Abstract: The notion of fluctuation indices, characterizing thermodynamic stability of statistical systems, is advanced. These indices are especially useful for investigating the stability of nonuniform and trapped atomic assemblies. The fluctuation indices are calculated for several systems with Bose-Einstein condensate. It is shown that: the ideal uniform Bose-condensed gas is thermodynamically unstable; trapped ideal gases are stable for the confining dimension larger than two; trapped gases, under the confining dimension two, are weakly unstable; harmonically trapped gas is stable only for the spatial dimension three; one-dimensional harmonically trapped gas is unstable; two-dimensional gas in a harmonic trap represents a marginal case, being weakly unstable; interacting nonuniform three-dimensional Bose-condensed gas is stable. There are no thermodynamically anomalous particle fluctuations in stable Bose-condensed systems.

Fluctuation indices for atomic systems with Bose-Einstein condensate

V.I. Yukalov 1,2,*

1 Bogolubov Laboratory of Theoretical Physics, Joint Institute for Nuclear Research, Dubna 141980, Russia
2 National Institute of Optics and Photonics, University of São Paulo, São Carlos 13560-970, Brazil

Received: 26 July 2010, Accepted: 29 July 2010
Published online: 31 August 2010

Key words: thermodynamic limit; stability conditions; Bose systems; particle fluctuations; trapped Bose gases; Bose-Einstein condensate

1. Introduction

Thermodynamic stability of statistical systems is an important notion characterizing the possibility of existence of equilibrium systems as such. There are several stability conditions that are required to be fulfilled in order that the system be thermodynamically stable [1]. In the present paper, we concentrate on the stability related to fluctuations of observable quantities. These fluctuations are to be thermodynamically normal as soon as one assumes that the considered system is in thermal equilibrium. In the other case, if the fluctuations of at least one of the observables are thermodynamically abnormal, this implies that this observable cannot be measured and the system equilibrium is actually destroyed by such fluctuations, which explains their naming as anomalous.

The problem of instability, caused by fluctuations, has recently attracted great attention with respect to nonuniform confined systems, such as trapped atomic gases. Especially intensive discussions on the type of particle fluctuations have accompanied the study of systems with Bose-Einstein condensate. Description of the main properties of the latter systems can be found in the book [2] and review articles [3–10].

In discussions of particle fluctuations in Bose-condensed systems, there have been the widely spread heresy that these fluctuations could be anomalous, been drastically different from such fluctuations in other systems. This controversy has been investigated in detail in
2. Fluctuation indices

2.1. Definition and stability conditions

The standard definition of thermodynamic limit implies that the number \( N \) of particles in the system and its volume \( V \) tend to infinity so that

\[
N \to \infty, \quad V \to \infty, \quad \frac{N}{V} \to \text{const}.
\]

(1)

This definition assumes that there is a well defined volume of the system.

However, for systems confined in trapping potentials, the volume may be not fixed. In such a case, it is necessary to resort to a more general definition of thermodynamic limit. The latter can be done as follows [10,14]. Let \( A_N \) be an extensive observable quantity for a system with the number of particles \( N \). Then the thermodynamic limit, related to this observable, is defined as

\[
N \to \infty, \quad A_N \to \infty, \quad \frac{A_N}{N} \to \text{const}.
\]

(2)

From here, it is seen that

\[
\lim_{N \to \infty} \frac{\ln |A_N|}{\ln N} \leq 1.
\]

(3)

In the particular case, when the system volume \( V \) is well defined, hence the extensive observable \( A_N \propto V \), definition (2) reduces to the standard form (1).

Fluctuations, associated with an observable, represented by a self-adjoint operator \( \hat{A} \), are described by the dispersion, or variance, of this operator, given by the statistical average

\[
\text{var}(\hat{A}) \equiv \langle (\hat{A} - \langle \hat{A} \rangle)^2 \rangle = \langle \hat{A}^2 \rangle - \langle \hat{A} \rangle^2.
\]

The fluctuation index, related to the observable quantity \( \langle \hat{A} \rangle \), represented by a self-adjoint operator \( \hat{A} \), is defined as the limit

\[
\varphi(\hat{A}) \equiv \lim_{N \to \infty} \frac{\ln \text{var}(\hat{A})}{\ln N}.
\]

(4)

Since the variance itself is an extensive observable, it has to satisfy the stability conditions

\[
\varphi(\hat{A}) \leq 1, \quad \lim_{N \to \infty} \frac{\text{var}(\hat{A})}{N} < \infty,
\]

(5)

in agreement with Eq. (3). The first of these conditions is necessary, characterizing the behavior of fluctuations in thermodynamic limit, while the second condition is necessary and sufficient. When both these conditions are valid, the system is stable. It may happen that the first condition is valid, but the second is not. In the latter case, we shall say that the system is weakly unstable.

Fluctuations, satisfying Eq. (5), are called thermodynamically normal, while fluctuations, for which conditions (5) are not valid, are termed thermodynamically anomalous. This is because an observable with normal fluctuations can be measured, but that with anomalous ones, cannot, as soon as the magnitude of fluctuations, hence the measurement uncertainty, is larger than the observable itself. A statistical system, where at least one of the observables exhibits anomalous fluctuations, cannot be in thermal equilibrium. Such a system is thermodynamically unstable.

2.2. Uniform ideal gas

Let us consider particle fluctuations in a system with Bose-Einstein condensate. The particle-number operator \( \hat{N} \) is the sum

\[
\hat{N} = \hat{N}_0 + \hat{N}_1
\]

of the terms corresponding to condensed particles (\( \hat{N}_0 \)) and uncondensed particles (\( \hat{N}_1 \)). In thermodynamic limit, by the Bogolubov theorem [15], the operator \( \hat{N}_0 \) becomes a nonoperator number, so that

\[
\text{var}(\hat{N}_0) \to 0 \quad (N \to \infty).
\]

This fact is discussed in detail in review [8]. Therefore, particle fluctuations are completely due to uncondensed particles,

\[
\text{var}(\hat{N}) = \text{var}(\hat{N}_1).
\]

(6)

For the ideal uniform Bose-condensed gas, confined in a volume \( V \), the condensation temperature is

\[
T_c = \frac{2\pi}{m} \left[ \frac{\rho}{\zeta(d/2)} \right]^{2/d},
\]

(7)
where $d$ is space dimensionality, $\rho$ is average density, and $\zeta(\cdot)$ is the Riemann zeta function. Below this temperature, the condensate fraction behaves as

$$n_0 = 1 - \left( \frac{T}{T_c} \right)^{d/2}, \quad (T \leq T_c).$$  \hspace{1cm} (8)

However, a finite critical temperature (7) exists only for $d \geq 3$. This is a general feature of the absence of spontaneous breaking of continuous symmetry in low-dimensional systems [16].

In the three-dimensional space, one has

$$\text{var}(\tilde{N}_1) = \left( \frac{MT}{\pi} \right)^2 \nu^{4/3}. \hspace{1cm} (9)$$

Taking into account Eq. (6) gives the fluctuation index

$$\varphi(\tilde{N}) = \frac{4}{3} \hspace{1cm} (10)$$

that contradicts the stability condition (5). This tells us that the ideal uniform Bose-condensed gas is unstable, being a pathological object with thermodynamically anomalous particle fluctuations.

### 2.3. Trapped Bose gas

An interesting question is whether the ideal Bose-condensed gas could be stabilized being trapped in an external potential. The most often used shape of the trapping potential is of the power-law form

$$U(r) = \sum_{\alpha=1}^{d} \frac{\omega_\alpha}{2} \left[ \frac{r_\alpha}{l_\alpha} \right]^{n_\alpha}, \hspace{1cm} (11)$$

in which $n_\alpha > 0$ and the trap frequencies and characteristic lengths are connected by the relations

$$\omega_\alpha = \frac{1}{ml_\alpha^2}, \quad l_\alpha = \frac{1}{\sqrt{m}\omega_\alpha}. \hspace{1cm} (12)$$

It is convenient to introduce the effective trap frequency and length by the geometric averages

$$\omega_0 \equiv \left( \prod_{\alpha=1}^{d} \omega_\alpha \right)^{1/d} = \frac{1}{ml_0^2}, \hspace{1cm} (13)$$

$$l_0 \equiv \left( \prod_{\alpha=1}^{d} l_\alpha \right)^{1/d} = \frac{1}{\sqrt{m}\omega_0}. \hspace{1cm} (14)$$

Another important quantity, defining the confining power of potential (11), is the \textit{confining dimension}

$$s \equiv \frac{d}{2} + \sum_{\alpha=1}^{d} \frac{1}{n_\alpha}, \hspace{1cm} (15)$$

where $d$ is the real-space dimension.

The properties of the ideal trapped Bose gas can be accurately described by the generalized quasiclassical approximation [14]. Bose-Einstein condensation occurs at the critical temperature

$$T_c = \left[ \frac{N}{Bg_s(1)} \right]^{1/s}, \hspace{1cm} (16)$$

in which

$$B \equiv \frac{2^s}{\pi^{d/2}} \sum_{\alpha=1}^{d} \frac{\Gamma(1 + 1/n_\alpha)}{\omega_\alpha^{1/2+1/n_\alpha}},$$

and the generalized Bose function

$$g_s(z) \equiv \frac{1}{\Gamma(s)} \int_{u_0}^{\infty} \frac{z^{u-1}}{e^u - z} \, du \hspace{1cm} (17)$$

is introduced [14], with the lower limit in the integral being

$$u_0 \equiv \frac{\omega_0}{2T}. \hspace{1cm} (18)$$

Note that the standard Bose function corresponds to the limiting case of $u_0 = 0$. Below the critical temperature (15), the condensate fraction is

$$n_0 = 1 - \left( \frac{T}{T_c} \right)^s \hspace{1cm} (T \leq T_c). \hspace{1cm} (19)$$

But the formal occurrence of a critical temperature does not necessarily mean the real existence of a stable Bose-condensed system. To check the stability with respect to particle fluctuations, we have to calculate the related fluctuation index. The trapping potential (11) extends to infinity, so that the system volume is not fixed. Hence, the general form of thermodynamic limit (2) is to be employed. As an extensive quantity, we can take the internal energy $E_N$, considering the thermodynamic limit in the form

$$N \to \infty, \quad E_N \to \infty, \quad \frac{E_N}{N} \to \text{const.} \hspace{1cm} (20)$$

For the internal energy, we find

$$E_N = Bsg_{1+s}(1) T^{1+s}, \hspace{1cm} (21)$$

which transforms limit (20) into

$$N \to \infty, \quad B \to \infty, \quad \frac{B}{N} \to \text{const.} \hspace{1cm} (22)$$

For the usual case of unipower trapping potentials, when $n_\alpha = n$, the confining power (14) is

$$s = \left( \frac{1}{2} + \frac{1}{n} \right)d. \hspace{1cm} (23)$$
And quantity (16) becomes
\[ B = \frac{2^s}{\pi^{d/2} \sqrt{\omega_0}} \Gamma^d \left( 1 + \frac{1}{n} \right). \]

Then the thermodynamic limit (22) reduces to
\[ N \to \infty, \quad \omega_0 \to 0, \quad N\omega_0^s \to \text{const}. \]

Looking at limit (22), there arises a temptation to treat the quantity \( B \) as an effective volume. The latter, however, is not uniquely defined. And the most important is that such a quantity \( B \) cannot be used as a thermodynamic variable. Attempting to use it as such would lead to inconsistent thermodynamic relations. That is, though \( B \) reminds something like an effective volume, there is no any sense of identifying it with the latter.

Under the thermodynamic limit (22), or (25), the critical temperature (15) behaves as
\[ T_c \propto N^{1-1/s} \to 0 \quad (s < 1), \]
\[ T_c \propto (\ln N)^{-1} \to 0 \quad (s = 1), \]
\[ T_c \to \text{const} \quad (s > 1). \]

For the confining dimension \( s \leq 1 \) the critical temperature tends to zero. Hence, only \( s > 1 \) provides a finite critical temperature.

Again, the occurrence of a condensation temperature does not guarantee the existence of a stable Bose-condensed system. We need to find the fluctuation indices. For the variance of the particle number, we get
\[ \var(\hat{N}) = \frac{g_s-1(1)}{g_s(1)} \left( \frac{T}{T_c} \right)^s N. \]

This becomes negative for \( s < 1 \), which contradicts the definition of the variance as a non-negative quantity. Thus, only \( s \geq 1 \) can be considered. With the generalized Bose function (17), we find
\[ \var(\hat{N}) = 2 \left( \frac{T}{\omega_0} \right)^2 \quad (s = 1), \]
\[ \var(\hat{N}) = \frac{N^{2-s} \zeta(s)}{2 \zeta(s)} \left( \frac{T}{T_c} \right)^2 \quad (1 < s < 2), \]
\[ \var(\hat{N}) = \frac{N^s}{\zeta(2)} \left( \frac{T}{T_c} \right)^2 \ln \left( \frac{2T_c}{\omega_0} \right) \quad (s = 2), \]
\[ \var(\hat{N}) = \frac{s-1}{s} \left( \frac{T}{T_c} \right)^s N \quad (s > 2). \]

This yields the fluctuation indices
\[ \var(\hat{N}) = 2 \quad (s = 1), \]
\[ \var(\hat{N}) = \frac{2}{s} \quad (1 < s < 2), \]
\[ \var(\hat{N}) = 1 + 0 \quad (s = 2), \]
\[ \var(\hat{N}) = 1 \quad (s > 2), \]

where the notation
\[ \lim_{N \to \infty} \frac{\ln N}{\ln N} \equiv 0 \]
is used.

Consequently, ideal trapped gas can form an absolutely stable Bose-condensed system only for \( s > 2 \). The case \( s = 2 \) is on the boundary of stability. Strictly speaking, \( \var(\hat{N}) \) diverges as \( N \) tends to infinity, but this divergence is weak, being of logarithmic type. This means that the Bose-condensed system, with the confining dimension \( s = 2 \), is weakly unstable.

Remembering definition (14) gives the stability condition
\[ \frac{d}{2} + \sum_{\alpha=1}^{d} \frac{1}{N_{\alpha}} > 2. \]

2.4. Harmonic trapping potential

The most commonly considered shape of trapping potentials is that of harmonic potential, when \( n_\alpha = 2 \). Then \( s = d \) and \( B = 1d^d \). The condensation temperature (15) gives
\[ T_c = \frac{N\omega_0}{\ln(2N)} \quad (d = 1), \]
\[ T_c = \omega_0 \left[ \frac{N}{\zeta(d)} \right]^{1/d} \quad (d \geq 2). \]

One often states that the formal existence of the critical temperature \( T_c \) implies the possibility of getting Bose-Einstein condensate in one- and two-dimensional harmonic traps. But, as has been stressed above, the mere occurrence of \( T_c \) does not guarantee that such a Bose-condensed system would be stable, hence, could really exist. We have to check the system stability.

The thermodynamic limit (25), for harmonic traps, takes the form
\[ N \to \infty, \quad \omega_0 \to 0, \quad N\omega_0^d \to \text{const}. \]

Variance (27) yields
\[ \var(\hat{N}) = 2 \left( \frac{T}{\omega_0} \right)^2 \quad (d = 1), \]
\[ \var(\hat{N}) = \left( \frac{T}{\omega_0} \right)^2 \ln \left( \frac{2T}{\omega_0} \right) \quad (d = 2), \]
As a result, the fluctuation indices are

\[ \var(\hat{N}) = 2 \quad (d = 1), \]
\[ \var(\hat{N}) = 1 + 0 \quad (d = 2), \]
\[ \var(\hat{N}) = 1 \quad (d = 3), \]

with the same notation for +0 as above.

This tells us that, according to the stability condition (5), only a three-dimensional harmonic trap can house stable ideal Bose-condensed gas. Bose-Einstein condensation cannot occur in one-dimensional harmonic traps. And two-dimensional gas in a harmonic trap is weakly unstable.

### 2.5. Interacting nonuniform gas

Let us consider an arbitrary nonuniform Bose system of atoms interacting through repulsive forces. The general expression, characterizing particle fluctuations, is given [4,17] by the variance

\[ \var(\hat{N}) = N + \int \rho(r) \rho(r') [g(r, r') - 1] \, dr \, dr', \]  

(35)

where the total particle density

\[ \rho(r) = \rho_0(r) + \rho_1(r) \]

is the sum of the condensate density \( \rho_0(r) \) and the density of uncondensed particles \( \rho_1(r) \), and \( g(r, r') \) is the pair correlation function. This expression is valid for any system whether equilibrium or not.

For an equilibrium system, we shall use the local density approximation [17] in the frame of the self-consistent mean-field approach [18-22]. Then the density of uncondensed particles can be written [17] in the form

\[ \rho_1(r) = \int n(k, r) \frac{dk}{(2\pi)^3}, \]

(37)

in which

\[ n(k, r) = \frac{\omega(k, r)}{2\varepsilon(k, r)} \coth \left[ \frac{\varepsilon(k, r)}{2T} \right] - \frac{1}{2} \]

is the local momentum distribution, the notation

\[ \omega(k, r) = mc^2(r) + \frac{k^2}{2m} \]

is used, and

\[ \varepsilon(k, r) = \sqrt{c^2(r)k^2 + \left( \frac{k^2}{2m} \right)^2} \]

is the local Bogolubov spectrum. The local sound velocity is defined by the equation

\[ mc^2(r) = [\rho_0(r) + \sigma_1(r)] \Phi_0, \]

(38)

where the interaction strength is given by

\[ \Phi_0 \equiv \int \Phi(r) \, dr = 4\pi a_s \frac{\sigma_0}{m} > 0, \]

with positive scattering length \( a_s \). And the anomalous average

\[ \sigma_1(r) = \int \sigma(k, r) \frac{dk}{(2\pi)^3} \]

(39)

is expressed through

\[ \sigma(k, r) = -\frac{mc^2(r)}{2\varepsilon(k, r)} \coth \left[ \frac{\varepsilon(k, r)}{2T} \right]. \]

Substituting in the right-hand side of variance (35) the Bogolubov shift [15] and keeping the terms up to second order with respect to the operators of uncondensed particles [4,17], we have

\[ \var(\hat{N}) = N + 2 \lim_{k \to 0} \int \rho(r) \left[ n(k, r) + \sigma(k, r) \right] \, dr. \]

(40)

Accomplishing here the limit \( k \to 0 \) yields

\[ \var(\hat{N}) = \frac{T}{m} \int \rho(r) \sigma^2(r) \, dr. \]

(41)

Bose-Einstein condensation is accompanied by the global gauge symmetry breaking, the latter being the necessary and sufficient condition for the former [8,23]. When Bose-Einstein condensate is present, the sound velocity \( c(r) \) is nonzero. Then the integral in Eq. (41) is proportional to \( N \). Therefore the fluctuation index, describing particle fluctuations, is \( \var(\hat{N}) = 1 \). The latter means that for an arbitrary nonuniform three-dimensional system of repulsive atoms, with Bose-Einstein condensate, particle fluctuations are thermodynamically normal.

### 3. Conclusion

The notion of fluctuation indices for operators, representing observable quantities, is introduced, characterizing the stability properties of statistical systems. Thermodynamically anomalous fluctuations imply the system instability, while stable systems exhibit thermodynamically normal fluctuations. The notion is illustrated by calculating the fluctuation indices for the number-of-particle operator for systems with Bose-Einstein condensate. It is shown that the ideal uniform Bose-condensed gas is unstable. The ideal gas can be stabilized in trapping potentials, provided that the confining dimension is larger than two. The
case of the confining dimension two is marginal, corresponding to a weakly unstable system. Atomic gases in harmonic traps are stable only in the three-dimensional case. Trapped one-dimensional gases are unstable, and trapped two-dimensional gases are weakly unstable. A three-dimensional Bose-condensed system of atoms, interacting through repulsive forces, is stable for arbitrary external potentials.

The particular nature of a condensate can be different. For short, we have been talking of atomic condensates. But there exist now several types of molecular condensates (see [24–28] and review [10]). The above consideration can be applied for any type of Bose condensates, whether atomic or molecular.

Only equilibrium systems have been considered in the paper. Fluctuations in nonequilibrium systems is a different topic (see, e.g., [29–35]). But the notion of fluctuation indices can be applied to nonequilibrium systems as well, since the definition of fluctuation indices (4) is equally valid for any type of averages, whether over equilibrium or nonequilibrium ensembles. The principal difference between equilibrium and nonequilibrium systems is that the stability conditions (5), generally, are not required for the latter. The strength of fluctuations in nonequilibrium systems can be of arbitrary magnitude. Though some restrictions on the fluctuation strength could be connected with steady and quasiequilibrium states.

The fluctuation indices, introduced in the present paper, provide a quantitative characteristic of fluctuation strength, associated with the operators of observables. The knowledge of these indices can help for deciding under what conditions and for what kind of traps one could realize stable atomic systems in experiment.

Acknowledgements Financial support from the Russian Foundation for Basic Research is acknowledged.

References

[1] R. Kubo, Thermodynamics (North-Holland, Amsterdam, 1968).
[2] C.J. Pethik and H. Smith, Bose-Einstein Condensation in Dilute Gases (Cambridge University, Cambridge, 2008).
[3] Ph.W. Courtelle, V.S. Bagnato, and V.I. Yukalov, Laser Phys. 11, 659 (2001).
[4] V.I. Yukalov, Laser Phys. Lett. 1, 435 (2004).
[5] J.O. Andersen, Rev. Mod. Phys. 76, 599 (2004).
[6] V.I. Yukalov and M.D. Girardeau, Laser Phys. Lett. 2, 375 (2005).
[7] A. Posazhennikova, Rev. Mod. Phys. 78, 1111 (2006).
[8] V.I. Yukalov, Laser Phys. Lett. 4, 632 (2007).
[9] N.P. Proukakis and B. Jackson, J. Phys. B 41, 203002 (2008).
[10] V.I. Yukalov, Laser Phys. 19, 1 (2009).
[11] V.I. Yukalov, Laser Phys. Lett. 2, 156 (2005).
[12] V.I. Yukalov, Phys. Lett. A 340, 369 (2005).
[13] V.I. Yukalov, Phys. Rev. E 72, 066119 (2005).
[14] V.I. Yukalov, Phys. Rev. A 72, 033608 (2005).
[15] N.N. Bogolubov, Lectures on Quantum Statistics, Vol. 2 (Gordon and Breach, New York, 1970).
[16] R. Peierls, Surprises in Theoretical Physics (Princeton University, Princeton, 1979).
[17] V.I. Yukalov, Laser Phys. Lett. 6, 688 (2009).
[18] V.I. Yukalov, Phys. Lett. A 359, 712 (2006).
[19] V.I. Yukalov, Laser Phys. Lett. 3, 406 (2006).
[20] V.I. Yukalov and E.P. Yukalova, Phys. Rev. A 74, 063623 (2006).
[21] V.I. Yukalov and E.P. Yukalova, Phys. Rev. A 76, 013602 (2007).
[22] V.I. Yukalov, Ann. Phys. 323, 461 (2008).
[23] E.H. Lieb, R. Seiringer, J.P. Solovej, and J. Yngvason, The Mathematics of the Bose Gas and Its Condensation (Birkhauser, Basel, 2005).
[24] J. Cubizolles, T. Bourdel, S.J. Kokkelmans, G.V. Shlyapnikov, and C. Salomon, Phys. Rev. Lett. 91, 240401 (2003).
[25] S. Jochim, M. Bartenstein, A. Altmeyer, G. Hendl, C. Chin, J.H. Denschlag, and R. Grimm, Phys. Rev. Lett. 91, 240402 (2003).
[26] M.W. Zwierlein, C.A. Stan, C.H. Schunck, S.M. Raupach, S. Gupta, Z. Hadzibabic, and W. Ketterle, Phys. Rev. Lett. 91, 250401 (2003).
[27] S. Dürr, T. Volz, A. Marte, and G. Rempe, Phys. Rev. Lett. 92, 020406 (2004).
[28] C.A. Regal, M. Greiner, and D.S. Jin, Phys. Rev. Lett. 92, 040403 (2004).
[29] L. Rondoni and C. Mejia-Monasterio, Nonlinearity 20, 1 (2007).
[30] D.J. Searles, L. Rondoni, and D.J. Evans, J. Stat. Phys. 128, 1337 (2007).
[31] D.A. Zezyulin, G.L. Alfmov, V.V. Konotop, and V.M. Pérez-García, Phys. Rev. A 78, 013606 (2008).
[32] V.I. Yukalov and V.S. Bagnato, Laser Phys. Lett. 6, 399 (2009).
[33] C. Weiss and N. Teichmann, Laser Phys. 19, 673 (2009).
[34] V.I. Yukalov, E.P. Yukalova, and V.S. Bagnato, Laser Phys. 19, 686 (2009).
[35] M. Ölshläger, G. Wirth, C.M. Smith, and A. Hemmerich, arXiv:1005.5488 (2010).