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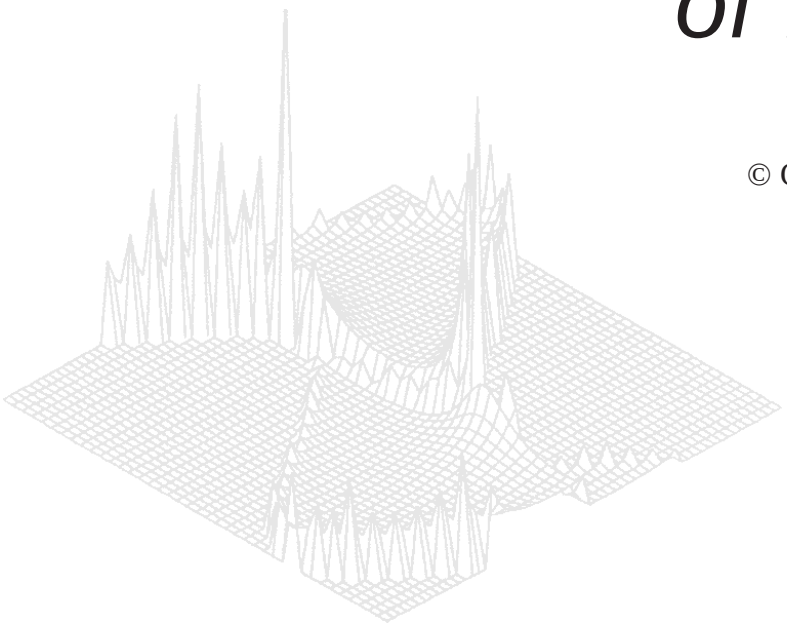

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Bose–Einstein Condensation of Atoms with Attractive Interaction in a Harmonic Trap*

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Abstract

It is well known that bosonic particles with attractive interaction in a uniform gas do not form a condensate. Here we investigate a dilute Bose gas and study stationary solutions of the Gross–Pitaevskii equation with attractive interaction. We have also used a higher order stabilising term in the presence of a harmonic confining potential. We show that there are three possible types of stationary solutions corresponding to stable, metastable and unstable phases. These results are discussed in relation to a ^{7}Li condensate.

In 1961 Gross and Pitaevskii independently proposed a study of the properties of the Bose condensate at zero temperature using a nonlinear equation now widely referred to as the Gross–Pitaevskii equation (GPE). This is a mean field equation for a slowly varying order parameter of the system of Bose particles. The original GPE accounted only for two-body collisions in the system through the quartic term in the GP functional. Subsequently many body processes can be taken into account (Popov 1983) with the modified GPE in the form

$$i\hbar\frac{\partial}{\partial t}\Psi = -\frac{\hbar^2}{2m}\Delta\Psi + \frac{4\pi\hbar^2 a}{m}\left|\Psi\right|^2\Psi + \frac{\delta\Sigma\left(\Psi,\Psi^+\right)}{\delta\Psi^+} + U(r)\Psi\,, \tag{1}$$

where Ψ denotes a collective wave function, a is the scattering length of the two-body collision process, Σ denotes all connected diagrams of the corresponding perturbation theory and U is one-body external potential. In a dilute gas, where many-body collisions are rare, Σ can be neglected. The linearisation of the resulting truncated equation is equivalent to the Bogoliubov approximation for the dilute Bose gas (ter Haar 1977).

For bosonic systems the existence of stable stationary solutions of the GPE provides preliminary evidence for the occurrence of the condensate at $T = 0$. It is well known that non-zero stable solutions of the GPE in the thermodynamic

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limit ($\Psi \to$ const at $r \to \infty$) exist only for a positive scattering length, i.e. when particles are repulsive. For a negative scattering length the spectrum of the linearised GPE has an imaginary component which indicates instability, and the complete solution of the nonlinear GPE is known to collapse in finite time (Zhakharov 1972). The same instability persists in the Bogoliubov spectrum, which leads to the conclusion that the Bose condensate does not exist for the systems with negative scattering length (see e.g. Landau and Lifshitz 1980 and ter Haar 1977).

During the past four years there have been experiments on ultracold dilute vapours of alkali atoms in magnetic traps which seem to exhibit Bose condensation in the nano-Kelvin temperature range (Anderson *et al.* 1995; Davis *et al.* 1995; Bradley *et al.* 1995, 1997). While ^{87}Rb and ^{23}Na are atoms of positive scattering lengths with repulsive potentials, Bose condensation is not a surprise in these systems. In the case of ^{7}Li, which has a negative scattering length (Abraham *et al.* 1995) and, according to theory (ter Haar 1977), is not supposed to Bose condense, traces of condensate have been observed (Bradley *et al.* 1995, 1997).

Several recent theoretical attempts have been made to understand condensation phenomena in dilute finite systems (Fetter 1996; Shuryak 1996; Bijlsma 1996; Krauth 1996; Kagan *et al.* 1996; Ruptecht *et al.* 1995; Ueda and Leggett 1998; Sackett *et al.* 1998; see also the two special journal issues on Bose–Einstein condensation published in 1996 and 1997).

In particular Baym and Pethick (1996) have used simple scaling arguments to show the spatial structure of the condensate as a result of interaction. Fetter (1996) has made a variational estimate of the critical condensate number ($N = 1440$) for the systems with negative scattering length and found that a stable condensate may exist below this critical number. Similar results have been obtained by Ruprecht *et al.* (1995) in their mean field calculations. Shuryak (1996) has argued that the metastable state of the condensate is due to an attractive interaction. The authors of these works only used terms up to $|\psi|^4$ in the GP functional. In this case, the stable condensate exists below some critical number of particles N, which is confirmed by our theory as well.

When the number of atoms is higher than the critical value, the collapse of the GPE with negative scattering length means that a system undergoes a transition to a denser state where Σ can no longer be neglected and higher-order terms in the perturbation series are to be taken in the GPE. Then these terms become crucial for stabilisation of the condensate in systems with an attractive potential. Mention may be made of the recent work of Sackett *et al.* (1998) and Kagan *et al.* (1998) who have emphasised the effect of three-body forces with regard to recombination in the condensate. We may mention that in a different context Pacheco and Prates Ramalho (1998) have shown that the three-body dispersive interaction, known as the Axilrod–Teller interaction, provides a repulsive contribution to the configurational energy.

In this paper we find stable and metastable stationary solutions of the GPE with negative scattering length and with a quintic stabilising term accounting for the three-body interaction:

$$i\hbar\frac{\partial}{\partial t}\Psi = -\frac{\hbar^2}{2m}\Delta\Psi + \frac{4\pi\hbar^2 a}{m}\left|\Psi\right|^2\Psi + \beta\left|\Psi\right|^4\Psi + U(r)\Psi\,, \tag{2}$$

where

$$U(r) = \tfrac{1}{2}\ m\omega^2 \left(x^2 + y^2 + z^2\right) . \tag{3}$$

In the experiments with ultracold gases the magnetic trap is anisotropic. However, in this work we use an isotropic potential for simplicity. Clearly, a small anisotropy will not affect the qualitative aspect of the results.

The free energy functional which generates equation (2) is

$$F = \int_V d^3r \left[\frac{\hbar^2}{2m} |\nabla\Psi|^2 + \frac{m\omega^2}{2} \left(x^2 + y^2 + z^2\right) |\Psi|^2 + \frac{2\pi\hbar^2 a}{m} |\Psi|^4 + \frac{\beta}{3} |\Psi|^6 \right] . \tag{4}$$

This functional is an integral of motion of the GPE. The number of particles in the system is given by another integral of motion

$$N = \int_V d^3r\, |\Psi|^2 . \tag{5}$$

It is convenient to remove the fast time dependence in the wave function by the substitution

$$\Psi(r,t) = \exp(-i\mu t/\hbar)\ \psi(r,t) , \tag{6}$$

where μ is the chemical potential of the system. For stationary solutions $\psi(r,t)$ does not depend on t. The stationary solutions comprise one parameter family with μ as a parameter. For the one parameter family, there is a continuous correspondence between the values F, N and μ. In other words, the values F, N and μ are located on a line in a three-dimensional space.

Equation (2) with the ansatz (6) can be written in the canonical form

$$i\hbar \frac{\partial\psi}{\partial t} = \frac{\delta}{\delta\psi^*}(F - \mu N) , \tag{7}$$

where $(\delta/\delta\psi^*)$ means a variational derivative. It can be seen from (7) that stationary solutions are the extrema of F for a constant N. Moreover, stationary solutions which have absolute minima of F at a given N are stable relative to small perturbations. Conversely, stationary solutions which have maxima of F at a given N are unstable. The stationary solutions which obey the local minima of F can be called metastable. All three types of solutions exist for the system under consideration. It can be shown (Grillakis *et al.* 1987) that for a one-parameter family of (ground state) stationary solutions the stability criterion which follows from the condition of local or absolute minimum of the free energy is

$$\frac{\partial N}{\partial \mu} > 0 . \tag{8}$$

Clearly, this criterion is for the stable and metastable solutions. To make definite conclusions about the stability of stationary solutions using the above criteria, we have to use both the dependences $F(N)$ and $N(\mu)$.

Since the external trap potential is taken to be symmetric, it is convenient to rewrite equation (2) using a spherical coordinate system. Also, since we are interested in the 'ground state' solutions, ϕ is taken to depend only on $R = (x^2 + y^2 + z^2)^{\frac{1}{2}}$ and the resulting equation reads

$$-\frac{\partial^2}{\partial r^2}\phi(r) - \frac{2}{r}\frac{\partial}{\partial r}\phi(r) + r^2\phi(r) + 8\pi\frac{a}{l}|\phi(r)|^2\phi(r) + \beta'|\phi(r)|^4\phi(r) = \mu'\phi(r), \tag{9}$$

where $l = (\hbar/m\omega)^{\frac{1}{2}}$ is the trapping length. To obtain equation (9) we used the following substitution:

$$\psi \to \frac{1}{l^{\frac{3}{2}}}\phi, \qquad R \to lr, \qquad \mu \to \hbar\tfrac{1}{2}\omega\mu', \qquad \beta \to \tfrac{1}{2}\hbar\omega l^6\beta'\,. \tag{10}$$

The energy of the system $E = \hbar\omega F$ and the number of particles N are given by

$$F = 4\pi\int_0^\infty r^2 dr\left[\tfrac{1}{2}\left|\frac{\partial}{\partial r}\phi\left(r\right)\right|^2 + \tfrac{1}{2}r^2\left|\phi\left(r\right)\right|^2 + 2\pi\frac{a}{l}\left|\phi\left(r\right)\right|^4 + \frac{\beta'}{6}\left|\phi\left(r\right)\right|^6\right],$$

$$N = 4\pi\int_0^\infty r^2 dr\left|\phi\left(r\right)\right|^2\,. \tag{11}$$

This one-dimensional equation is subject to the boundary conditions

$$\frac{\partial}{\partial r}\phi(r)|_{r\to 0} = 0, \quad \phi t(r) \to 0 \quad \text{as} \quad r \to \infty\,. \tag{12}$$

The function ϕ can be taken to be real in equations (9) and (11).

Numerical solution of equation (9) subject to (12) is obtained by the following procedure. First we chose $\phi(0)$ to be a constant and then find a solution of (9) at some remote point, say r_0, using this value and $\phi'(0) = 0$. Then varying the initial value of $\phi(0)$ we try to achieve the condition $\phi(r_0) = 0$. This will give us a stationary solution of the GPE. Since r_0 can be chosen arbitrarily large and solutions of the problem are expected to fall quickly for large r, the solution is practically independent of r_0.

In the calculations we take parameters close to those in the experiment (Baym and Pethick 1996) for ^{7}Li, i.e. $a = -27a_0$ and $\omega/2\pi = (\omega_y + \omega_x)/2\pi = 140$ Hz. The results of the calculations are shown in Fig. 1 as the functions $N(\mu)$ and $F(\mu)$, and in Fig. 2 which shows a plot of the free energy versus number of particles in the condensate $F(N)$. For the parameter β, which results from three-body collisions, no experimental estimate is available. In Fig. 1 we have chosen several values of β' to demonstrate the qualitative features of the solutions. When $\beta' = 0$ (see the curve I) there are two solutions with the same number of particles but for different μ. The solutions of the first branch (up to the point A) are stable due to the criterion (8). The solutions of the second branch (to the right of point A) are unstable. These stability results can also be confirmed

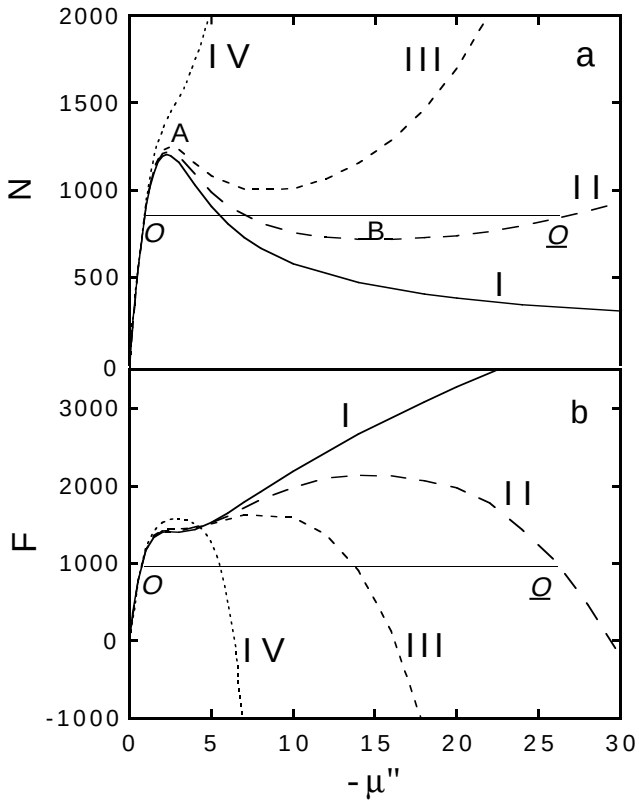

Fig. 1. (a) Number of particles N and (b) the free energy F versus the chemical potential μ. For clarity the lowest eigenvalue of the harmonic oscillator is subtracted from the chemical potential μ. Curve I corresponds to $\beta' = 0$, curve II to $\beta' = 3 \times 10^{-7}$, curve III to $\beta' = 6 \times 10^{-7}$, and curve IV to $\beta' = 2{\cdot}4 \times 10^{-6}$. The points O and $\underline{O}$ are the ones where the stable solution becomes metastable for the curve II.

using Fig. 2a. The solutions of the lower branch have an absolute minimum of free energy and they are stable. The solutions of the upper branch have a local maximum of free energy and therefore they are unstable. These results are in agreement with those of Fetter (1996) who predicted stability of the condensate below some critical number N. In his calculations the critical number was 1440, whereas in our case this number is ≈ 1200. The deviation can be related to a slightly different set of parameters which Fetter used for estimates and to the inaccuracy of the variational approach developed by Fetter (1996). The calculations for $\beta' = 0$, but for a positive scattering length a, have been done previously by many authors (see e.g. Ruprecht *et al.* 1995). In this case the condensate is always stable.

Another extreme case appears when β' is higher than a certain threshold (curves IV in Figs 1 and 2). In this case, the free energy is a single-valued function of N which, for the ground state, is a minimum and the condensate is again always stable.

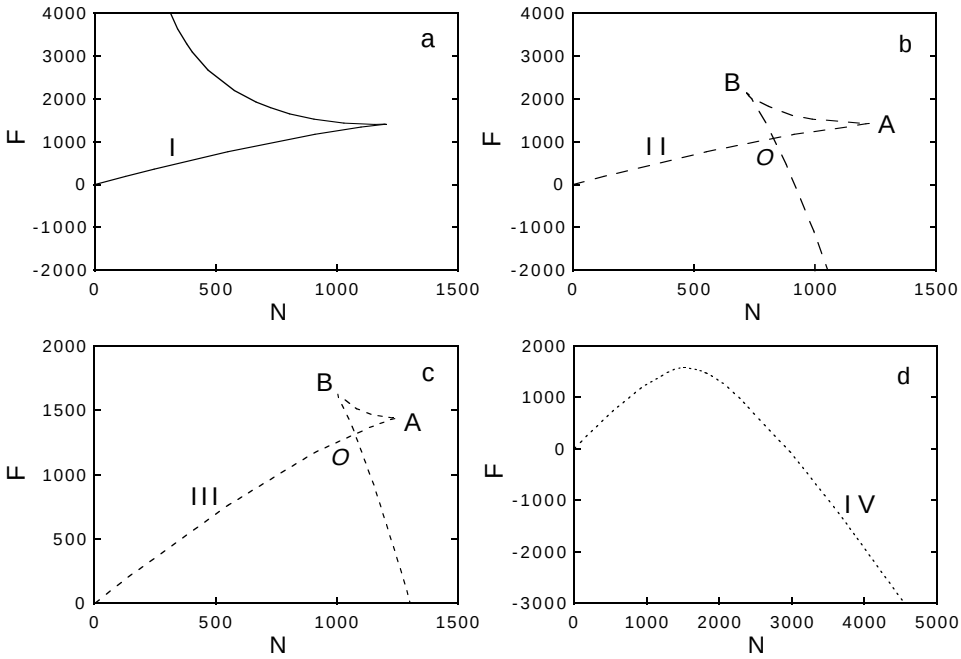

Fig. 2. Free energy F versus the number of particles in the condensate N for the four values of β' given in Fig. 1.

The most interesting case appears at intermediate values of β' (curves II and III). One can distinguish three different intervals in these graphs: $[0, A]$, $[A, B]$ and $[B, +\infty]$. In the first interval $[0, A]$, the stationary solution is stable. Stability in this interval is controlled by the external parabolic potential. The term $|\Psi|^6$ in equation (4) does not play any significant role in this interval and the $N(\mu)$ and $F(\mu)$ functions are nearly independent of β'. The stabilising effect of the external potential has already been observed in the literature (Dalfovo and Stringari 1996). It results from the suppression of the Fourier component $(k \to 0)$ of the linearised GPE.

When the number of particles in the condensate reaches some critical number [point A with zero derivative $dN/d\mu$ in the diagram $N(\mu)$], the system becomes unstable relative to perturbations which tend to collapse it to a denser phase. The critical number of particles in the condensate is directly proportional to the trapping length l. This can be easily shown by changing ω in the energy functional (4), so that the ratio between the new and the old rotational frequency is $\omega/\omega' = (l'/l)^2 = \gamma^2$. Then the energy functional and the number of particles become

$$F = \frac{4\pi}{\gamma^2} \int_0^\infty r'^2 dr' \left[\tfrac{1}{2} \left| \frac{\partial}{\partial r'} \phi(r') \right|^2 + \tfrac{1}{2} r'^2 \left| \phi(r') \right|^2 + 2\pi \frac{a}{l\gamma} \left| \phi(r') \right|^4 \right],$$

$$N = 4\pi \int_0^\infty r'^2 dr' \left| \phi(r') \right|^2 . \tag{13}$$

Now we perform the substitution $\phi \to \gamma^{\frac{1}{2}}\phi'$. Then equations (13) become

$$F' = \frac{4\pi}{\gamma}\int_0^\infty r'^2 dr' \left[\frac{1}{2}\left|\frac{\partial}{\partial r'}\phi'(r')\right|^2 + \frac{1}{2}r'^2\left|\phi'(r')\right|^2 + 2\pi\frac{a}{l}\left|\phi'(r')\right|^4\right],$$

$$N' = 4\pi\gamma\int_0^\infty r'^2 dr' \left|\phi'(r')\right|^2 . \tag{14}$$

It is now obvious that equation (14) leads to the stationary GPE (2) for ϕ' with the old scattering length a. So, for all ω solutions the GPE is the same and only the energy and number of particles N will change inversely proportional to ω. The maximum density of the particles in the condensate thus becomes

$$\rho_{\max} = \frac{3N'}{4\pi l'^3} = \frac{\text{const}}{\gamma^2} . \tag{15}$$

The maximum density increases for small traps and decreases for shallow traps. In the thermodynamic limit the density becomes zero as expected.

The minimal number of particles required for the formation of a stable denser phase is represented in Figs 1 and 2 by the point B on curve II. The term of sixth order in the functional (4) at this point becomes approximately comparable in value with the fourth order term. Solutions which correspond to the parts of the curves II and III between the points A and B are unstable as follows from (8). The solutions in the intervals $[0, A]$ and $[B, +\infty]$ are stable due to the criterion (8). However, the free energy in these intervals is an absolute minimum only outside the interval between the points O and $\underline{O}$. Then F becomes a local minimum inside the intervals $[O, A]$ and $[B, \underline{O}]$, as follows from the diagrams in Figs 2*b* and 2*c*. Hence, the intervals $[0, A]$ and $[B, +\infty]$ are subdivided into regions where solutions are stable (the curves with the lowest F) or metastable (the intervals $[O, A]$ and $[B, \underline{O}]$), as can be seen from Figs 2*b* and 2*c*. Points of equal energy (points O) in the dilute and denser phase are connected in Fig. 1*a* by the line O–$\underline{O}$.

Fig. 1*a* is similar to a phase diagram for the first order phase transition (Zhakharov 1972). Indeed, the process of forming a denser phase consists of forming 'grains' of a denser phase which are increased with time—a typical first order transition scenario. How long the process of formation of the denser phase takes—whether the gas–liquid transition happens before the system reaches the denser condensate state or whether 'evaporation' of particles from the 'grains' prevents the system from achieving a denser phase—is beyond the scope of this article. A discussion can be found in Stoof (1994). With a decreasing value of β the 'transition line' $O - \underline{O}$ becomes lower. If β is significantly smaller than that taken in our trial calculations, then this line approaches $N = 0$, as seen in Figs 1 and 2.

The form of the external confinement potential does not seem very important at the qualitative level. A calculation with a potential well of the size l with infinite walls yields nearly the same results. The number of particles in a dilute condensate is directly proportional to the size of such a well. In the

thermodynamic limit the stable dilute phase of the condensate does not seem to exist.

In summary, we studied a confined Bose–Einstein condensate in systems with negative scattering length in the presence of a phenomenological three-body stabilising term. We found a localised solution of the GPE and investigated the stability of these solutions. We have shown that the equation has stable, metastable and unstable solutions. The diagram of the stability of solutions is similar to a diagram for the first order phase transition in statistical physics. Recently, this point has been further elaborated by Gammal *et al.* (1999). We found that there is a dilute condensate phase stabilised by an external potential and the denser condensate phase where the next orders in the expansion of Σ become important. The transition to the denser condensate phase is expected to be of first order. A further interesting case would be to study the dynamical solution of the NLSE in the presence of a three-body interaction including both elastic and inelastic processes. The inelastic interaction processes lead to three-body recombination. It is likely that by including the latter the stability of the condensate may be affected. This aspect needs further investigation.

Acknowledgments

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References

Abraham, E. R. I., McAlexander, W. I., Sackett, C. A., and Hulet, R. G. (1995). *Phys. Rev. Lett.* **74**, 1315.
Anderson, M. H., Ensher, J. R., Matthews, M. R., Weiman, C. E., and Cornell, E. A. (1995). *Science* **269**, 198.
Baym, G., and Pethick, C. (1996). *Phys. Rev. Lett.* **76**, 6.
Bijlsma, M., and Stoof, H. T. C. (1996). *Phys. Rev.* A **54**, 5085.
Bogolubov, N. N. (1947). *Izv. Akad. Nauk SSSR* **11**, 77.
Bradley, C. C., Sackett, C. A., Tollett, J. J., and Hulet, R. G. (1995). *Phys. Rev. Lett.* **75**, 168.
Bradley, C. C., *et al.* (1997). *Phys. Rev. Lett.* **78**, 985.
Dalfovo, F., and Stringari, S. (1996). *Phys. Rev.* A **53**, 2477.
Davis, K. B., Mewes, M. O., Andrews, M. R., van Druten, N. J., Durfee, D. S., Kurn, D. M., and Ketterle, W. (1995). *Phys. Rev. Lett.* **75**, 3969.
Fetter, A. (1996). *Phys. Rev.* A **53**, 4245.
Gammal, A., *et al.* (1999). cond-mat/9904184.
Grillakis, M., Shatah, J., and Strauss, W. (1987). *J. Function. Anal.* **74**, 160.
Gross, E. P. (1961). *Nuovo Cimento* **20**, 454.
Kagan, Yu., Muryshev, A. E., and Shlyapnikov, G. V. (1998). Preprint cond-mat/9801168.
Kagan, Yu., Shlyaprikov, G. V., and Walraven, J. T. M. (1996). *Phys. Rev. Lett.* **76**, 2670.
Krauth, W. (1996). *Phys. Rev. Lett.* **77**, 3695.
Landau, L. D., and Lifshitz, E. M. (1980). 'Statistical Physics', Parts 1&2 (Pergamon: Oxford).
Pacheco, J. M., and Prates Ramalho, J. P. (1998). *Phys. Rev. Lett.* **79**, 3873.
Pitaevskii, L. P. (1961). *Sov. Phys. JETP* **13**, 451.
Popov, V. N. (1983). 'Functional Integrals in Quantum Field Theory and Statistical Physics', p. 123 (Reidel: Dordrecht).

Ruprecht, P. A., Holland, M. J., Burnett, K., and Edwards, M. (1995). *Phys. Rev.* A **51**, 4704.
Sackett, C. A., Stoof, H. T. C., and Hulet, R. G. (1998). *Phys. Rev. Lett.* **80**, 2031.
Shuryak, E. V. (1996). *Phys. Rev.* A **54**, 3151.
Special issue on BEC (1996). *J. Res. NIST* **101**, Number 4.
Special Issue on BEC (1997). *J. Modern Opt.* **44**, Number 10.
Stoof, H. T. C. (1994). *Phys. Rev.* A **49**, 3824.
ter Haar, D. (1977). 'Lectures on Selected Topics in Statistical Mechanics' (Pergamon: London).
Ueda, M., and Leggett, A. J. (1998). *Phys. Rev. Lett.* **80**, 1576.
Zhakharov, V. E. (1972). *Zh. Eksp. Teor. Fiz.* **62**, 1745 [Engl. trans. *Sov. Phys. JETP* **35**, 908].

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