}') = B\,\delta^3(\mathbf{r}-\mathbf{r}')\ , \tag{10}$$

where $B = 4\pi\hbar^2 a_s/m$ is the scattering amplitude and a_s the s-wave scattering length. In this way one obtains the so-called time-dependent GP equation[5,6]

$$i\hbar\frac{\partial}{\partial t}\phi(\mathbf{r},t) = \Big[-\frac{\hbar^2}{2m}\nabla^2 + V_0(\mathbf{r}) + B(N-1)|\phi(\mathbf{r},t)|^2\Big]\phi(\mathbf{r},t)\ , \tag{11}$$

that is the starting point of many calculations.[4] Note that the GP equation is accurate to describe the condensate of weakly-interacting bosons only near zero temperature, where thermal excitations can be neglected. At finite temperature, one must consider a generalized GP equation plus the Bogoliubov equations, which describe the quasi-particle elementary excitations of the condensate.[7]

IV. TRIAL WAVE-FUNCTION OF THE CONDENSATE

In this section we use a Gaussian trial wave-function to describe the ground-state of the Bose condensate and to minimize the GP action.

We consider a triaxially asymmetric harmonic trapping potential of the form

$$V_0(\mathbf{r}) = \frac{1}{2}m\omega_0^2\left(\omega_1^2x^2 + \omega_2^2y^2 + \omega_3^2z^2\right)\ , \tag{12}$$

where ω_i $(i=1,2,3)$ are adimensional constants proportional to the spring constants of the potential along the three axes. In the rest of this section we write the lengths in units of the characteristic length of the trap $a_0 = \sqrt{\hbar/(m\omega_0)}$, the time in units ω_0^{-1}, the action in units $\hbar$ and the energy in units $\hbar\omega_0$. By using the delta pseudo-potential to model the interaction between particles, the GP action is explicitly given by

$$S_{GP} = N\int dt\, d^3\mathbf{r}\ \phi^*(\mathbf{r},t)\Big[i\frac{\partial}{\partial t} + \frac{1}{2}\nabla^2 - V_0(\mathbf{r}) - \frac{1}{2}B(N-1)|\phi(\mathbf{r})|^2\Big]\phi(\mathbf{r},t)\ , \tag{13}$$

where $B = 4\pi a_s/a_0$ in our units.

We want minimize this GP action S_{GP} by choosing an appropriate single-particle trial wave-function. A good choice is the following

$$\phi(\mathbf{r},t) = \Big[\frac{1}{\pi^3\sigma_1^2(t)\sigma_2^2(t)\sigma_3^2(t)}\Big]^{1/4} \prod_{i=1,2,3} \exp\left\{-\frac{x_i^2}{2\sigma_i^2(t)} + i\beta_i(t)x_i^2\right\} \ , \tag{14}$$

with $(x_1,x_2,x_3) \equiv (x,y,z)$. σ_i and β_i are the time-dependent variational parameters. The σ_i are the widths of the condensate in the three axial directions. Note that, in order to describe the time evolution of the variational function, the phase factor $i\beta_i(t)x_i^2$ is needed.[11,12] The choice of a Gaussian shape for the condensate is well justified in the limit of weak interatomic coupling, because the exact ground-state of the linear Schrödinger equation with harmonic potential is a Gaussian. Moreover, for the description of the collective dynamics of Bose-Einstein condensates, it has already been shown that the variational technique based on Gaussian trial functions leads to reliable results even in the large condensate number limit.[15−17]

By inserting the trial wave-function, after spatial integration, the GP action becomes

$$S_{GP} = N\int dt\ L(\dot\beta_i,\beta_i,\sigma_i) \ , \tag{15}$$

where the effective Lagrangian is given by

$$L = -\frac{1}{2}\Big[\sum_{i=1}^{3}(\dot\beta_i\sigma_i^2 + \frac{1}{2\sigma_i^2} + 2\sigma_i^2\beta_i^2 + \frac{1}{2}\omega_i^2\sigma_i^2) + \frac{\tilde g}{\sigma_1\sigma_2\sigma_3}\Big] \ , \tag{16}$$

with $g = (2/\pi)^{1/2}(a_s/a_0)$ and $\tilde g = g(N-1)$. Again, by imposing the least action principle, we find six Euler-Lagrange equations

$$\beta_i = -\frac{\dot\sigma_i}{2\sigma_i} \ , \qquad \ddot\sigma_i + \omega_i^2\sigma_i = \frac{1}{\sigma_i^3} + \frac{\tilde g}{\sigma_1\sigma_2\sigma_3\sigma_i} \ , \tag{17}$$

with $i = 1,2,3$. Note that the time dependence of β_i is fully determined by that of σ_i. Moreover, for $\tilde g = 0$ the six equations are exact solutions of the time-dependent GP equation. The last three differential equations are the classical equations of motion of a system with coordinates σ_i and total energy per particle given by

$$\frac{E}{N} = \frac{1}{2}\Big[\sum_{i=1}^{3}\frac{1}{2}\dot\sigma_i^2\Big] + U(\sigma_1,\sigma_2,\sigma_3) \ , \tag{18}$$

where the potential energy is given by

$$U(\sigma_1,\sigma_2,\sigma_3) = \frac{1}{2}\Big[\sum_{i=1}^{3}(\frac{1}{2}\omega_i^2\sigma_i^2 + \frac{1}{2\sigma_i^2}) + \frac{\tilde{g}}{\sigma_1\sigma_2\sigma_3}\Big] \; . \tag{19}$$

We use the previous equations to calculate the ground-state energy and the low-energy excitations of the condensate.

The ground-state energy per particle of the Bose condensate is simply $E^{(0)}/N = U(\vec{\sigma}^*)$, where $\vec{\sigma}^* = (\sigma_1^*, \sigma_2^*, \sigma_3^*)$ is the the minimum of the effective potential energy U. This equilibrium point is identified by the following equations:

$$\omega_1^2\sigma_1^4 - \tilde{g}\frac{\sigma_1}{\sigma_2\sigma_3} = 1 \; , \quad \omega_2^2\sigma_2^4 - \tilde{g}\frac{\sigma_2}{\sigma_1\sigma_3} = 1 \; , \quad \omega_3^2\sigma_3^4 - \tilde{g}\frac{\sigma_3}{\sigma_1\sigma_2} = 1 \; . \tag{20}$$

The low-energy collective excitations of the condensate are the small oscillations of variables σ_i's around the equilibrium point. The calculation of the normal mode frequencies for the motion of the condensate is reduced to an eigenvalue problem for the Hessian matrix Λ, given by

$$\Lambda_{ij} = \frac{\partial^2 U}{\partial\sigma_i\partial\sigma_j}\Big|_{\vec{\sigma}=\vec{\sigma}^*} \; . \tag{21}$$

In the case $\tilde{g}=0$, the stationary solution is simply $\sigma_i^* = \omega_i^{1/2}$ $(i=1,2,3)$ and the energy per particle of the non-interacting condensate is given by $E^{(0)}/N = (\omega_1+\omega_2+\omega_3)/2$. The Hessian matrix Λ of the potential energy U is diagonal and the frequency modes are simply $\Omega_i = 2\omega_i$ $(i=1,2,3)$.

The general solution for stationary state and eigenvalue problem of the collective mode frequencies can be obtained numerically,[17] but analytical results are available in the Thomas-Fermi limit. In such limit, i.e. when $\tilde{g} \gg 1$, the right-hand side in the equations of the equilibrium point, related to the kinetic pressure, can be neglected and the following expression for the equilibrium point is obtained

$$\sigma_1^* = \Big(\frac{\tilde{g}\;\omega_2\;\omega_3}{\omega_1^4}\Big)^{1/5} \; , \quad \sigma_2^* = \Big(\frac{\tilde{g}\;\omega_1\;\omega_3}{\omega_2^4}\Big)^{1/5} \; , \quad \sigma_3^* = \Big(\frac{\tilde{g}\;\omega_1\;\omega_2}{\omega_3^4}\Big)^{1/5} \; . \tag{22}$$

The energy per particle of the ground-state results

$$\frac{E^{(0)}}{N} = \frac{5}{4}\Big(\tilde{g}\;\omega_1\;\omega_2\;\omega_3\Big)^{2/5} \; , \tag{23}$$

and the Hessian matrix Λ is given by

$$\Lambda = \begin{pmatrix} 3 \;\; \omega_1^2 \\ \omega_1 \omega_2 \\ \omega_1 \omega_3 \\ \omega_1 \omega_2 \\ 3 \;\; \omega_2^2 \\ \omega_2 \omega_3 \\ \omega_1 \omega_3 \\ \omega_2 \omega_3 \\ 3 \;\; \omega_3^2 \end{pmatrix} . \tag{24}$$

Note that $\tilde{g}$ does not appear in the matrix. The eigenfrequencies Ω of the collective motion are found as the solutions of the equation[14]

$$\Omega^6 - 3 \left(\omega_1^2 + \omega_2^2 + \omega_3^2 \right) \Omega^4 + 8 \left(\omega_1^2 \, \omega_2^2 + \omega_1^2 \, \omega_3^2 + \omega_2^2 \, \omega_3^2 \right) \Omega^2 - 20 \, \omega_1^2 \, \omega_2^2 \, \omega_3^2 = 0 \; . \tag{25}$$

This equation has been also obtained by Stringari[4] using a hydrodynamical approach, which is effective in the Thomas-Fermi limit.

For an axially symmetric trap, where $\omega_1 = \omega_2 = \omega_\perp \neq \omega_3$, the previous equations give $\sigma_1^* = \sigma_2^* = (\tilde{g}\omega_3/\omega_\perp^3)^{1/5}$, $\sigma_3^* = (\tilde{g}\omega_\perp/\omega_3^3)^{1/5}$, $E^{(0)}/N = (5/4)\tilde{g}^{2/5}\omega_\perp^{4/5}\omega_3^{2/5}$, and

$$\Omega_{1,2} = \sqrt{2\omega_\perp^2 + \frac{3}{2}\omega_3^2 \pm \frac{1}{2}\sqrt{16\omega_\perp^4 + 9\omega_3^4 - 16\omega_\perp^2\omega_3^2}} \; , \quad \Omega_3 = \sqrt{2} \, \omega_\perp \; . \tag{26}$$

Because of the axial symmetry of the trap, the angular momentum along the z axis is conserved and one can thus label the modes by angular (l) and azimuthal (m_z) quantum numbers. One finds[4,11] $m_z = 0$ for the coupled monopole $(l = 0)$ and quadrupole $(l = 2)$ modes $\Omega_{1,2}$, and $|m_z| = 2$ for the quadrupole $(l = 2)$ mode Ω_3. Note that the experimental results obtained on sodium vapors at MIT are in excellent agreement with these theoretical values.[18]

For an isotropic harmonic trap with frequency ω, we obtain $\sigma_i^* = (\tilde{g}/\omega^2)^{1/5}$ $(i = 1, 2, 3)$, $E^{(0)}/N = (5/4)\tilde{g}^{2/5}\omega^{6/5}$, and $\Omega_{1,2} = \sqrt{5} \, \omega$, $\Omega_3 = \sqrt{2} \, \omega$. Here, differently from the axially symmetric case, the frequencies do not depend on m_z. In particular, $\sqrt{5}\omega$ is the monopole oscillation, also called breathing mode, characterized by radial quantum number $n_r = 1$ and angular quantum number $l = 0$. Instead $\sqrt{2}\omega$ is the quadrupole ($l = 2$) surface ($n_r = 0$) oscillation.

It is worth noting that the variational formalism makes it possible to investigate the case of negative scattering length. In this case, the large N limit of the Thomas-Fermi approximation does not apply because the condensate number cannot exceed a critical value. Let us consider again the isotropic trap with frequency ω. For the ground-state, the number of particles satisfies the following equation

$$N = 1 + \frac{1}{g}(\omega^2 \sigma_0^5 - \sigma_0) \ , \tag{27}$$

where $\sigma_0 = \sigma_i^*$ $(i = 1, 2, 3)$ is mean radius of the condensate, that is the same in the three axial directions. It follows that, for $g > 0$, with $N = 1$ we have $\sigma_0 = 1$ and with $N \to \infty$ then $\sigma_0 \to \infty$. Instead, for $g < 0$, the mean radius σ_0 decreases by increasing the number of bosons N to a critical radius $\sigma_0^c = (5\omega^2)^{-1/4}$ with a critical number of bosons given by $N^c = 1 + |g|^{-1}\omega^{-1/2}(5^{-1/4} - 5^{-5/4})$. Moreover, one finds a simple expression for the monopole ($l = 0$) frequency of surface oscillation of the condensate, namely[16]

$$\Omega = \left[5\omega^2 - \sigma_0^{-4} \right]^{1/2} . \tag{28}$$

We have seen that $\sigma_0 = 1$ for $N = 1$ or $g = 0$. Moreover, when $N > 1$, it is $\sigma_0 > 0$ for $g > 0$ and $\sigma_0^c < \sigma < 1$ for $g < 0$. Regarding the frequency Ω, one easily verifies that $\Omega \to \sqrt{5}\omega$ for $\sigma_0 \to \infty$ and $\Omega \to 0$ for $\sigma_0 \to \sigma_0^c$. Note that, for the triaxial trap, at the critical point the two highest frequencies diverge and the lowest one falls to zero.[17]

It is important to observe that it is possible to include in the Gaussian trial wave-function other three parameters describing the position of the center of mass of the condensate. Due to the harmonic confinement, the motion of the center of mass (dipole mode) is periodic and the frequencies of oscillation are equal to those of the harmonic trap.[11,12]

V. TRIAL WAVE-FUNCTION OF VORTEX STATES

Let us consider states having a vortex line along the z axis and all bosons flowing around it with quantized circulation. The observation of these states would be a signature of macroscopic phase coherence of trapped BEC. The time-dependent variational approach can be used to describe also these vortex states of the condensate in a axially symmetric trap

$$V_0(\mathbf{r}) = \frac{1}{2}\left(\omega_\perp^2 r^2 + \omega_3^2 z^2\right) , \tag{29}$$

where $r = \sqrt{x^2+y^2}$, $\theta =$arctg(y/x) and z are the cylindrical coordinates.

The trial wave function of the vortex states of the condensate can be chosen as

$$\phi_k\left(\mathbf{r},t\right) = \Big[\frac{1}{k!\pi^3 {\sigma_\perp}^{4k+4}(t)\sigma_3^2(t)}\Big]^{1/4} r^k e^{ik\theta} \exp\left\{-\frac{r^2}{2\sigma_\perp^2(t)} - \frac{z^2}{2\sigma_3^2(t)} + i\beta_\perp(t) r^2 + i\beta_3(t) z^2\right\} , \tag{30}$$

where k is the vortex quantum number and $\sigma_\perp$, σ_3, $\beta_\perp$ and β_3 are the time-dependent variational parameters. This trial wave-function describes exactly the vortex states of a non-interacting gas of bosons in the harmonic trap.

By following the same procedure of the previous section, namely by inserting the trial wave-function in the GP action, and after spatial integration, one gets

$$S_{GP} = N\int dt \; L(\dot\beta_\perp, \dot\beta_3, \beta_\perp, \beta_3, \sigma_\perp, \sigma_3) , \tag{31}$$

where the effective Lagrangian is given by

$$L = -\frac{1}{2}\Big[(k+1)(\dot\beta_\perp\sigma_\perp^2 + \frac{1}{2\sigma_\perp^2} + 2\sigma_\perp^2\beta^2 + \frac{1}{2}\omega_\perp^2\sigma^2) +$$

$$+(\dot\beta_3\sigma_3^2 + \frac{1}{2\sigma_3^2} + 2\sigma_3^2\beta_3^2 + \frac{1}{2}\omega_3^2\sigma_3^2) + \frac{\tilde g(k)}{\sigma_\perp^2\sigma_3}\Big] , \tag{32}$$

with $g = (2/\pi)^{1/2}(a_s/a_0)$ and $\tilde g(k) = g(N-1)(2k)!/(2^{2k}k!^2)$. The four Euler-Lagrange equations of the system are given by

$$\beta_\perp = -\frac{\dot\sigma_\perp}{2\sigma_\perp} , \qquad \beta_3 = -\frac{\dot\sigma_3}{2\sigma_3} , \tag{33}$$

$$(k+1)\ddot{\sigma}_\perp + (k+1)\omega_\perp^2 \sigma_\perp = \frac{(k+1)}{\sigma_\perp^3} + \frac{\tilde{g}(k)}{\sigma_\perp^3 \sigma_3} \; , \qquad \ddot{\sigma}_3 + \omega_3^2 \sigma_3 = \frac{1}{\sigma_3^3} + \frac{\tilde{g}(k)}{\sigma_\perp^2 \sigma_3^2} \; . \tag{34}$$

The time dependence of $\beta_\perp$ and β_3 is fully determined by that of $\sigma_\perp$ and σ_3; moreover, for $\tilde{g} = 0$ (non-interacting condensed vortex) these four equations are exact. The last two differential equations correspond to the classical equations of motion of a system with energy per particle

$$\frac{E_k}{N} = \frac{1}{2}\Big[(k+1)\dot{\sigma}_\perp^2 + \frac{1}{2}\dot{\sigma}_3^3\Big] + U(\sigma_\perp, \sigma_3) \; , \tag{35}$$

where the potential energy is given by

$$U(\sigma_\perp, \sigma_3) = \frac{1}{2}\Big[(k+1)\omega_\perp^2 \sigma_\perp^2 + \frac{1}{2}\omega_3^2 \sigma_3^2 + \frac{(k+1)}{\sigma_\perp^2} + \frac{1}{2\sigma_3^2} + \frac{\tilde{g}(k)}{\sigma_\perp^2 \sigma_3}\Big] \; . \tag{36}$$

The equilibrium point $(\sigma_\perp^*, \sigma_3^*)$, corresponding to the minimum of the effective potential energy, is given by the following equations:

$$(k+1)\omega_\perp^2 \sigma_\perp^4 - \tilde{g}(k)\frac{1}{\sigma_3} = (k+1) \; , \qquad \omega_3^2 \sigma_3^4 - \tilde{g}(k)\frac{\sigma_3}{\sigma_\perp^2} = 1 \; . \tag{37}$$

In the non-interacting case ($\tilde{g} = 0$) the stationary solution is simply $\sigma_\perp^* = \omega_\perp^{1/2}$ and $\sigma_3^* = \omega_3^{1/2}$. The stationary energy of the non-interacting vortex state is exactly given by

$$\frac{E_k^{(0)}}{N} = (k+1)\omega_\perp + \frac{1}{2}\omega_3 \; . \tag{38}$$

It is important to observe that the energy grows only linearly with the vortex quantum number k, in contrast to the homogenous case[7] where the vortex energy grows as k^2. In addition, the two ($m_z = 0$) frequency modes are $\Omega_1 = 2\omega_\perp$ and $\Omega_2 = 2\omega_3$ and do not depend on the vortex quantum number k.

In the Thomas-Fermi limit ($\tilde{g} >> 1$), the analytic expression of the equilibrium point reads

$$\sigma_\perp^* = \left[\frac{\tilde{g}(k)\;\omega_3}{(k+1)^{3/2}\omega_\perp^3}\right]^{1/5} \; , \qquad \sigma_3^* = \left[\frac{\tilde{g}(k)\;(k+1)\;\omega_\perp^2}{\omega_3^4}\right]^{1/5} \; . \tag{39}$$

The stationary energy of the vortex state results

$$\frac{E_k^{(0)}}{N} = \frac{5}{4}\Big((k+1)\,\tilde{g}(k)\,\omega_\perp^2\,\omega_3\Big)^{2/5} \; . \tag{40}$$

¿From this formula it is easy to calculate the critical frequency $\bar{\Omega}_c$ at which a vortex can be produced. One has to compare the energy of a vortex state in frame rotating with angular frequency $\bar{\Omega}$, that is $E_k^{(0)} - \bar{\Omega} L_z$, with the energy E^0 of the ground state (with no vortices).[7] Since the angular momentum per particle is $\hbar k$, the critical frequency is given by $\hbar\bar{\Omega}_c = (E_k^{(0)}/N - E^{(0)}/N)/k$. By using our previous formula, we get

$$\bar{\Omega}_c = \frac{5}{4} k^{-1} \omega_\perp^{4/5} \omega_3^{2/5} \Big[\tilde{g}(k)^{2/5}(k+1)^{2/5} - \tilde{g}(0)^{2/5}\Big] \; . \tag{41}$$

In the presence of a vortex, for frequencies smaller than the critical frequency $\bar{\Omega}_c$, the system is not thermodynamically stable (global stability), but can be locally stable (metastability) against small deformations of the system. Rohksar[19] has shown that the vortex state is locally unstable for $\bar{\Omega} = 0$. Actually, in a harmonic trap, there is local instability for $0 \leq \bar{\Omega} < \bar{\Omega}_s$, where the frequency $\bar{\Omega}_s$ ($\bar{\Omega}_s < \bar{\Omega}_c$) can be estimated numerically.[20] On the other hand, we have recently shown that, in toroidal traps, vortices can be locally stable also in absence of external forced rotation.[21]

It is important to observe that, in our present treatment, the condensate has a unique vortex line, which is fixed along the z axis. Butts and Rokhsar[22] have numerically shown that increasing the rotational frequency $\bar{\Omega}$ well beyond $\bar{\Omega}_c$ will favour the creation of more complex vortical configurations, associated with the occurrence of 2 or more vortex lines.

To calculate the collective oscillations in the Thomas-Fermi limit, we follow the same procedure of the previous section. The Hessian matrix Λ of the potential energy U at the equilibrium point is given by

$$\Lambda = \begin{pmatrix} 8 \quad (k \; + \; 1) \quad \omega_\perp^2 \\ 2\,(k+1)^{1/2}\,\omega_\perp\,\omega_3 \\ 2\,(k+1)^{1/2}\,\omega_\perp\,\omega_3 \\ 3 \qquad\qquad\quad \omega_3^2 \end{pmatrix} \; . \tag{42}$$

Again the $\tilde{g}(k)$ dependence drops out. Moreover, the mass matrix of the kinetic energy is not the identity matrix but instead

$$M = \begin{pmatrix} 2 & (k+1) \\ 0 & \\ 0 & \\ 1 & \end{pmatrix} . \tag{43}$$

The eigenfrequencies Ω of the collective motion are found as the solutions of the equation $|\Lambda - \Omega^2 M| = 0$, which gives the $m_z = 0$ frequencies

$$\Omega_{1,2} = \sqrt{2\omega_\perp^2 + \frac{3}{2}\omega_3^2 \pm \frac{1}{2}\sqrt{16\omega_\perp^4 + 9\omega_3^4 - 16\omega_\perp^2\omega_3^2}} . \tag{44}$$

This is an interesting result: The $m_z = 0$ frequencies of a harmonically trapped condensate do not depend on the vortex quantum number k. Note that Zambelli and Stringari[23] have shown, by using a sum-rule approach, that the $m_z \neq 0$ collective frequencies do instead depend on k. Nevertheless, all the modes are k sensitive because of the amplitudes, which are given by $< r^2 >^{1/2} = (k+1)^{1/2}\sigma_\perp$ and $< z^2 >^{1/2} = \sigma_3/\sqrt{2}$.

Finally, we study an isotropic trap with frequency ω. We have $\sigma_\perp^* = \sigma_3^*$ only for $\tilde{g} = 0$. In order to obtain some analytic results also in the case of negative scattering length, we consider the vortex trial wave-function with a unique variational parameter σ, i.e. we put $\sigma_\perp = \sigma_3 = \sigma$. For the ground-state, the number of particles satisfies the equation $N = 1 + g(k)^{-1}(\omega^2\sigma_0^5 - \sigma_0)(1 + 2/3k)$, where σ_0 is mean radius of the condensate in the stationary configuration and $g(k) = g(2k)!/(2^{2k}k!^2)$. It follows that for $g < 0$, the critical number of bosons for the collapse of the wave-function is given by $N^c = 1 + |g(k)|^{-1}\omega^{-1/2}(5^{-1/4} - 5^{-5/4})(1 + 2/3k)$. Thus, compared with the condensed state without vortices, the critical number of trapped atoms in the vortex state increases. This variational result is in full agreement with the $k = 1$ numerical results of Dalfovo and Stringari.[24]

VI. CONCLUSIONS

We have studied a Bose-Einstein condensate trapped in a harmonic potential by using a variational method based on the minimization of the Gross-Pitaevskii action with a Gaussian ansatz for the shape of the macroscopic wave function of the condensate. Our analysis has been applied to the whole range of coupling strengths between particles (attractive and repulsive interaction) to study both the ground-state and vortex states. In particular, for vortex states, we have determined the critical rotational frequency at which a single vortex becomes globally stable. Moreover, we have calculated the collective oscillations and the critical number of bosons for the collapse of the condensate in the case of attractive interaction. Nowadays it is experimentally possible to trap and condense a very large number of alkali atoms (more than 10^9) and to obtain a less diluite system. Thus, the study of the time-dependent variational approach without the independent-particle approximation begins to appear an interesting problem also for Bose gases in an external potential (the case of a superfluid film containing a vortex has been discussed in Ref. 9 and 10). This will be one of our future projects.

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