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A renormalized Gross–Pitaevskii theory and vortices in a strongly interacting Bose gas

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Abstract

We consider a strongly interacting Bose–Einstein condensate in a spherical harmonic trap. The system is treated by applying a slave-boson representation for hardcore bosons. A renormalized Gross–Pitaevskii theory is derived for the condensate wavefunction that describes the dilute regime (like the conventional Gross–Pitaevskii theory) as well as the dense regime. We calculate the condensate density of a rotating condensate for both the vortex-free condensate and the condensate with a single vortex and determine the critical angular velocity for the formation of a stable vortex in a rotating trap.

1. Introduction

In this paper, we shall study two aspects of a strongly interacting Bose gas at high density. One is related to a consistent treatment of a strongly interacting Bose gas in terms of an effective Gross–Pitaevskii (GP) equation with renormalized parameters. The second aspect is related to the formation of a vortex in a trapped condensate in the presence of strong interaction.

The stationary form of the conventional GP equation

$$\left[-\frac{\hbar^2}{2m} \nabla^2 - \mu + V(\mathbf{r}) + g|\Phi(\mathbf{r})|^2 \right] \Phi(\mathbf{r}) = 0 \quad (1)$$

describes the condensate order parameter Φ of a Bose gas in a trapping potential at zero temperature, where μ is the chemical potential and g the repulsive coupling constant [1–3]. In the absence of a trapping potential, a solution of equation (1) is given by

$$|\Phi|^2 = \frac{\mu}{g}. \quad (2)$$

This describes a linearly increasing condensate density (the latter is proportional to $|\Phi|^2$) with respect to the chemical potential. Although it takes the repulsion into account by a factor $1/g$ which is decreasing with increasing coupling constant g , the saturation of n_0 cannot be seen in this solution. From the physical point of view, in a realistic description for large densities,

the particle density must saturate because there is a finite scattering volume around each particle. Furthermore, for increasing particle density, the condensate density should reach a maximum and for even larger densities, decrease again until its total destruction, because of the increasing interparticle interaction. This behaviour has also been found by variational perturbation theory [4] and diffusion Monte Carlo calculations [5]. In other words, the strong effect of the repulsion in a dense condensate is not really described by the conventional GP equation. In order to describe condensates at higher densities, the second-order term in the low-density expansion of the energy density has been taken into account which lead to a modified GP theory [1, 5–7].

Although in many experimentally realized situations the BEC is in the weakly interacting regime where it is well described by GP theory, it might be possible to reach the strongly interacting regime. The main problem at high particle densities is the instability of the Bose gas from the formation of molecules due to three-particle interactions [8]. Here, we will assume that molecule formation does not occur. This might be unrealistic for some systems, but in others it is not, e.g. for Bose gases in optical lattices.

It has been shown that the slave-boson approach to a hardcore Bose gas provides a mean-field equation, similar to the GP equation, that leads to a saturation of the condensate $n_0 \leq 1$ [9–13]. Here we will discuss a simplified version of this mean-field equation which is the same type of nonlinear Schrödinger equation as in the GP approach. However, in contrast to the latter the parameters are renormalized such that equation (2) becomes

$$|\Phi_R|^2 = \frac{\mu_R}{g_R},$$

where the renormalized parameters μ_R and g_R are functions of the bare parameters μ and n_0 . At the phase transition between the non-condensed Bose gas and the BEC μ_R vanishes, then increases linearly with increasing μ , reaches a maximum and decreases again until the condensate is destroyed totally due to strong interaction effects. We use this approach to calculate the condensate density profile of a trapped BEC.

The formation of vortices in a rotating condensate is understood as a local destruction of the condensate. From the depletion effect due to strong interaction it can be anticipated that the tendency of vortex formation is enhanced in a dense Bose gas. This implies a reduction of the critical angular velocity Ω_c with increasing density by the interaction. Vortex formation in rotating traps in the region beyond the validity of GP has also been studied by the modified GP theory and by variational Monte Carlo methods [7].

The paper is organized as follows: in the following section we survey the results of the slave-boson approach for a hardcore Bose gas on a lattice and derive a corresponding mean-field theory for a continuous system in an external trap potential. Then we derive the renormalized GP equation and evaluate solutions with and without a straight vortex and determine the critical angular velocity for the vortex formation.

2. The model

The slave-boson representation of a strongly interacting Bose gas is based on the idea that the bosons fill the space with finite density, where each particle occupies a lattice cell related to a sphere with radius a_s (s -wave scattering length) [10]. Singly occupied and empty sites are described by two complex fields b_x and e_x , respectively [11]. Here, b_x^* and b_x represent a creation and annihilation process of a boson at site x , while e_x^* and e_x represent the creation and annihilation of a ‘hole’. In the functional integral representation [14], the grand canonical

partition function in classical approximation is given as

$$Z = \int \exp \left[-\beta \sum_{x,x'} b_x^* e_x t_{x,x'} e_{x'}^* b_{x'} + \beta \sum_x \mu_x |b_x|^2 \right] \times \prod_x \delta(|e_x|^2 + |b_x|^2 - 1) db_x db_x^* de_x de_x^*, \quad (3)$$

where $1/\beta = k_B T$ is the thermal energy. In a d -dimensional lattice,

$$\hat{t}_{x,x'} = \begin{cases} -J/(2d) & \text{if } x, x' \text{ nearest neighbours} \\ 0 & \text{else} \end{cases}$$

is the nearest-neighbour tunneling rate and $\mu_x = \mu - V_x$ is the space-dependent chemical potential that includes the trapping potential V_x . Instead of μ_x we will write only μ subsequently and assume implicitly that the effective chemical potential can depend on space. The fields e and b are dimensionless. Moreover, we rescale all physical energies by a multiple of the hopping rate αJ to obtain dimensionless quantities:

$$\hat{t} \rightarrow \hat{t}' = \frac{1}{\alpha J} \hat{t}, \quad \mu \rightarrow \mu' = \frac{1}{\alpha J} \mu, \quad \beta \rightarrow \beta' = \alpha J \beta. \quad (4)$$

The hopping term is quartic in the field variables, due to the fact that a hopping process is characterized as an ‘exchange process’ of a boson and an empty site. The δ function enforces the constraint that each lattice site is either singly occupied or empty but excludes a multiple occupation.

A similar approach has been applied to the Bose–Hubbard model which allows multiple occupation, by introducing additional fields, one for each occupation number [12, 13]. The well-known zero-temperature phase diagram with Mott-insulating phases for integer lattice fillings $n = 0, 1, 2, \dots$ (‘lobes’) was found. In contrast, our hardcore Boson model is restricted to the two lattice fillings $n = 0, 1$ which is a simplification, but contains all relevant aspects of Bose–Einstein condensation with repulsive interaction. A second simplification of our approach is that we neglect quantum fluctuations by treating the grand-canonical partition function in classical approximation. This allows us to integrate the constraint exactly. On the other hand, it restricts the applicability of our approach to non-zero temperatures.

Two new fields are introduced by a Hubbard–Stratonovich transformation, the complex field Φ_x which describes the condensate wavefunction and the real field φ_x which is related to the total density of bosons [10]:

$$Z = \int \exp \left\{ -\beta' \left[\sum_{x,x'} \Phi_x^* (\mathbf{1} - \hat{t}')_{x,x'}^{-1} \Phi_{x'} + \sum_x \varphi_x^2 + \sum_x (e_x, b_x) \begin{pmatrix} 2\varphi_x + 1 & \Phi_x \\ \Phi_x^* & -\mu' \end{pmatrix} \begin{pmatrix} e_x^* \\ b_x^* \end{pmatrix} \right] \right\} \times \prod_x \delta(|b_x|^2 + |e_x|^2 - 1) db_x db_x^* de_x de_x^* d\Phi_x d\Phi_x^* d\varphi_x. \quad (5)$$

Integration over the fields Φ and φ leads back to equation (3). On the other hand, the fields b_x and e_x can be integrated in (5) because they appear in the exponent as quadratic forms. This leads to the partition function

$$Z = \int e^{-S_b - S_l} \prod_x d\Phi_x d\Phi_x^* \quad (6)$$

with the kinetic part of the action

$$S_b = \beta' \sum_{x,x'} \Phi_x (\mathbf{1} - \hat{t}')_{x,x'}^{-1} \Phi_{x'}^* \quad (7)$$

and the potential part

$$S_1 = - \sum_x \log \left(\int_{-\infty}^{\infty} e^{-\beta' \varphi_x^2} \frac{\sinh \left[\beta' \sqrt{(\varphi_x + \frac{\mu'}{2})^2 + |\Phi_x|^2} \right]}{\beta' \sqrt{(\varphi_x + \frac{\mu'}{2})^2 + |\Phi_x|^2}} d\varphi_x \right) := - \sum_x Z_x. \quad (8)$$

The condensate density can be identified with

$$n_0 = \frac{|\Phi_x|^2}{(1 + 1/\alpha)^2}, \quad (9)$$

as argued in the appendix, and the total particle density is given by the expectation value [10]

$$n_{\text{tot}} = \langle \varphi_x \rangle + \frac{1}{2}. \quad (10)$$

We apply a saddle-point approximation to the integration in equation (6). This is controlled by the minimized action, which means that we have to solve the equation

$$\frac{\partial S}{\partial \Phi_x^*} = 0.$$

This yields the mean-field equation

$$\beta' \sum_{x'} (\mathbf{1} - \hat{t}')_{x,x'}^{-1} \Phi_{x'} - \left[\frac{\partial}{\partial (|\Phi_x|^2)} \log Z_x \right] \Phi_x = 0. \quad (11)$$

In order to derive a mean-field equation which is applicable to a continuous trapping potential, we perform the continuum approximation of (11). If the field $\Phi_{\mathbf{r}}$ is varying only very slowly between neighbouring lattice sites, we can approximate

$$(\mathbf{1} - \hat{t}')_{x,x'}^{-1} \approx \frac{1}{1 + 1/\alpha} \left(\delta_{x,x'} + \frac{1}{1 + 1/\alpha} \alpha J (J \delta_{x,x'} + \hat{t}_{x,x'}) \right),$$

and perform the substitution

$$\sum_{x'} (J \delta_{x,x'} + \hat{t}_{x,x'}) \rightarrow -J a^2 \nabla^2.$$

This leads to the equation

$$\left[-\frac{J a^2}{6} \nabla^2 + (1 + \alpha) J - \frac{(1 + 1/\alpha)^2}{\beta} \frac{\partial}{\partial (|\Phi(\mathbf{r})|^2)} \log Z(\mathbf{r}) \right] \Phi(\mathbf{r}) = 0 \quad (12)$$

with

$$Z(\mathbf{r}) = \int e^{-\beta' \varphi_{\mathbf{r}}^2} \frac{\sinh \left[\beta' \sqrt{(\varphi_{\mathbf{r}} + \mu'/2)^2 + |\Phi(\mathbf{r})|^2} \right]}{[\beta' \sqrt{(\varphi_{\mathbf{r}} + \mu'/2)^2 + |\Phi(\mathbf{r})|^2}]} d\varphi_{\mathbf{r}}$$

for the spatially dependent order parameter $\Phi(\mathbf{r})$ in a three-dimensional space and a is the lattice constant of the discrete system. In the continuum a loses its identity as a lattice constant, but describes a characteristic length scale in equation (12), and can be interpreted as the spatial extension of a boson. Thus, it should be of the same order of magnitude as the s -wave scattering length a_s [1]. Equation (12) is the analogue of the GP equation in the case of our slave-boson approach. The parameters can be identified with those of the conventional GP equation: the mass m of the particles is given by the hopping constant J and the lattice

constant a via

$$\frac{\hbar^2}{2m} \equiv \frac{Ja^2}{6}. \quad (13)$$

3. Renormalized Gross–Pitaevskii equation

The continuum limit of the action defined by equation (7) and (8) is

$$S = \int \left\{ \beta' \Phi^*(\mathbf{r}) \left[-\frac{\alpha}{(1+\alpha)^2} \frac{a^2}{6} \nabla^2 + \frac{1}{1+1/\alpha} \right] \Phi(\mathbf{r}) - \log Z(\mathbf{r}) \right\} d^d r. \quad (14)$$

Applying the variational principle

$$\frac{\partial S}{\partial \Phi_x^*} = 0,$$

we obtain the full mean-field equation (12) directly. If the order parameter Φ is small, we can expand the potential part of the action up to fourth order:

$$\frac{1}{1+1/\alpha} |\Phi|^2 - \frac{1}{\beta'} \log Z(\mathbf{r}) = a_0(\mu') + a_2(\mu') |\Phi|^2 + \frac{1}{2} a_4(\mu') |\Phi|^4 + \mathcal{O}(|\Phi|^6), \quad (15)$$

where we have introduced the coefficients

$$a_0(\mu') = -\frac{1}{\beta'} \log Z(\mathbf{r}) \Big|_{\Phi=0} \quad (16)$$

$$a_2(\mu') = -\frac{1}{\beta'} \frac{\partial}{\partial |\Phi|^2} \log Z(\mathbf{r}) \Big|_{\Phi=0} + \frac{1}{1+1/\alpha} \quad (17)$$

$$a_4(\mu') = -\frac{1}{\beta'} \frac{\partial^2}{(\partial |\Phi|^2)^2} \log Z(\mathbf{r}) \Big|_{\Phi=0}. \quad (18)$$

Further, we introduce the rescaled field

$$\Phi_R(\mathbf{r}) = \frac{1}{1+1/\alpha} \Phi(\mathbf{r}),$$

which we identify with the condensate wavefunction of our renormalized GP theory. We now introduce the renormalized coefficients

$$\mu_R(\mu, J) \equiv -\frac{(1+\alpha)^2}{\alpha} J a_2(\mu')$$

and

$$g_R(\mu, J) \equiv \frac{(1+\alpha)^4}{\alpha^3} J a_4(\mu').$$

After neglecting the term of order $|\Phi|^6$ in the expansion (15), we get the renormalized Gross–Pitaevskii (RGP) equation

$$\left[-\frac{Ja^2}{6} \nabla^2 - \mu_R(\mu, J) + g_R(\mu, J) |\Phi_R(\mathbf{r})|^2 \right] \Phi_R(\mathbf{r}) = 0. \quad (19)$$

It has the same form as the conventional GP equation (1), when μ and g are replaced by μ_R and g_R . Their μ -dependence is plotted in figure 1. In the case of a trapping potential, where the chemical potential μ is space dependent, μ_R and g_R are space dependent as well. While g_R is always positive, μ_R can change sign. A BEC exists if $\mu_R > 0$. The phase transition

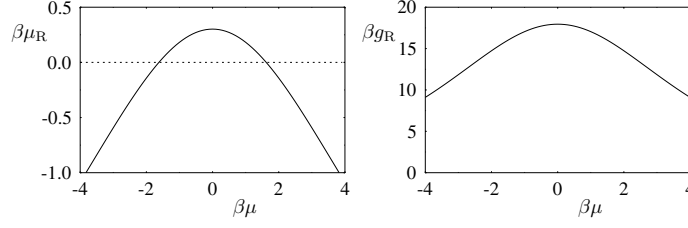


Figure 1. Coefficients μ_R and g_R of the RGP theory plotted against the chemical potential μ for the tunneling rate $\alpha J = k_B T$. Both functions are symmetric in μ . A BEC exists if $\mu_R > 0$. The two points where $\mu_R = 0$ mark the phase transition between the non-condensate and the BEC. The coefficient g_R is always positive.

between the BEC and the non-condensate phase, i.e. the point at which the condensate order parameter vanishes, is given by the relation $\mu_R(\mu, J) = 0$.

4. Results

4.1. Zero-temperature result

In the zero-temperature limit we can integrate the φ -field in equation (8) exactly by a saddle-point integration, as shall be shown in this paragraph. Therefore, we write

$$Z(\mathbf{r}) = \frac{1}{2\beta'}(Z_- - Z_+),$$

where

$$Z_{\pm} = \int_{-\infty}^{\infty} \frac{e^{-\beta' f_{\pm}(\varphi, |\Phi|^2)}}{\sqrt{(\varphi + \frac{\mu'}{2})^2 + |\Phi|^2}} d\varphi$$

and

$$f_{\pm}(\varphi, |\Phi|^2) = \varphi^2 \pm \sqrt{\left(\varphi + \frac{\mu'}{2}\right)^2 + |\Phi|^2}.$$

It is possible to perform a saddle-point approximation by expanding the functions f_{\pm} up to second order in φ around their minimum φ_0 :

$$f_{\pm}(\varphi, |\Phi|^2) = f_{\pm}(\varphi_0, |\Phi|^2) + \frac{1}{2} \frac{\partial^2 f_{\pm}}{\partial \varphi^2}(\varphi_0, |\Phi|^2)(\varphi - \varphi_0)^2 + \mathcal{O}(\varphi^2).$$

In the limit of large β , the saddle-point integration becomes exact and yields

$$Z_{\pm} = \sqrt{\frac{\pi}{(\varphi_0 + \frac{\mu'}{2})^2 + |\Phi|^2}} \frac{e^{-\beta' f_{\pm}(\varphi_0, |\Phi|^2)}}{\sqrt{\frac{\beta'}{2} \frac{\partial^2 f_{\pm}(\varphi_0, |\Phi|^2)}{\partial \varphi^2}}}.$$

The minimum is found to satisfy the equation

$$|\Phi|^2 = \left(\varphi_0 + \frac{\mu'}{2}\right)^2 \left(\frac{1}{4\varphi_0^2} - 1\right),$$

and we have

$$f_{\pm}(\varphi_0) = \varphi_0^2 - \frac{1}{2} - \frac{\mu'}{4\varphi_0}; \quad \frac{\partial^2 f_{\pm}(\varphi_0)}{\partial \varphi^2} = 2 - \frac{8|\Phi|^2 \varphi_0^3}{(\varphi_0 + \frac{\mu'}{2})^3}.$$

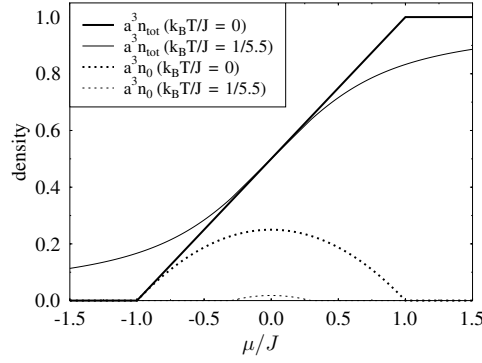


Figure 2. Condensate density n_0 and total density n_{tot} of a translational invariant system, plotted against chemical potential for zero-temperature (thick lines) and finite temperature (thin lines).

We find the following zero-temperature result for a translational invariant condensate ($\Phi_x \equiv \Phi = \text{const}$) from the mean-field equation (12): for the condensate density we find

$$n_0 = \frac{|\Phi|^2}{(1 + 1/\alpha)^2} = \begin{cases} \frac{1}{4} \left(1 - \frac{\mu^2}{J^2}\right) & \text{if } -J < \mu < J \\ 0 & \text{else,} \end{cases} \quad (20)$$

and the total particle density given by equation (10) is

$$n_{\text{tot}} = \varphi_0 + \frac{1}{2} = \begin{cases} 0 & \text{if } \mu \leq -J \\ \frac{1}{2} \left(1 - \frac{\mu}{J}\right) & \text{if } -J < \mu < J \\ 1 & \text{if } J \leq \mu. \end{cases} \quad (21)$$

The solution of the mean-field equation is plotted in figure 2 for zero temperature and near the critical temperature T_c where the BEC breaks down. In the dilute regime at $T = 0$, the chemical potential can be written as $\mu = -J + \Delta\mu$, where $\Delta\mu \ll J$. In this limiting case we find $\mu_R = \Delta\mu + \mathcal{O}(\Delta\mu^2)$ and $g_R = 2J$, which is consistent with the conventional GP equation with a shifted chemical potential.

4.2. Vortex-free trapped condensate

Assuming a dense condensate, where the repulsive interaction between bosons dominates their kinetic energy, we neglect the differential term in equations (12) and (14). This is called the Thomas–Fermi (TF) approximation [1]. In the following we use a spherical trapping potential

$$V(\mathbf{r}) = \frac{m}{2} \omega_{\text{ho}}^2 \mathbf{r}^2. \quad (22)$$

In typical experiments, the oscillator length $d_{\text{ho}} = \sqrt{\hbar/m\omega_{\text{ho}}}$ is of the order of a few μm [1], where ω_{ho} is the trap frequency measured in Hz. Considering, for instance, ^{85}Rb atoms near a Feshbach resonance [15], we can study a Bose gas in a dense regime with a scattering length $a_s \sim a \sim 200 \text{ nm}$. In our calculations we choose the parameters

$$\beta' = 1, \quad \frac{k_B T}{\hbar \omega_{\text{ho}}} = 36.93, \quad \frac{a}{d_{\text{ho}}} = 0.1215, \quad (23)$$

and keep the hopping constant J fixed. Thus all energies can be scaled with J .

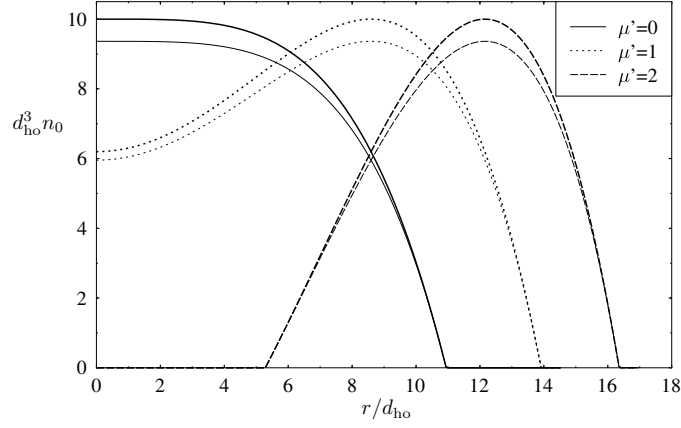


Figure 3. Condensate density $n_0 = |\Phi|^2/a^3(1+1/\alpha)^2$ of a vortex-free condensate in a spherical trap with the numerical parameters given in equation (23) and different values of the chemical potential μ' calculated from the full slave-boson mean-field equation (24) (thick lines) and within RGP approximation (25) (thin lines).

To calculate the profile of the condensate density in a BEC without vortex, we solve the TF equation

$$(1 + 1/\alpha) - (1 + 1/\alpha)^2 \frac{\partial}{\partial |\Phi(\mathbf{r})|^2} \log Z(\mathbf{r}) = 0. \quad (24)$$

In the RGP approximation (19), the solution is

$$|\Phi_R(\mathbf{r})|^2 = \frac{\mu_R}{g_R} = -\frac{a_2(\mu')}{(1 + 1/\alpha)^2 a_4(\mu')}. \quad (25)$$

Solutions for typical values of the parameters are plotted in figure 3. The results we get from the renormalized GP approximation show only small deviations from the numerical solutions of equation (24). We find a condensate depletion at the trap centre for $\mu' = 1$. This is due to the fact that the condensate is partly suppressed by strong interaction effects [4, 5, 11]. For $\mu' = 2$ the condensate is completely destroyed at the trap centre. We find particle numbers in the condensate of the order $N_0 \approx 10^4 \dots 10^5$.

We note that the total particle density n_{tot} is much larger than the condensate density n_0 and takes values of about $0.5a^{-3}$ at the trap centre. Thus the interaction between the non-condensed and the condensed parts of the Bose gas plays a significant role. This implies that the conventional GP equation, which neglects the non-condensed part, is not reliable in this parameter regime.

4.3. Rotating condensate with a single vortex

In the case of a trap rotating about the z -axis with an angular velocity Ω , one must include the additional angular momentum term $-\Omega L_z \Phi(\mathbf{r})$ on the left-hand side of the differential equation (12), where L_z is the z -component of the angular momentum operator. This term must also be kept in the TF approximation. The condensate wavefunction may then develop a vortex. We assume here a straight single vortex along the z -axis. This can be described by using cylindrical coordinates and the ansatz $\Phi(\mathbf{r}) = \phi(r_\perp, z) e^{i\varphi}$, where r_\perp is the distance from the z -axis and φ the polar angle. The angular momentum operator is given as $L_z = -i \frac{\partial}{\partial \varphi}$.

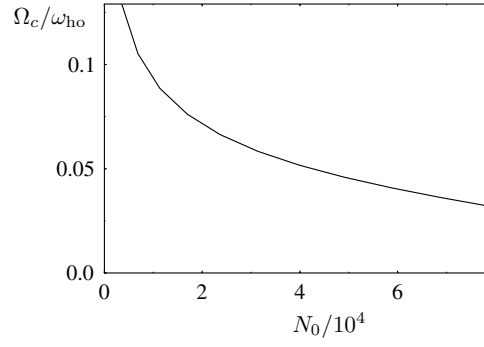


Figure 4. Critical angular velocity plotted against the total number of particles in the condensate.

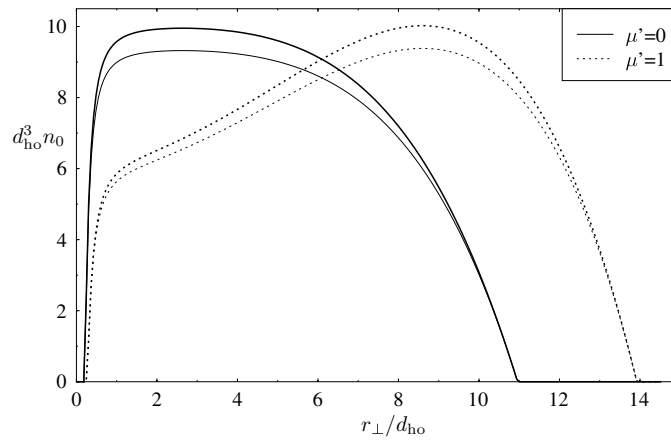


Figure 5. Condensate density of a condensate with a single vortex, with same parameters as in figure 3, calculated from the full mean-field equation (26) (thick lines) and within RGP approximation (27) (thin lines). The rotating frequencies of the trap were chosen to be close to the critical angular frequency Ω_c .

This gives rise to an additional term $(\Omega/\alpha J - a^2/\alpha(6r_{\perp}^2))|\Phi(\mathbf{r})|^2/(1+1/\alpha)^2$ in the action (14). Instead of equation (24) we have to solve

$$(1+1/\alpha) + \left(\frac{a^2}{\alpha 6r_{\perp}^2} - \frac{\Omega}{\alpha J} \right) - (1+1/\alpha)^2 \frac{\partial}{\partial |\Phi(\mathbf{r})|^2} \log Z(\mathbf{r}) = 0, \quad (26)$$

and the solution in the RGP approximation is

$$|\Phi_R(\mathbf{r})|^2 = -\frac{1}{(1+1/\alpha)^4 a_4(\mu')} \left[\left(\frac{a^2}{\alpha 6r_{\perp}^2} - \frac{\Omega}{\alpha J} \right) + (1+1/\alpha)^2 a_2(\mu') \right]. \quad (27)$$

A condensate that is rotating with given angular velocity Ω forms a stable vortex, if its total energy is lower than that of a vortex free condensate. This is equivalent to the condition

$$S^{\text{vort}}(\Omega) - S < 0 \quad (28)$$

which can be checked numerically by using the TF approximation of equation (14) for a condensate with vortex $S_{\text{FT}}^{\text{vort}}(\Omega)$ and without vortex S_{TF} . The critical angular velocity Ω_c

above which the vortex is stable is plotted against the number of condensed bosons N_0 in figure 4, where N_0 is given as

$$N_0 = \int \frac{1}{a^3} |\Phi_R(\mathbf{r})|^2 d^3\mathbf{r}. \quad (29)$$

The RGP approximation is in good agreement with the results of the full mean-field equation. The decreasing critical angular velocity for higher values of N_0 indicates that a high interaction energy favours the formation of a vortex. This agrees with results derived from the GP equation by perturbation theory [16] as well as numerically [17].

Typical solutions for shapes of condensate density profiles of BECs with a stable single vortex are shown in figure 5. In contrast to the case without a vortex, the condensate is always completely destroyed at the trap centre, a feature that also shows up in the conventional GP approximation [1]. Again, the RGP approximation is in good agreement with the numerical results from (26).

5. Conclusion

The slave-boson approach allowed us to study the condensation of a trapped high-density Bose gas in a regime where the conventional Gross–Pitaevskii approach is not valid. Starting from the saddle-point approximation, we have derived a renormalized Gross–Pitaevskii equation with a space-dependent coupling constant. This provides good results in comparison with the more complicated slave-boson saddle-point calculations. At high densities, we have found a depletion of the condensate at the trap centre due to the interaction between the condensate and the non-condensate parts of the Bose gas. This feature is not covered by the conventional Gross–Pitaevskii equation. The behaviour of the critical angular velocity for the formation of a single vortex agrees qualitatively with previous results in the literature but supports also the formation of a vortex for increasing N_0 .

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Appendix

For a Bose system with creation operators a_x^+ and annihilation operators a_x at a lattice site x , an appropriate definition of the condensate density is [3]

$$n_0 := \lim_{x-x' \rightarrow \infty} \langle a_x^+ a_{x'} \rangle. \quad (A.1)$$

In our slave-boson representation, a creation process of a particle is associated with the product $b_x^* e_x$ and an annihilation process with $e_x^* b_x$, thus

$$n_0 = \lim_{x-x' \rightarrow \infty} \langle b_x^* e_x e_{x'}^* b_{x'} \rangle. \quad (A.2)$$

Here, the expectation value is defined with respect to the functional integral (5) by

$$\langle \dots \rangle = \frac{1}{Z} \int \dots \exp[\dots] \prod_x \delta(|b_x|^2 + |e_x|^2 - 1) db_x db_x^* de_x de_x^* d\Phi_x d\Phi_x^* d\varphi_x.$$

We are interested in the connection between the correlation function $\langle \Phi_x \Phi_{x'}^* \rangle$ and the condensate density. For this purpose we integrate the field Φ to transform the correlation

function of the field Φ back to a correlation function of the fields b and e . Therefore, we perform the integration

$$\begin{aligned}
& \beta'^2 \int \Phi_y \Phi_{y'}^* \exp \left[\beta' \sum_{x,x'} \Phi_x (\mathbf{1} - \hat{t}')^{-1} \Phi_{x'}^* + \beta' \sum_x \Phi_x b_x^* e_x + \beta' \sum_x \Phi_x^* e_x^* b_x \right] \prod_x d\Phi_x d\Phi_x^* \\
&= \frac{\partial}{\partial(b_y^* e_y)} \frac{\partial}{\partial(b_{y'} e_{y'}^*)} \int \exp \left[\beta' \sum_{x,x'} \Phi_x (\mathbf{1} - \hat{t}')^{-1} \Phi_{x'}^* \right. \\
&\quad \left. + \beta' \sum_x \Phi_x b_x^* e_x + \beta' \sum_x \Phi_x^* e_x^* b_x \right] \prod_x d\Phi_x d\Phi_x^* \\
&= \frac{\partial}{\partial(b_y^* e_y)} \frac{\partial}{\partial(b_{y'} e_{y'}^*)} \det \beta' (\mathbf{1} - \hat{t}') \exp \left[\beta' \sum_{x,x'} b_x^* e_x (\mathbf{1} - \hat{t}') e_{x'}^* b_{x'} \right] \\
&= \beta'^2 \det(\mathbf{1} - \hat{t}') \left[(\mathbf{1} - \hat{t}')_{y,y'} + \beta' \sum_{x,x'} b_x^* e_x e_{x'}^* b_{x'} (\mathbf{1} - \hat{t}')_{y',x'} \right] \\
&\quad \times \exp \left[\beta' \sum_{x,x'} b_x^* e_x (\mathbf{1} - \hat{t}')_{x,x'} e_{x'}^* b_{x'} \right].
\end{aligned}$$

Since we are interested in the limit $y - y' \rightarrow \infty$, and the matrix $\hat{t}'_{y,y'}$ includes nearest-neighbour hopping only, the term $(\mathbf{1} - \hat{t}')_{y,y'}$ does not contribute. This yields for far distant lattice points y, y' the expression

$$\langle \Phi_y \Phi_{y'}^* \rangle = \sum_{x,x'} \langle b_x^* e_x e_{x'}^* b_{x'} \rangle (\mathbf{1} - \hat{t}')_{x,y} (\mathbf{1} - \hat{t}')_{y',x'}.$$

In this sum, only those terms contribute, where x, y as well as x', y' are nearest neighbours. In the limit $y - y' \rightarrow \infty$ we can assume $\langle b_x^* e_x e_{x'}^* b_{x'} \rangle = \langle b_y^* e_y e_{y'}^* b_{y'} \rangle$. Thus we can use

$$\sum_x (\mathbf{1} - \hat{t}')_{x,y} = \sum_{x'} (\mathbf{1} - \hat{t}')_{y',x'} = (1 + 1/\alpha)^2. \quad (\text{A.3})$$

We get

$$\lim_{y-y' \rightarrow \infty} \langle \Phi_y \Phi_{y'}^* \rangle \approx (1 + 1/\alpha)^2 \lim_{y-y' \rightarrow \infty} \langle b_y^* e_y e_{y'}^* b_{y'} \rangle \quad (\text{A.4})$$

and therefore

$$n_0 \approx \frac{1}{(1 + 1/\alpha)^2} \lim_{y-y' \rightarrow \infty} \langle \Phi_y \Phi_{y'}^* \rangle. \quad (\text{A.5})$$

On the mean-field level, this justifies our identification of the condensate density in equation (9).

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