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Variational approach for the two-dimensional trapped Bose Einstein condensate

Ludovic Pricoupenko

*Laboratoire de Physique Théorique des Liquides, Université Pierre
et Marie Curie, 4 place Jussieu, 75252 Paris Cedex 05, France.*

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We present a formalism which takes into account the back action of the non-condensed fraction on the condensate field in a two-dimensional trapped Bose Einstein condensate. For this purpose, we use the many-body variational gaussian approach while interactions are described using a generalized pseudo-potential. By this way, we predict a non trivial equation of state beyond the ultra-dilute limit and solve stability problems encountered in similar but non-variational formalisms for a single vortex configuration at finite temperature.

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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 well known gaussian variational approach in 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 Λ -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 scheme [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 modelisation 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 Bogoliubov or HFB in the literature) 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 temperature.

We consider N bosons of mass m in a very anisotropic trap characterized by a high axial frequency ω_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 (ϵ) 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 ψ_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} is the 2D scattering length. This quantity 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 (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 , we must have :

$$na_z^2 \ll 1 \quad . \quad (3)$$

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Another and equivalent way to implement the zero-range approach is to solve the Schrödinger equation using the Λ -potential [15] defined by:

$$\langle \vec{R}, \vec{r} | V^\Lambda | \psi_2 \rangle = g_\Lambda \delta^{(2)}(\vec{r}) \mathcal{R}_\Lambda \left[\psi_2(\vec{R} - \frac{\vec{r}}{2}, \vec{R} + \frac{\vec{r}}{2}) \right]. \quad (4)$$

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

$$g_\Lambda = -\frac{2\pi\hbar^2}{m} \frac{1}{\ln(q\Lambda a_{2D})}, \quad (5)$$

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

$$\mathcal{R}_\Lambda = \lim_{r \rightarrow 0} \{1 - \ln(q\Lambda r) r \partial_r\}. \quad (6)$$

By construction, the observables are independent of the parameter Λ 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 Λ -dependent. In this type of formalism, Λ appears as a new degree of freedom which is a way of improving the results. Taking for example the Born approximation in the two-body case, one can easily check that the exact scattering amplitude at energy ϵ is obtained using an uniform $\Lambda = -i\sqrt{m\epsilon}/\hbar$. In this case, Λ 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 [18] using the Λ -potential (4). In Ref.[15], it has been already shown that this type of approximation is Λ -dependent. We explain in the following the criterium 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 Φ and a quantum fluctuation $\hat{\phi} = \hat{\psi} - \Phi$. The HFB scheme consists in choosing as a trial density operator the exponential of the most general quadratic form of the fields $\{\hat{\phi}, \hat{\phi}^\dagger\}$. For practical implementation of the formalism, we diagonalize the trial quadratic form by performing a special Bogolubov transformation

$$\hat{\phi}(\vec{R}) = \sum_n \left\{ \hat{b}_n u_n(\vec{R}) + \hat{b}_n^\dagger v_n^*(\vec{R}) \right\}. \quad (7)$$

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

$$\begin{aligned} \left[-\frac{\hbar^2}{2m} \Delta + V_{\text{ext}} + \hbar\Sigma_{11} - \mu \right] u_n + \hbar\Sigma_{12} v_n &= \hbar\omega_n u_n \\ \left[-\frac{\hbar^2}{2m} \Delta + V_{\text{ext}} + \hbar\Sigma_{11}^* - \mu \right] v_n + \hbar\Sigma_{12}^* u_n &= -\hbar\omega_n v_n, \end{aligned} \quad (8)$$

where the external potential is $V_{\text{ext}} = m\omega_L^2 R^2/2$. From the variational principle [14], we deduce the self-energies

$$\hbar\Sigma_{11}(\vec{R}) = 2g_\Lambda \langle \hat{\psi}^\dagger(\vec{R}) \hat{\psi}(\vec{R}) \rangle \quad (9)$$

$$\hbar\Sigma_{12}(\vec{R}) = g_\Lambda \mathcal{R}_\Lambda \left[\langle \hat{\psi}(\vec{R} - \frac{\vec{r}}{2}) \hat{\psi}(\vec{R} + \frac{\vec{r}}{2}) \rangle \right], \quad (10)$$

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

$$\left[-\frac{\hbar^2}{2m} \Delta + V_{\text{ext}} + 2g_\Lambda \tilde{n} - \mu \right] \Phi + \hbar\Sigma_{12} \Phi^* = 0, \quad (11)$$

where \tilde{n} is the non-condensed density. In Eq.(10), the Λ -potential fully applies on the pairing field explaining why the formalism is free of Ultra Violet divergencies [15]. Eqs.(8) are often interpreted as the analog of the Bogolubov-De Gennes equations obtained in the perturbative approach. However, strictly speaking, the associated eigen-energies $\hbar\omega_n$ do not coincide with the ones appearing in the linearized time-dependent treatment (the so-called RPA formalism). This explains quite generally, why the spurious mode associated to a phase change in the condensate wave function is a solution of the time dependent equations but not of the static equations (8). In the homogeneous case, this leads to the presence of a gap in the "static spectrum", and more generally, to the presence of an unphysical mode of non-zero energy. This well known problem prevented to apply the full variational scheme for many years [19]. Indeed, the spurious energy scale in the "static spectrum" is not compatible with a consistent description of thermodynamical properties. In other words, the eigen-frequencies calculated in the RPA formalism have to be small corrections with respect to the "static spectrum". As we will see now, the Λ -freedom offers the opportunity to solve this problem. For that purpose, we recall that Eq.(9) corresponds to a first order Born approximation so that unlike an exact approach, HFB is explicitly Λ -dependent. The key point is then to choose a specific realization of the field Λ noted in the following Λ^* such that the condensate mode

$$u_0(\vec{R}) = \Phi(\vec{R}) \quad ; \quad v_0(\vec{R}) = -\Phi^*(\vec{R}), \quad (12)$$

is a solution of Eqs.(8). This requirement which renders the static and dynamic formalisms consistent, leads to the condition $\hbar\Sigma_{12} = g_\Lambda \Phi^2$ [20, 21], so that at each point \vec{R} in the condensate, $\Lambda^*(\vec{R})$ is an implicit solution of the equation:

$$\mathcal{R}_{\Lambda^*} \left[\langle \hat{\phi}(\vec{R} - \frac{\vec{r}}{2}) \hat{\phi}(\vec{R} + \frac{\vec{r}}{2}) \rangle \right] = 0. \quad (13)$$

In this way, Eqs.(8,11) are very similar to the one obtained in Refs.[11, 12] where a treatment of phase fluctuations not taken into account here is included. This similarity is tightly linked to the fact that the Λ -potential introduces the T-matrix in the formalism at the Born approximation level. However, the two formalisms do

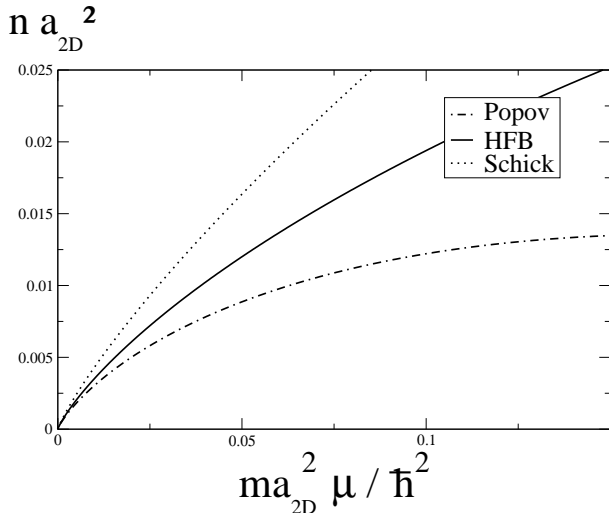


FIG. 1: Equation Of State of the 2D homogeneous Bose gas. Dotted line: EOS deduced from Schick's formula $\mu = 4\pi\hbar^2 n / (m \ln(na_{2D}^2))$ [23]. Full line: full variational approach (HFB). Dashed dotted line: Perturbative EOS obtained using the path integral method [9].

not coincide: using the full variational scheme allows a self-consistent determination of the energy at which the T-matrix appearing in Eqs.(8,11) is evaluated. On the contrary, in Ref.[11] this energy is fixed at $-2\mu_{loc}$, where μ_{loc} is the local chemical potential. In the limit where $a_{3D} \ll a_z$, from Eq.(13) we obtain at finite temperature :

$$g_{\Lambda^*}(T) \simeq \frac{4\pi\hbar^2 a_{3D}}{ma_z\sqrt{2\pi}} \left(1 + \frac{\tilde{\kappa}_T}{\Phi^2} \right) , \quad (14)$$

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 $\hbar\omega_n$. Remarkably, Eq.(14) coincides with the HFB-G2 prescription [16].

As a first application, we consider the homogeneous medium at zero temperature. From Eqs.(8,11,13), we deduce a standard Bogolubov spectrum and a self-consistent equation for Λ^* :

$$\frac{\hbar^2 \Lambda^{*2}}{m} = g_{\Lambda^*} |\Phi|^2 , \quad (15)$$

giving directly the energy at which the T-matrix has to be evaluated for having a gapless spectrum. From $\mu = g_{\Lambda^*} (|\Phi|^2 + 2\tilde{n})$ and (15) we deduce the EOS shown in Fig.(1). In the ultra-dilute limit $na_{2D}^2 \ll 1$, we recover the exact perturbative result obtained using the path integral formalism [9]:

$$n = \frac{m\mu}{4\pi\hbar^2} \ln \left(\frac{4\hbar^2}{e^{(2\gamma+1)} m\mu a_{2D}^2} \right) . \quad (16)$$

For increasing values of the 2D atomic density, the predicted EOS deviates from the perturbative and Schick's formulas. 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. Note that the EOS can be studied in traps, keeping in mind that the chemical potential is constrained to values compatible with the 2D regime. In situations where the density varies rapidly, for example in presence of vortices, or also at finite temperature not only Eqs.(8,11) but also Eq.(13) 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 [24]. 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 an anomalous mode (the lowest core localized state), having a negative energy ($\hbar\omega_a$) when the trap rotation frequency is zero [25]. In 3D rotating BEC experiments, this type of instability which causes the spiralling of the vortex core out of the condensate has been observed [26], and we expect a similar behavior in 2D. We then consider an off-equilibrium situation where the trap is at rest and all the modes except the anomalous one are thermalized. In a first step, we use the gapless HFB equations and evaluate arbitrarily the T-matrix at energy $-2\mu_{loc}$. This prescription is very close to the approach of Ref.[17], where the mean-field coupling constant is uniform. As shown in Fig.2,

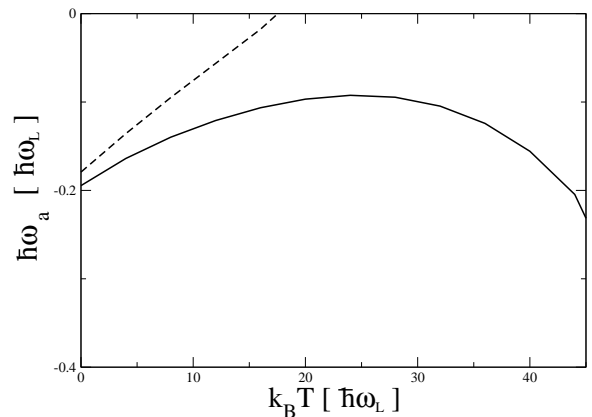


FIG. 2: Typical evolution of the anomalous mode energy of a single vortex in a non rotating trap as a function of the temperature. The presence of a negative energy mode in the spectrum leads to the so-called thermodynamical instability of the single vortex [25]. Dashed line: the coupling constant used in the gapless equations is arbitrarily evaluated using the two-body T-matrix at energy $-2\mu_{loc}$. Full line: full variational scheme; at finite temperature, the anomalous mode energy is not stabilized.

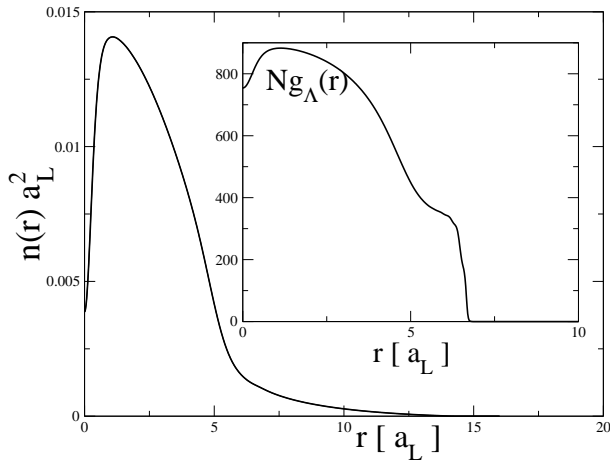


FIG. 3: Typical density profile of a single vortex at finite temperature ($k_B T = 20\hbar\omega_L$), obtained using the full variational approach when the anomalous mode is not thermalized. Inset: mean-field coupling constant in harmonic oscillator units, obtained by solving Eq.(13).

this non-variational approach predicts also an unphysical stabilization at sufficiently high temperature. On the

contrary, using the full variational scheme where Eq.(13) 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 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 [17], the unexpected stabilization in the non-variational approach is linked to the mean field term $g_\Lambda \tilde{n}$ in Eq.(11) which plays the role of a pinning potential. In the formalism presented here, the structure of g_Λ changes dramatically with increasing temperatures (for example, the curve dives at the vicinity of the core). As a consequence, the spurious pinning effect is avoided.

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. The T-matrix appears as a natural object in this formalism, which includes known results on the 2D BEC and gives crucial improvements in situations where similar but non-variational approaches fail.

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