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# Variational approach for the two-dimensional trapped Bose Einstein condensate

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We construct a many-body Gaussian variational approach for the two-dimensional trapped Bose gas in the condensate phase. Interaction between particles is modeled by a generalized pseudo-potential of zero range that allows recovering perturbative results in the ultra-dilute limit, while back action of non-condensate particles on the condensate part is taken into account for higher density. As an application, we derive the equation of state and solve stability problems encountered in similar mean-field formalisms for a single vortex configuration.

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Both for fundamental reasons and for eventual future applications, ultra cold atomic gases trapped in reduced geometries has become a challenging field. Two-dimensional (2D) configurations are especially interesting for their various expected features including the interplay between the Bose Einstein and the Kosterlitz-Thouless transitions, the concept of tunable BEC [1] and in the rotating case the possible realization of a gas with fractional statistics [2]. A quasi-2D BEC has been produced using polarized hydrogen atoms adsorbed on a helium film [3], with clear evidence of the quasi-condensate phase. Several experimental groups [4, 5, 6, 7] are now interested in quasi-2D configurations using optical and magneto-optical traps which are expected to be more flexible for varying physical parameters such as the atomic density or the interaction strength. On the theoretical side, the general formalisms deeply differ from usual many body treatments in that they take into account both thermal phase fluctuations and the specific scattering properties [8, 9, 10, 11, 12, 13].

In this Letter we use the Gaussian variational approach of the many-body problem to study the condensate phase for the 2D BEC [14]. We show that describing interactions between atoms with the so-called  $\Lambda$ -potential [15] is a very simple way to construct a gapless and consistent theory. In 3D configurations, this formalism has been already developed [15] and allows to recover in a purely variational way the gapless HFB-G2 prescription [16]. In the 2D regime, this way of taking into account the back action of non-condensed particles on the condensate field has not been yet implemented and brings new features. The Letter is composed of three parts. In the first part, we describe the modelization of the system and recall some basics of the two-body problem in 2D using the zero range approximation. In the second part, we develop the Gaussian variational approach (called also Hartree Fock Bogolubov or HFB) for the 2D trapped Bose gas and show the links with the HFB-G2 scheme. In the last part we apply the formalism in two distinct situations. We first calculate the Equation Of State (EOS) at zero temperature in the homogeneous limit. This first result generalizes the known perturbative EOS. Finally, as a test of the formalism we study the thermodynamical

instability of a single vortex in a non rotating trap. We conclude that unlike unexpected results obtained in similar but non variational approaches [17], the system remains unstable at finite temperatures.

We consider  $N$  bosons of mass  $m$  in a very anisotropic trap characterized by a high axial frequency  $\omega_z$  and small longitudinal frequencies  $\omega_x = \omega_y = \omega_L \ll \omega_z$ . In the following, we suppose that the system is in a quasi two-dimensional geometry. This situation is achieved when the typical energy ( $\epsilon$ ) of a two body scattering process is sufficiently low as compared to the axial frequency  $|\epsilon| \ll \hbar\omega_z$ . In this regime, the system is somehow frozen along the tight direction in the ground state of the axial trapping potential and we can restrict our study to the longitudinal  $xy$ -plane. Before going into the approximate treatment of the many body problem, let us recall some basics of the two-body case in a planar trap ( $\omega_L = 0$ ). We note the spatial coordinates in the plane ( $\vec{r}_1, \vec{r}_2$ ), the relative and center of mass coordinates are respectively  $\vec{r} = \vec{r}_1 - \vec{r}_2$  and  $\vec{R} = \frac{\vec{r}_1 + \vec{r}_2}{2}$ . In the zero range approach, the two-body wave function  $\psi_2$  obeys the free Schrödinger equation for  $r \neq 0$ , while the interaction is taken into account by imposing the contact condition :

$$\psi_2(\vec{r}_1, \vec{r}_2) = A(\vec{R}) \ln\left(\frac{r}{a_{2D}}\right) \quad \text{for } r \rightarrow 0 \quad , \quad (1)$$

where  $a_{2D}$  (the “2D scattering length”) is obtained from the usual scattering length  $a_{3D}$  and from the characteristic length of the trap  $a_z$  using the relation [8]:

$$a_{2D} = 2.092 a_z \exp\left(-\sqrt{\frac{\pi}{2}} \frac{a_z}{a_{3D}}\right). \quad (2)$$

Note that the short range part of the wave function is not described by relation (1) [8] which gives only the correct asymptotic behavior for  $r \gg a_z$ . However, the zero range approach is justified when the mean inter-particle distance is much larger than the axial width  $a_z = \sqrt{\frac{\hbar}{m\omega_z}}$ . In term of the 2D atomic density  $n$ , this gives  $na_z^2 \ll 1$ . Another and equivalent way to implement the zero-range approach is to solve the Schrödinger equation

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using the  $\Lambda$ -potential [15] defined by:

$$\langle \vec{R}, \vec{r} | V^\Lambda | \psi_2 \rangle = g_\Lambda \delta^{(2)}(\vec{r}) \mathcal{R}_\Lambda \left[ \psi_2(\vec{R} - \frac{\vec{r}}{2}, \vec{R} + \frac{\vec{r}}{2}) \right]. \quad (3)$$

In this potential,  $g_\Lambda$  is the two-body T-matrix evaluated at energy  $-\hbar^2 \Lambda^2 / m$ :

$$g_\Lambda = -\frac{2\pi\hbar^2}{m} \frac{1}{\ln(q\Lambda a_{2D})}, \quad (4)$$

where  $q = e^\gamma/2$ ,  $\gamma$  is the Euler's constant and  $\mathcal{R}_\Lambda$  is a regularizing operator:

$$\mathcal{R}_\Lambda = \lim_{r \rightarrow 0} \{1 - \ln(q\Lambda r) r \partial_r\}. \quad (5)$$

By construction, the observables are independent of the parameter  $\Lambda$  which can be considered as a free field of the exact theory, function of the center of mass coordinates  $\vec{R}$  [15]. However, we recall that some approximate treatments are  $\Lambda$ -dependent. In this type of formalism,  $\Lambda$  appears as a new degree of freedom which is a way of improving the results. Taking for example the first order Born approximation in the two-body case, one can easily check that the exact scattering amplitude at energy  $\epsilon$  is obtained using an uniform  $\Lambda = -i\sqrt{m\epsilon}/\hbar$ . In this case,  $\Lambda$  is directly linked to the energy of the scattering process and has a straightforward physical meaning.

Now, we implement the variational Gaussian approach in the case of a 2D condensate in the external potential  $V_{\text{ext}} = m\omega_L^2 R^2/2$  [18] using the  $\Lambda$ -potential (3). In Ref.[15], it has been already shown that this type of approximation is  $\Lambda$ -dependent. We explain in the following the criterion we use for a systematic determination of the field  $\Lambda(\vec{R})$ . In order to simplify the discussion, we break the  $U(1)$  symmetry by splitting the atomic field  $\hat{\psi}$  into a classical field  $\Phi$  and a quantum fluctuation  $\hat{\phi} = \hat{\psi} - \Phi$  [19]. The HFB scheme consists in choosing as a trial density operator the exponential of the most general quadratic form of the fields  $\{\hat{\phi}, \hat{\phi}^\dagger\}$ . Diagonalization of the quadratic form is obtained using a Bogolubov transformation:

$$\hat{\phi}(\vec{R}) = \sum_n \left\{ \hat{b}_n u_n(\vec{R}) + \hat{b}_n^\dagger v_n^*(\vec{R}) \right\}, \quad (6)$$

where  $\{\hat{b}_n, \hat{b}_n^\dagger\}$  are the usual creation and annihilation bosonic operators for a quasi-particle of quantum number  $n$ , while the amplitudes  $\{u_n, v_n\}$  verify the modal equations:

$$\begin{aligned} \left[ -\frac{\hbar^2}{2m} \Delta + V_{\text{ext}} + \hbar\Sigma_{11} - \mu \right] u_n + \hbar\Sigma_{12} v_n &= \hbar\omega_n u_n \\ \left[ -\frac{\hbar^2}{2m} \Delta + V_{\text{ext}} + \hbar\Sigma_{11}^* - \mu \right] v_n + \hbar\Sigma_{12}^* u_n &= -\hbar\omega_n v_n. \end{aligned} \quad (7)$$

From the variational principle [14] we deduce the self-energies:

$$\hbar\Sigma_{11}(\vec{R}) = 2g_\Lambda \langle \hat{\psi}^\dagger(\vec{R}) \hat{\psi}(\vec{R}) \rangle \quad (8)$$

$$\hbar\Sigma_{12}(\vec{R}) = g_\Lambda \mathcal{R}_\Lambda \left[ \langle \hat{\psi}(\vec{R} - \frac{\vec{r}}{2}) \hat{\psi}(\vec{R} + \frac{\vec{r}}{2}) \rangle \right], \quad (9)$$

and also a generalized Gross-Pitaevskii equation for the classical field

$$\left[ -\frac{\hbar^2}{2m} \Delta + V_{\text{ext}} + 2g_\Lambda \tilde{n} - \mu \right] \Phi + \hbar\Sigma_{12} \Phi^* = 0, \quad (10)$$

where  $\tilde{n}$  is the non-condensed density. Let us insist on the fact that the modal equations (7) do not coincide with the ones appearing in the linearized time-dependent treatment (the so-called RPA formalism; see for example Ref.[14]). As a consequence, while the condensate mode associated to a phase change in the condensate wave function is a solution of the time dependent equations with a zero eigen-frequency, it is not in general solution of Eqs.(7). In the homogeneous case, this leads to the presence of a gap in the spectrum defined through Eqs.(7), and in the inhomogeneous case, to the presence of an unphysical mode of non-zero eigen-frequency. Unfortunately, the existence of a spurious energy scale introduced by this mode prevents from a consistent description of the thermodynamical properties of the system. We show in the following that this problem can be solved without modifying the equations deduced from the variational principle. For that purpose, we recall that Eq.(8) corresponds to a first order Born approximation so that unlike an exact approach, HFB is explicitly  $\Lambda$ -dependent. The key point is then to choose a specific realization of the field  $\Lambda$ , noted in the following  $\Lambda^*$ , such that the condensate mode:

$$u_0(\vec{R}) = \Phi(\vec{R}) \quad ; \quad v_0(\vec{R}) = -\Phi^*(\vec{R}), \quad (11)$$

solution of the time dependent equations, is also solution of Eqs.(7) with a zero frequency. This requirement leads to the condition  $\hbar\Sigma_{12} = g_\Lambda \Phi^2$  [21], so that at each point  $\vec{R}$  in the condensate,  $\Lambda^*(\vec{R})$  is an implicit solution of the equation [23]:

$$\mathcal{R}_\Lambda \left[ \langle \hat{\phi}(\vec{R} - \frac{\vec{r}}{2}) \hat{\phi}(\vec{R} + \frac{\vec{r}}{2}) \rangle \right] = 0. \quad (12)$$

In the limit  $a_{3D} \ll a_z$  where interatomic collisions are weakly modified by the transverse confinement, Eq.(12) leads at finite temperature to the HFB-G2 prescription [16] introduced in the 3D configuration:

$$g_{\Lambda^*}(T) \simeq \frac{4\pi\hbar^2 a_{3D}}{m a_z \sqrt{2\pi}} \left( 1 + \frac{\tilde{\kappa}_T}{\Phi^2} \right), \quad (13)$$

where  $\tilde{\kappa}_T(\vec{R}) = \sum_n 2g_n u_n(\vec{R}) v_n^*(\vec{R})$  is the thermal contribution of the pairing field and  $g_n$  is the usual Bose occupation factor for the mode of energy  $\hbar\omega_n$ .

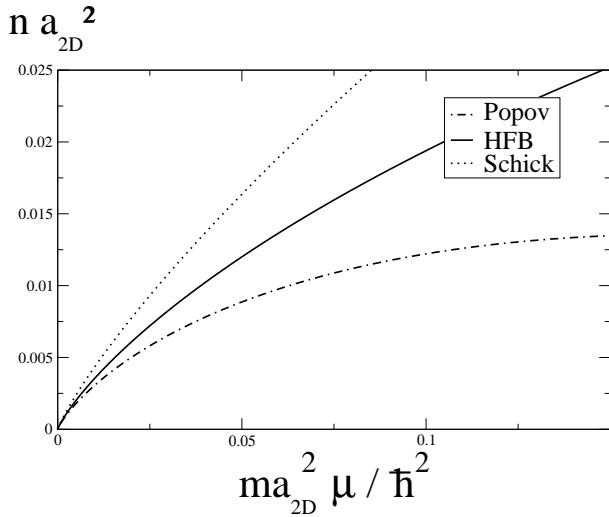


FIG. 1: Equation Of State of the 2D homogeneous Bose gas. Dotted line: EOS deduced from Schick's formula  $\mu = 4\pi\hbar^2 n / (m \ln(na_{2D}^2))$  [24]. Full line: full variational approach (HFB). Dashed dotted line: Perturbative EOS [9, 13].

As a first application, we consider the homogeneous medium at zero temperature. From Eqs.(7,10,12), we deduce a standard Bogolubov spectrum and a self-consistent equation for  $\Lambda^*$ :

$$\frac{\hbar^2 \Lambda^{*2}}{m} = g_{\Lambda^*} |\Phi|^2, \quad (14)$$

giving directly the energy at which the T-matrix has to be evaluated for having a gapless spectrum. From  $\mu =$

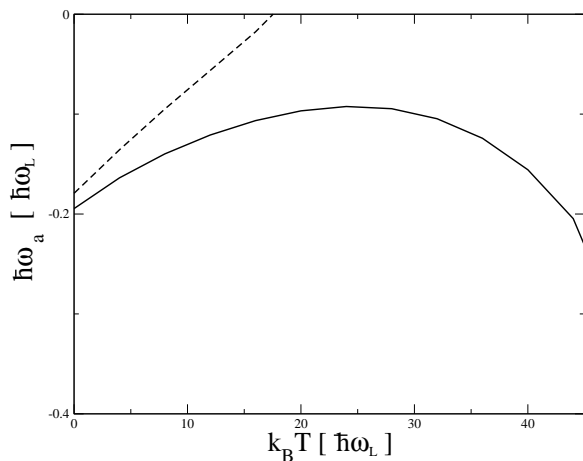


FIG. 2: Typical evolution of the anomalous mode energy of a single vortex in a non rotating trap as a function of the temperature. The presence of a negative energy mode in the spectrum leads to the so-called thermodynamical instability of the single vortex [26]. Dashed line: the coupling constant used in the gapless equations is arbitrarily evaluated using the two-body T-matrix at energy  $-2\mu_{oc}$ . Full line: full variational scheme; at finite temperature, the anomalous mode energy is not stabilized.

$g_{\Lambda^*} (|\Phi|^2 + 2\bar{n})$  and (14) we deduce the EOS shown in Fig.(1). In the ultra-dilute limit  $na_{2D}^2 \ll 1$ , we recover the exact perturbative result [9, 13]:

$$n = \frac{m\mu}{4\pi\hbar^2} \ln \left( \frac{4\hbar^2}{e^{(2\gamma+1)} m \mu a_{2D}^2} \right). \quad (15)$$

For increasing values of the 2D atomic density, the predicted EOS deviates from Eq.(15) (for a value of the 2D gas parameter greater than  $3 \cdot 10^{-5}$ , the relative difference between the two EOS is more than 5%). Note that similarly to the 3D situation, there is an upper bound for the values of the density that can be studied [15], here at  $T = 0$ ,  $n < n_{crit} = \exp(-2\gamma) / \pi a_{2D}^2$ . At  $n = n_{crit}$ ,  $\mu \rightarrow \infty$  and  $\Phi \rightarrow 0$ , this gives a fundamental limit of applicability of the present formalism. In 2D traps, we have checked that at zero temperature, for static configurations, the full variational approach gives the same results as the LDA. In situations where the density varies rapidly, for example in presence of vortices, or also at finite temperature not only Eqs.(7,10) but also Eq.(12) have to be solved numerically. We consider then as a last example, the case of a single vortex in a non rotating trap at finite temperature [25]. This configuration is especially interesting as a test of the present formalism. Indeed, a previous self-consistent but not variational approach [17] has led to the conclusion that a vortex which is thermodynamically unstable at vanishing temperatures, could be stabilized at finite temperature. We recall that this instability is due to the existence of a core localized state having a negative energy ( $\hbar\omega_a$ ) when the trap rotation frequency is zero [26]. In 3D rotating BEC experiments, this type of instability which causes the spiraling of the vortex core out of the condensate has been observed [27], and we expect a similar behavior in 2D. We then consider an off-equilibrium situation where the trap is at rest and

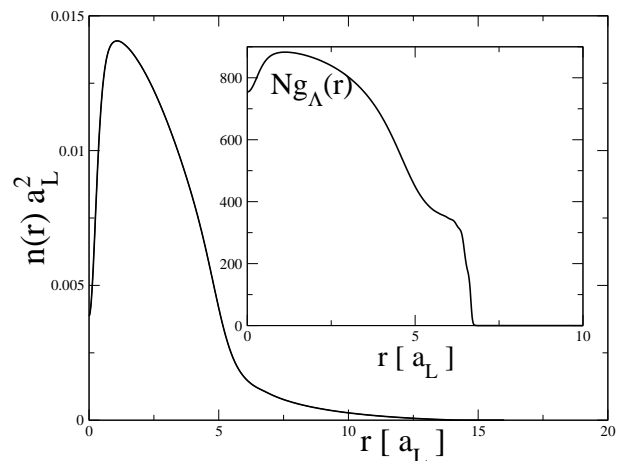


FIG. 3: Typical density profile of a single vortex at finite temperature ( $k_B T = 20\hbar\omega_L$ ), obtained using the full variational approach when the anomalous mode is not thermalized. Inset: mean-field coupling constant in harmonic oscillator units, obtained by solving Eq.(12).

all the modes except the anomalous core localized state are thermalized. In a first step, we have checked that accordingly to Ref.[17], stabilization occurs when the coupling constant  $g_\Lambda$  is arbitrarily set to a constant value in the “gapless” HFB equations. In a second step, we have used a more realistic prescription by assuming that the T-matrix entering the “gapless” equations is taken at energy  $-\hbar^2\Lambda^2/m = -2\mu_{\text{loc}}$  ( $\mu_{\text{loc}}$  is the local chemical potential). As shown in Fig.2, this non-variational approach predicts also an unphysical stabilization at sufficiently high temperature. On the contrary, using the full variational scheme where Eq.(12) is solved numerically, the anomalous mode is never stabilized (see Fig.2). In Fig.(3), we show a typical density profile and the associated mean-field coupling constant  $g_{\Lambda^*}$  obtained at finite temperature as a function of the distance from the core (we have used the notation  $a_L = \sqrt{\hbar/m\omega_L}$ ). As explained in Ref.[17], the unexpected stabilization in the non-variational approach is linked to the mean-field term  $g_{\Lambda^*}\tilde{n}$  in Eq.(10) which acts as a pinning potential. In the formalism presented here, the low energy modes

which have a very different structure with respect to the homogeneous case, crucially determine the behavior of the coupling constant  $g_{\Lambda^*}$  through Eq.(12). As a consequence, the homogeneous result Eq.(14) cannot be applied: the lowest modes which become widely occupied with increasing temperatures, shape the structure of  $g_{\Lambda^*}$ . For example in Fig.(3), the coupling constant dives at the origin (recall that the structure at the vicinity of the core plays a central role in the pinning process) and presents a buttress at the edge of the condensate due to the population of the surface modes.

In conclusion, we have presented an approach for the 2D trapped BEC which takes into account the back action of the non-condensed fraction on the condensate field at finite temperature. This formalism includes known results on the 2D BEC and solves stability problems encountered in similar but non variational approaches.

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