

# Ground-state of a two-dimensional Bose gas in a harmonic trap

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## Abstract

We study the ground state properties of a two-dimensional Bose gas in an harmonic trap potential using the recently proposed mean-field equation that takes into account the correct dimensionality effect. In contrast to the three-dimensional case, the interaction term depends logarithmically on the scattering length and density. We compare our results with other approaches with various forms for the two-dimensional coupling.

## I. INTRODUCTION

The observation of Bose-Einstein condensation (BEC) in externally confined atomic vapors [1] has stimulated a big interest in the theoretical and experimental work on interacting systems of bosons. The thermodynamic, ground-state static and dynamic properties of condensates are extensively investigated and the main results are compiled in a number of reviews. [2] Most of the excitement stems from the possibility of understanding properties of a macroscopic quantum state. Apart from fundamental physics considerations, the Bose-Einstein condensed systems offer interesting applications of atom laser and atom optics.

The BEC phenomenon in two-dimensional systems has attracted considerable amount of interest from the point of view of understanding effects of dimensionality. As the homogeneous 2D system of bosons would not undergo BEC at a finite temperature, the prospects of observing BEC in systems with an external potential [3] provides a strong motivation for such investigations. It was argued by Mullin [4] that BEC is not possible for strictly 2D systems even in a trapping potential in the thermodynamic limit. However, by varying the trapping field so that it is very narrow in one direction, it should be possible to separate the single-particle states of the oscillator potential into well-defined bands, and occupying the lowest band should produce an effectively two-dimensional system. Growing number of recent experiments [5–10] point to the possibility of realizing quasi-two-dimensional (Q2D) trapped atomic gases, and measurements on the BEC transition temperature and other properties are expected to follow.

The studies on the BEC in 2D systems can be broadly divided into two categories. In the first group the interaction effects are treated parametrically without reference to the actual interaction potential or the scattering length which describes it as in 3D formulation of the interacting boson condensates. [11–14] Included in the same mold of calculations

there has been path integral Monte Carlo simulations [15] at finite temperature to give indications of a BEC transition in two-dimensional systems. In the second group, some effort is made to relate the 2D interaction strength to the 3D scattering length [16–18] or to solve the scattering problem in strictly 2D to obtain the relevant dependence of the interaction coupling on the scattering length. Kim *et al.* [19] using the scattering theory in 2D, found that the interaction strength depends logarithmically on the scattering length. Shevchenko [20,21] in a series of papers studied interacting 2D Bose gas in a nonuniform field arriving at the conclusion even though a Bose-Einstein condensation does not take place, the system exhibits superfluidity. Recently, Kolomeisky *et al.* [22] in their treatment of low-dimensional Bose liquids suggested a modified form for the mean-field description of 2D condensates. Lieb, Seiringer, and Yngvason [23] have rigorously analyzed this and related approximations as applied to the practical cases of interest. Petrov, Holzmann, and Shlyapnikov [24] using scattering theory arguments obtained a slightly more detailed form of the effective interaction coupling for Q2D systems that distinguishes different density regimes.

The central aim of this paper is to calculate the ground-state properties of 2D Bose condensates based on the formulation given by Shevchenko [21] and Kolomeisky *et al.* [22] and study the effects of density dependent interaction strength. There are several works that consider Q2D Bose condensates in harmonic trap potentials using a model for the effective interaction strength. In contrast to the strictly 2D problem, the Q2D model takes into account the influence of the transverse direction in terms of the confinement frequency  $\omega_z$ . Recent experiments [5–10] indicate that such realizations will be possible in the near future.

In the following we first discuss the mean-field description of Bose condensates within the local-density approximation. Specializing to the case of 2D bosons in an harmonic trap at zero temperature, we calculate the condensate wave function and compare it with the predictions of other models suggested in the literature. We conclude with a brief summary.

## II. THEORY

The ground-state properties of a condensed system of bosons at zero temperature are described by the Gross-Pitaevskii equation. [25] In the presence of external trapping potentials, therefore an inhomogeneous Bose system, it is useful to adopt the local-density approximation which regards the system locally homogeneous. The mean-field energy functional in the local-density approximation can very generally be written as [26]

$$E = \int d\mathbf{r} \left[ \frac{\hbar^2}{2m} |\nabla\psi|^2 + V_{\text{ext}}(\mathbf{r})|\psi|^2 + \epsilon(\rho)|\psi|^2 \right], \quad (1)$$

where  $\epsilon(\rho)$  is the ground-state energy (per particle) of the homogeneous system, and  $\rho = |\psi|^2$  is the density. Variation of the energy functional with respect to  $\psi^*$ , subject to the normalization condition  $\int d\mathbf{r} |\psi|^2 = N$ , yields the nonlinear Schrödinger equation

$$-\frac{\hbar^2}{2m} \nabla^2\psi + V_{\text{ext}}(\mathbf{r})\psi + \frac{\partial[\epsilon(\rho)\rho]}{\partial\rho} \psi = \mu\psi, \quad (2)$$

where  $\mu$  is the chemical potential. The local-density approximation was used by Fabrocini and Polls [27] and Nunes [26] to study the high density effects in 3D condensates, by making use of the 3D homogeneous hard-sphere Bose gas results from perturbation theory. These studies showed that the modifications to GP equation become important as the number of particles  $N$  and the hard-sphere radius  $a$  are increased making the system less dilute.

We now apply the above scheme to a 2D system of bosons in an harmonic isotropic trapping potential  $V_{\text{ext}}(\mathbf{r}) = m\omega_{\perp}^2 r^2/2$ . Perturbation theory calculations for a homogeneous system of 2D hard-disk bosons yield [28]

$$\epsilon(\rho) = \frac{\hbar^2}{2m} \frac{4\pi\rho}{|\ln \rho a^2|}, \quad (3)$$

for the ground-state energy (per particle). The corresponding mean-field equation for the condensate wave function thus reads [22]

$$-\frac{\hbar^2}{2m} \nabla^2 \psi(r) + \frac{1}{2} m\omega_{\perp}^2 r^2 \psi(r) + \frac{\hbar^2}{2m} \frac{8\pi}{|\ln \psi^2 a^2|} |\psi(r)|^2 \psi(r) = \mu \psi. \quad (4)$$

The energy functional corresponding to this equation has also been suggested by Shevchenko. [21] We shall call Eq. (4) the 2D Gross-Pitaevskii equation, and compare it with other suggested forms to describe the ground state of 2D Bose condensates. We note that Eq. (4) is quite different than its 3D counterpart, in that the dimensionless interaction term  $g = 1/|\ln \psi^2 a^2|$  not only depends on the hard-disk radius  $a$  logarithmically, but it also depends on  $|\psi|^2$ , making the GP equation highly nonlinear. In 3D the density dependent interactions arise as corrections or modifications to the GP equation, whereas in 2D the mean-field interaction is density dependent. Here, we cast the nonlinear term in the form  $\frac{\hbar^2}{2m} g \psi^3$ . In the following we shall present numerical results of the solution of Eq. (4) and compare them with other approximations.

In the previous applications [26,27,29] of the local-density approximation in 3D condensates, effects beyond the mean-field theory (GP equation) has been explored by including higher order terms in the homogeneous energy density  $\epsilon(\rho)$ . In 2D, the correct mean-field description is given by Eq. (4). To go beyond the mean-field theory one would have to use the Another possible correction to the mean-field description has been suggested by Andersen and Haugerud. [30] In their treatment the kinetic energy functional is modified to include a gradient term

$$E_{\text{kin}} = \frac{\hbar^2}{2m} \int d\mathbf{r} \left[ 1 - \frac{2}{3} \frac{1}{|\ln |\psi|^2 a^2|} \right] |\nabla \psi|^2. \quad (5)$$

In our numerical calculations to be presented and discussed in the next section, we have tested the significance of corrections brought by the gradient term. We have found that it has negligible effect on the condensate profile  $\psi(r)$  and other physical quantities for the range of  $N$  and scattering length values we examined.

### III. RESULTS AND DISCUSSION

We solve the 2D Gross-Pitaevskii equation given in Eq. (4) numerically using the steepest descent method [31,27] which is known to produce accurate results. We also minimize the

corresponding energy functional over a set of spline test functions, as has been done by Krauth [32] in his comparison of quantum Monte Carlo simulations with mean-field solutions. In both cases our numerical results are in good agreement. A further check of our numerical calculations is provided by the virial relation. Under the scaling transformation  $\mathbf{r} \rightarrow \lambda \mathbf{r}$ , so that  $\psi(\mathbf{r}) \rightarrow \psi(\mathbf{r})/\lambda$ , and using the variational nature of the energy we obtain

$$E_{\text{kin}} - E_{\text{ext}} + E_{\text{int}} + 2\pi \int d\mathbf{r} \frac{|\psi(\mathbf{r})|^4}{|\ln|\psi|^2 a^2|^2} = 0. \quad (6)$$

In this form of the virial relation, we have omitted the gradient correction to the kinetic energy, since numerically it is found to be negligibly small. Our solution of the GP equation satisfies the virial relation to a high degree.

In Fig. 1 we show the scaled condensate wave function for 2D bosons in a harmonic trap for systems with particle numbers  $N = 10^4$  and  $N = 10^5$ . We have chosen  $a/a_{\text{HO}} = 4.33 \times 10^{-3}$ , the  $s$ -wave scattering length of  $^{87}\text{Rb}$  atoms, for the hard-disk radius describing the interaction strength. In a recent paper Lieb, Seiringer and Yngvason [23] argued that a simplified form of Eq. (4) would be sufficient for the leading order calculations. They suggested that the logarithmic term be replaced by  $\ln \bar{\rho} a^2$ , where  $\bar{\rho}$  is a mean density, defined by  $\bar{\rho} = \frac{1}{N} \int \rho_1^{\text{TF}}(\mathbf{r})^2 d\mathbf{r}$ . Here,  $\bar{\rho}$  is expressed in terms of an average over  $\rho_1^{\text{TF}}(\mathbf{r})$ , the Thomas-Fermi density when the logarithmic term is absent. The Thomas-Fermi (TF) approximation simply neglects the kinetic energy in Eq. (4) since the interaction term dominates for the most part except in the outer region. For the harmonic trapping potential in 2D, we find  $\bar{\rho} a_{\text{HO}}^2 = N^{1/2}/3\pi$ . We compare in Fig. 1 the resulting condensate wave function for the proposed  $g \sim |\ln \bar{\rho} a^2|^{-1}$  model. We observe that when Eq. (4) is used interaction term has a bigger effect and the condensate shows depletion near the center compared to the approximation suggested by Lieb, Seiringer, and Yngvason. [23] In 2D, the dilute limit is characterized by the condition  $\rho a^2/|\ln \rho a^2| \ll 1$ . For our chosen parameters of typical values this condition is fulfilled. It is then interesting to observe the effects of logarithmic term on the overall shape of the condensate wave function.

In their description of the quasi-2D condensates in harmonic traps, Bhaduri *et al.* [16] have used  $g = \sqrt{2/\pi} (a/a_{\text{HO}}^z)$  for the dimensionless coupling constant (interaction). Here  $a_{\text{HO}}^z$  is the harmonic oscillator length of the confinement in the transverse direction. We define the asymmetry parameter  $\lambda = a_{\text{HO}}/a_{\text{HO}}^z$  as the ratio between the 2D harmonic oscillator length and that for the  $z$ -direction, so that the interaction becomes  $g = \sqrt{2/\pi} (a/a_{\text{HO}}) \lambda$ . To see how such a model compares with the 3D Gross-Pitaevskii equation, we show in Fig. 2  $\psi(r)$  for several values of  $\lambda$ . For the system with  $N = 10^5$  and  $a/a_{\text{HO}} = 4.33 \times 10^{-3}$ , we find that  $\lambda = 50$  describes the condensate wave function quite accurately. Thus, such an approximation will have great utility in modeling the 2D dynamics of Bose condensates in terms of the parameters of the external trapping potentials. The 2D Gross-Pitaevskii equation suggested by Kim *et al.* [19] makes use of the scattering theory to obtain  $g = |\ln ka|^{-1}$ , where  $k$  is some inverse length scale. This differs from the above models somewhat but a proper choice of  $k$  would produce a similar condensate wave function for practical purposes.

## FIGURES

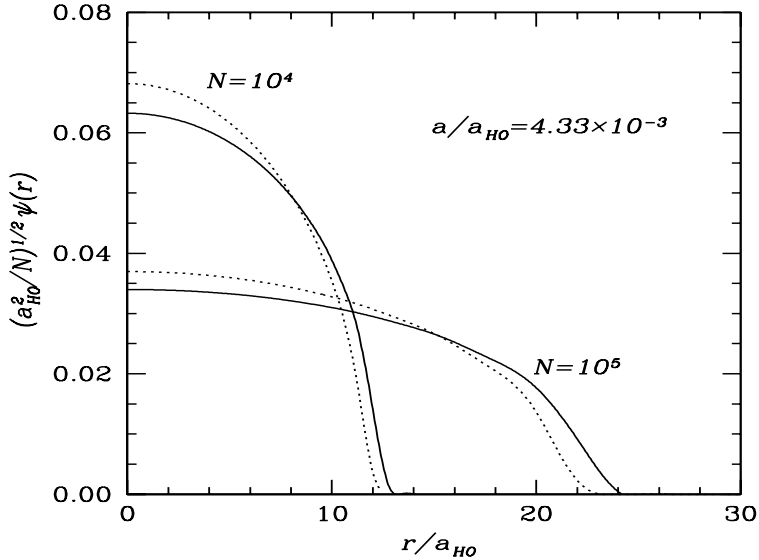


FIG. 1. The condensate wave function  $\psi(r)$  as a function of the radial distance for a system of  $N = 10^4$  and  $N = 10^5$  atoms and hard-disk radius  $a/a_{\text{HO}} = 4.33 \times 10^{-3}$ . The solid and dotted lines indicate the solutions of the mean-field equation with  $\ln |\psi|^2 a^2$  and  $\ln \bar{\rho} a^2$  factors, respectively, as explained in the text.

The interaction term in the local-density approximation based 2D GP equation we employ does not allow for negative scattering lengths, because of its quadratic dependence on  $a$ . In the Q2D model of Petrov, Holtzmann, and Shlypanikov [24] the attractive mean-field interaction is shown to have a resonant character, namely, becoming repulsive for very large values of  $a_{\text{HO}}^z$ . This would mean a large asymmetry parameter  $\lambda$  as defined previously, and hence a more 2D-like condensate. We have not systematically compared our results with the predictions of coupling constant proposed by Petrov, Holtzmann, and Shlypanikov [24] but surmise that variable asymmetry parameter  $\lambda$  would yield results similar to the previous examples.

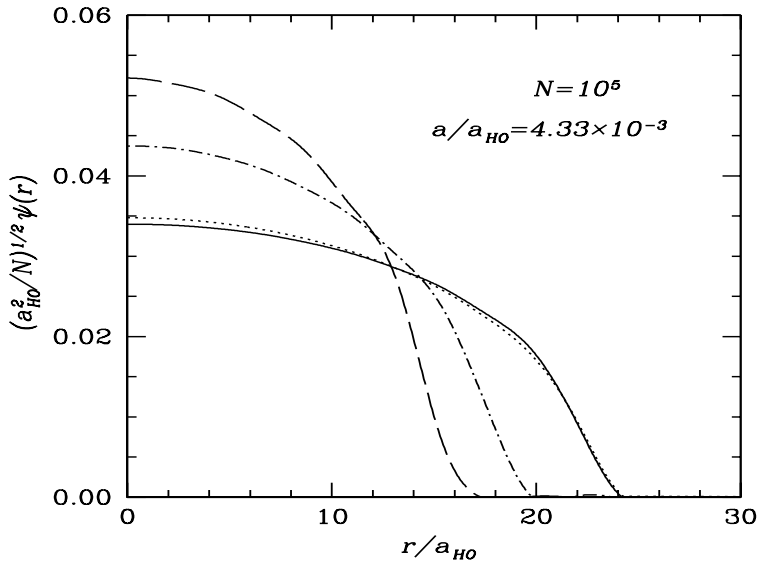


FIG. 2. The condensate wave function  $\psi(r)$  with  $|\ln \psi^2 a^2|^{-1}$  correction (solid line) as a function of the radial distance for a system of  $N = 10^5$  atoms and hard-disk radius  $a/a_{\text{HO}} = 4.33 \times 10^{-3}$ , compared to that with the simplified interaction. The dashed, dot-dashed, and dotted lines correspond to the asymmetry parameter  $\lambda = 10$ ,  $\lambda = 20$ , and  $\lambda = 50$ , respectively.

Recent experiments by Cornish *et al.* [33] have demonstrated the feasibility of tuning the scattering length through Feshbach resonances. This opens the possibility of studying the effects of interactions and regimes those described beyond the Gross-Pitaevskii equation more systematically. To understand how the condensate wave function is affected by the interaction strength (i.e. hard-disk radius  $a$ ), we display in Fig. 3 the solution of Eq. (4) for three different values of  $a$ . We observe that for a fixed number of particles, as  $a$  increases the condensate wave function is depleted in the center and middle regions and is extended to a larger spatial region. In all the examples shown in Fig. 3 our chosen parameters fulfill the diluteness condition, thus the form of the GP equation should be adequate. For much larger values of  $N$  and  $a$ , it may be necessary to include the higher order corrections provided by the perturbative results for homogeneous 2D bosons.

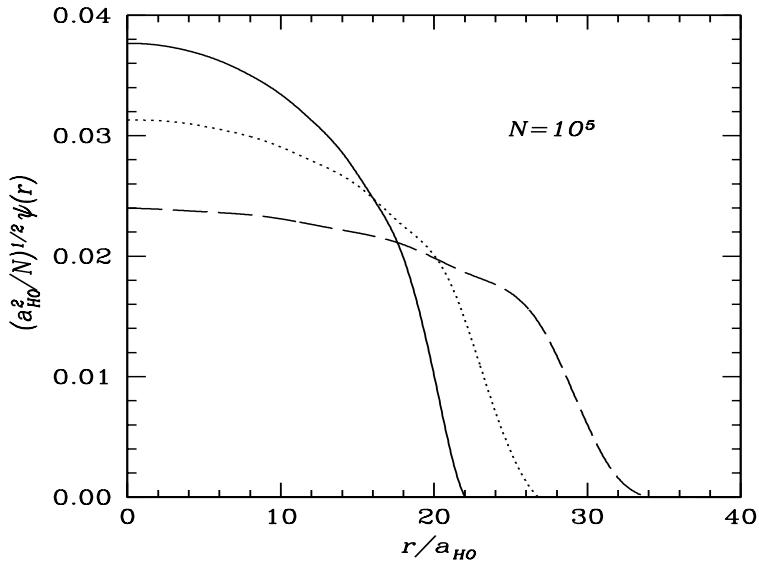


FIG. 3. The condensate wave function  $\psi(r)$  as a function of the radial distance for a system of  $N = 10^5$  atoms, at different values of the hard-disk radius  $a$ . The solid, dotted, and dashed lines correspond to  $a/a_{\text{HO}} = 10^{-3}$ ,  $a/a_{\text{HO}} = 10^{-2}$ , and  $a/a_{\text{HO}} = 5 \times 10^{-2}$ , respectively.

In summary, we have compared several forms of the 2D Gross-Pitaevskii equation as suggested in the literature. We have found that the local-density approximation based approach without any adjustable parameters yields quantitatively different results compared to simplified models. However, taking the tightly confined direction into account in terms of the asymmetry parameter provides qualitative and quantitative agreement with the Q2D models. It would be interesting to extend the calculations presented here in several directions. First, the finite temperature effects would be necessary to elucidate the thermodynamics of the system around the Bose-Einstein transition temperature. The role of the  $|\ln \psi^2 a^2|^{-1}$  correction to the GP equation and the interaction with non-condensed thermal particles awaits a separate study. Even at zero temperature the ground-state energy and wave function of the vortex state would be interesting to explore. To better understand the significance of interaction and high-density effects, precision Monte Carlo simulations would be useful as a test of the range of validity of the mean-field approximations.

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## REFERENCES

- [1] M. H. Anderson, J. R. Ensher, M. R. Matthews, C. E. Wieman, and E. A. Cornell, *Science* **269**, 198 (1995); K. B. Davis, M.-O. Mewes, M. R. Andrews, N. J. van Druten, D. S. Durfee, D. M. Kurn, and W. Ketterle, *Phys. Rev. Lett.* **75**, 3969 (1995); C. C. Bradley, C. A. Sackett, and R. G. Hulet, *Phys. Rev. Lett.* **78**, 985 (1997).
- [2] F. Dalfovo, S. Giorgini, L. Pitaevskii, and S. Stringari, *Rev. Mod. Phys.* **71**, 463 (1999); A. S. Parkins and D. F. Walls, *Phys. Rep.* **303**, 1 (1998); A. J. Leggett, *Rev. Mod. Phys.* **73**, 307 (2001); Ph. W. Courteille, V. S. Bagnato, V. I. Yukalov, *Laser Phys.* **11**, 659 (2001).
- [3] V. Bagnato and D. Kleppner, *Phys. Rev. A* **44**, 7439 (1991); S. I. Shevchenko, *Sov. J. Low Temp. Phys.* **16**, 64 (1990).
- [4] W. J. Mullin, *J. Low Temp. Phys.* **110**, 167 (1998).
- [5] E. A. Hinds, M. G. Boshier, and I. G. Hughes, *Phys. Rev. Lett.* **80**, 645 (1998).
- [6] H. Gauck, M. Hartl, D. Schneble, H. Schnitzler, T. Pfau, and J. Mlynek, *Phys. Rev. Lett.* **81**, 5298 (1998).
- [7] V. Vuletić, C. Chin, A. J. Kerman, and S. Chu, *Phys. Rev. Lett.* **81**, 5768 (1998); V. Vuletić, A. J. Kerman, C. Chin, and S. Chu, *ibid.* **82**, 1406 (1999); V. Vuletić, C. Chin, A. J. Kerman, and S. Chu, *ibid.* **83**, 943 (1999).
- [8] I. Bouchoule, H. Perrin, A. Kuhn, M. Morinaga, and C. Salomon, *Phys. Rev. A* **59**, 8 (1999); M. Morinaga, I. Bouchoule, J.-C. Karam, and C. Salomon, *Phys. Rev. Lett.* **83**, 4037 (1999).
- [9] S. Dettmer, D. Hellweg, P. Ryytty, J. J. Arlt, W. Ertmer, K. Sengstock, D. S. Petrov, G. Y. Shlyapnikov, H. Kreutzmann, L. Santos, and M. Lewenstein, preprint cond-mat/0105525.
- [10] A. Görlitz, J. M. Vogels, A. E. Leanhardt, C. Raman, T. L. Gustavson, J. R. Abo-Shaeer, A. P. Chikkatur, S. Gupta, S. Inouye, T. P. Rosenband, D. E. Pritchard, and W. Ketterle, *Phys. Rev. Lett.* **87**, 130402 (2001).
- [11] T. Haugset and H. Haugerud, *Phys. Rev. A* **57**, 3809 (1998).
- [12] M. Bayindir and B. Tanatar, *Phys. Rev. A* **58**, 3134 (1998).
- [13] J. G. Kim and E. K. Lee, *J. Phys. B* **32**, 5575 (1999).
- [14] S. K. Adhikari, *Phys. Lett. A* **265**, 91 (2000).
- [15] S. Heinrichs and W. J. Mullin, *J. Low Temp. Phys.* **113**, 231 (1998); S. Pearson, T. Pang, and C. Chen, *Phys. Rev. A* **58**, 4811 (1998).
- [16] R. K. Bhaduri, S. M. Reimann, S. Viefers, A. G. Choudhury, and M. K. Srivastava, *J. Phys. B* **33**, 3895 (2000).
- [17] Y. S. Kivshar and T. J. Alexander, preprint cond-mat/9905048.
- [18] J. G. Kim, K. S. Kang, B. S. Kim, and E. K. Lee, *J. Phys. B* **33**, 2559 (2000).
- [19] S.-H. Kim, C. Won, S. D. Oh, and W. Jhe, preprint cond-mat/9904087.
- [20] S. I. Shevchenko, *JETP* **73**, 1009 (1991).
- [21] S. I. Shevchenko, *Sov. J. Low Temp. Phys.* **18**, 223 (1992).
- [22] E. B. Kolomeisky, T. J. Newman, J. P. Straley, and X. Qi, *Phys. Rev. Lett.* **85**, 1146 (2000).
- [23] E. H. Lieb, R. Seiringer, and J. Yngvason, preprint cond-mat/0005026, *Commun. Math. Phys.*

- [24] D. S. Petrov, M. Holzmann, and G. V. Shlyapnikov, Phys. Rev. Lett. **84**, 2551 (2000).
- [25] E. P. Gross, Nuovo Cimento **20**, 454 (1961); L. P. Pitaevskii, Zh. Eksp. Teor. Fiz. **40**, 646 (1961) [Sov. Phys. JETP **13**, 451 (1961)].
- [26] G. S. Nunes, J. Phys. B **32**, 4293 (1999).
- [27] A. Fabrocini and A. Polls, Phys. Rev. A **60**, 2319 (1999).
- [28] M. Schick, Phys. Rev. A **3**, 1067 (1971).
- [29] A. Banerjee and M. P. Singh, Phys. Rev. A **64**, 063604 (2001).
- [30] J. O. Andersen and H. Haugerud, preprint cond-mat/0012101.
- [31] F. Dalfovo and S. Stringari, Phys. Rev. A **53**, 2477 (1996).
- [32] W. Krauth, Phys. Rev. Lett. **77**, 3695 (1996).
- [33] S. L. Cornish, N. R. Claussen, J. L. Roberts, E. A. Cornell, and C. E. Wiemann, Phys. Rev. Lett. **65**, 1795 (2000).