Condensate Statistics in Interacting and Ideal Dilute Bose Gases

V. V. Kocharovsky,[1,2] Vl. V. Kocharovsky,[2] and Marlan O. Scully[1,3]
[1]*Department of Physics and Institute for Quantum Studies, Texas A&M University, College Station, Texas 77843*
[2]*Institute of Applied Physics of the Russian Academy of Science, Nizhny Novgorod, Russia*
[3]*Max-Planck Institut fur Quantenoptik, 85748 Garching, Germany*
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We obtain analytical formulas for the statistics, in particular, for the characteristic function and all cumulants, of the Bose-Einstein condensate in dilute weakly interacting and ideal equilibrium gases in the canonical ensemble via the particle-number-conserving operator formalism of Girardeau and Arnowitt. We prove that the ground-state occupation statistics is not Gaussian even in the thermodynamic limit. We calculate the effect of Bogoliubov coupling on suppression of ground-state occupation fluctuations and show that they are governed by a pair-correlation, squeezing mechanism.

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Two interesting recent papers [1,2] have addressed the question of condensate fluctuations in the interacting Bose gas. Recently we have been working on the canonical-ensemble approach to the condensation of N bosons in a trap using a nonequilibrium (laserlike) analysis [3,4] on the one hand, and a particle-number-conserving operator formalism [5–7] on the other.

We here give explicit expressions for the characteristic function and all cumulants of the probability distribution of the number of atoms in the (bare) ground state of a trap both for the ideal and weakly interacting dilute Bose gas in equilibrium. We find that the Bose-Einstein condensate (BEC) statistics is not Gaussian; i.e., higher cumulants do not vanish even in the thermodynamic limit. We calculate the effect of Bogoliubov coupling between excited atoms on the suppression of the BEC fluctuations in a box ("homogeneous gas") at moderate temperatures and their enhancement at very low temperatures. Our approach is based on the canonical-ensemble quasiparticle formulation which allows us to extend the Bogoliubov method to the solution of the canonical ensemble BEC problem. We discover a deep (not accidental) parallel between the fluctuations of ideal and interacting bosons.

We show that the ansatz for the BEC fluctuations suggested in [2] is misleading, and the Giorgini, Pitaevskii, Stringari result for the variance of the ground-state occupation fluctuations [1] is correct. The present paper extends the results of the pioneering work of Ref. [1].

The analysis of [1] is carried out within the traditional, particle-number-nonconserving Bogoliubov approach. An ambiguity whether, and to what extent, collective phonon-like excitations change the number of condensed atoms was the main argument in [2] against [1].

However, we find that it is possible to take into account the particle number constraint, $\hat{n}_0 + \sum_{\mathbf{k}\neq 0} \hat{n}_{\mathbf{k}} = N$, from the very beginning by a proper reduction of the many-body Hilbert space so that one can work with the new, unconstrained quasiparticles [6]. Our analysis is based on the particle-number-conserving Girardeau-Arnowitt formalism [5], $\hat{\beta}_{\mathbf{k}}^{+} = \hat{a}_{\mathbf{k}}^{+}\hat{\beta}_0$, $\hat{\beta}_{\mathbf{k}} = \hat{\beta}_0^{+}\hat{a}_{\mathbf{k}}$, $\hat{\beta}_0 = (1+\hat{n}_0)^{-1/2}\hat{a}_0$, where $\hat{a}_{\mathbf{k}}^{+}$ and $\hat{a}_{\mathbf{k}}$ are usual creation and annihilation operators for the trap bare $\mathbf{k}$ mode. The $\hat{\beta}_{\mathbf{k}}^{+}$ and $\hat{\beta}_{\mathbf{k}}$ are the new canonical-ensemble quasiparticle operators which obey the Bose canonical commutation relations, $[\hat{\beta}_{\mathbf{k}}, \hat{\beta}_{\mathbf{k}'}^{+}] = \delta_{\mathbf{k},\mathbf{k}'}$. We focus on the important situation when the variance is much less than the mean number of the ground-state atoms, $\langle (n_0 - \bar{n}_0)^2\rangle^{1/2} \ll \bar{n}_0$. In such a case, the relative role of the states with zero ground-state occupation, $n_0 = 0$, is less important, so that we can approximate the canonical-ensemble subspace $\mathcal{H}^{\mathrm{CE}}$ by the subspace $\mathcal{H}^{\mathrm{CE}}_{n_0\neq 0}$. This approximation is valid starting with even a small ground-state fraction $\bar{n}_0 \ll N$. But this is not good near T_c as we discuss later.

The physical meaning of the canonical-ensemble quasiparticles is that they describe transitions between the ground ($\mathbf{k} = 0$) and excited ($\mathbf{k} \neq 0$) states of a trap. All quantum properties of the condensed atoms have to be expressed via the canonical-ensemble quasiparticle operators $\hat{\beta}_{\mathbf{k}}^{+}$ and $\hat{\beta}_{\mathbf{k}}$. In particular, we have the identity $\hat{n}_0 = N - \hat{n}$, where $\hat{n} = \sum_{\mathbf{k}\neq 0} \hat{n}_{\mathbf{k}}$ and the occupation operators of the excited states are $\hat{n}_{\mathbf{k}} = \hat{a}_{\mathbf{k}}^{+}\hat{a}_{\mathbf{k}} = \hat{\beta}_{\mathbf{k}}^{+}\hat{\beta}_{\mathbf{k}}$.

In [8] quasiparticle operators similar in spirit to those of [5] were introduced which, unlike $\hat{\beta}_{\mathbf{k}}$, did not obey the Bose commutation relations exactly. As was shown by Girardeau [5], this is important because the commutation corrections can accumulate in a perturbation series for quantities like an S matrix. A warning concerning a similar subtlety was stressed some time ago [9].

The canonical-ensemble quasiparticle approach allows us to find the crossover between the ideal-gas and interaction-dominated regimes of the BEC fluctuations. These and related problems including BEC fluctuations become of essential interest in view of fascinating experiments on BEC in dilute Bose systems [10,11] and the possibility of measurement of the two-point correlation function [12]. The fact that the canonical (or

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microcanonical) ensemble has to be used, since the grand canonical ensemble predicts wrong BEC fluctuations, was stressed in [13] and analyzed further in [14,15].

Turning now to the analysis, we derive all cumulants [16] κ_r and characteristic function $\Theta_n(u) = \mathrm{Tr}\{e^{iu\hat{n}}\hat{\rho}\}$,

$$\log\Theta_n(u) = \sum_{r=1}^{\infty} \kappa_r \frac{(iu)^r}{r!}, \qquad \kappa_r = \sum_{m=1}^{r} \sigma_r^{(m)} \tilde{\kappa}_m ,$$

for a gas with a density matrix $\hat{\rho}$ in terms of "generating cumulants" $\tilde{\kappa}_m$, where $\sigma_r^{(m)} = \frac{1}{m!}\sum_{k=0}^{m}(-1)^{m-k}\binom{m}{k}k^r$ are the Stirling numbers of the second kind. For a box (square well trap) of a volume $V = L^3$ with periodic boundary conditions, we find that for the ideal gas

$$\tilde{\kappa}_m = (m-1)! \sum_{\mathbf{k}\neq 0} \frac{1}{[\exp(\varepsilon_{\mathbf{k}}^{(0)}/T) - 1]^m}, \qquad \varepsilon_{\mathbf{k}}^{(0)} = \frac{\mathbf{k}^2}{2M}, \tag{1}$$

and for a weakly interacting via interatomic potential $U_{\mathbf{k}}$ gas with Bogoliubov coupling, $\hat{\beta}_{\mathbf{k}} = u_{\mathbf{k}}\hat{b}_{\mathbf{k}} + v_{\mathbf{k}}\hat{b}^{+}_{-\mathbf{k}}$, $v_{\mathbf{k}} = A_{\mathbf{k}}u_{\mathbf{k}} = A_{\mathbf{k}}/\sqrt{1 - A_{\mathbf{k}}^2}$ (Bogoliubov Bose gas),

$$\tilde{\kappa}_m = \frac{(m-1)!}{2}\sum_{\mathbf{k}\neq 0}\left[\frac{1}{[z(A_{\mathbf{k}}) - 1]^m} + \frac{1}{[z(-A_{\mathbf{k}}) - 1]^m}\right],$$
$$z(A_{\mathbf{k}}) = (A_{\mathbf{k}} - e^{\varepsilon_{\mathbf{k}}/T})/(A_{\mathbf{k}}e^{\varepsilon_{\mathbf{k}}/T} - 1). \tag{2}$$

Here $\varepsilon_{\mathbf{k}} = [(\hbar^2\mathbf{k}^2/2M + \bar{n}_0U_{\mathbf{k}}/V)^2 - (\bar{n}_0U_{\mathbf{k}}/V)^2]^{1/2}$, $A_{\mathbf{k}} = (\varepsilon_{\mathbf{k}} - \hbar^2\mathbf{k}^2/2M)V/\bar{n}_0U_{\mathbf{k}} - 1$, M is the atomic mass, and $\mathbf{k} = 2\pi\mathbf{l}/L$, where $\mathbf{l} = \{l_x, l_y, l_z\}$ are integers. The generating cumulants are related to the centered moments $\mu_m = \langle(n - \bar{n})^m\rangle$ by simple formulas $\mu_1 = \tilde{\kappa}_1$, $\mu_2 = \tilde{\kappa}_2 + \tilde{\kappa}_1$, $\mu_3 = \tilde{\kappa}_3 + 3\tilde{\kappa}_2 + \tilde{\kappa}_1$, etc. Here and below all cumulants are given for the distribution of the excited-state number operator $\hat{n}$ which is a simple "mirror" image of the distribution of the ground-state number operator, $\rho(n) = \rho_0(n_0 = N - n) = \frac{1}{2\pi}\int_{-\pi}^{\pi} e^{-iun}\Theta_n(u)\,du$.

Our explicit expressions for the cumulants of the BEC fluctuations, Eq. (2), $m \geq 2$, are based on the solution $\bar{n}_0(T)$ of the self-consistency equation (2), $m = 1$, that coincides precisely with that for the grand-canonical dilute gas in the first-order Popov approximation [17]. The latter is well established for the analysis of the finite-temperature properties of the dilute gas and is not valid only near T_c, $T_c - T < a(N/V)^{1/3}T_c \ll T_c$, where $a = MU_0/4\pi\hbar^2$ is a usual s-wave scattering length. A mean-field theory of this kind describes the mean condensate occupation with good accuracy (see review [18]).

We note that our squared variance $\Delta n_0^2 = \Delta n^2 = \mu_2$ for the ideal Bose gas (IBG) from Eq. (1) and for the Bogoliubov Bose gas (BBG) from Eq. (2)

$$\Delta n^2_{\mathrm{IBG}} = \sum_{\mathbf{k}\neq 0}[(z_{\mathbf{k}} - 1)^{-2} + (z_{\mathbf{k}} - 1)^{-1}] \to D, \tag{3}$$

$$\Delta n^2_{\mathrm{BBG}} = 2^{-1}\sum_{\mathbf{k}\neq 0}\{[z(A_{\mathbf{k}}) - 1]^{-2} + [z(-A_{\mathbf{k}}) - 1]^{-2} + [z(A_{\mathbf{k}}) - 1]^{-1} + [z(-A_{\mathbf{k}}) - 1]^{-1}\} \to D/2, \tag{4}$$

coincide with the values obtained earlier [1,13]. Here the arrow indicates the limit $\tilde{\varepsilon}_1 \ll T$, $D = N^{4/3}(T/T_c)^2 s_4/\pi^2[\zeta(3/2)]^{4/3}$, $s_4 = \sum_{\mathbf{l}\neq 0}\mathbf{l}^{-4} \approx 16.53$.

There are essential differences between the IBG and BBG (see Fig. 1). First, the energy gap between the ground state and the first excited state in a trap is increased by the interaction, that is, $\tilde{\varepsilon}_1 = \sqrt{\varepsilon_1^2 + 2\varepsilon_1\bar{n}_0(T)U_0/V} > \varepsilon_1 = (2\pi\hbar/L)^2/2M$. More importantly BBG fluctuations are only $1/2$ as large as in an IBG for the moderate temperatures, $\tilde{\varepsilon}_1 \ll T < T_c$, when a strong coupling ($A_{\mathbf{k}} \approx -1$) contribution dominates in Eq. (2). The factor $1/2$ comes from the fact that $z(\pm A_{\mathbf{k}} = \mp 1) = \pm 1$, so that the first

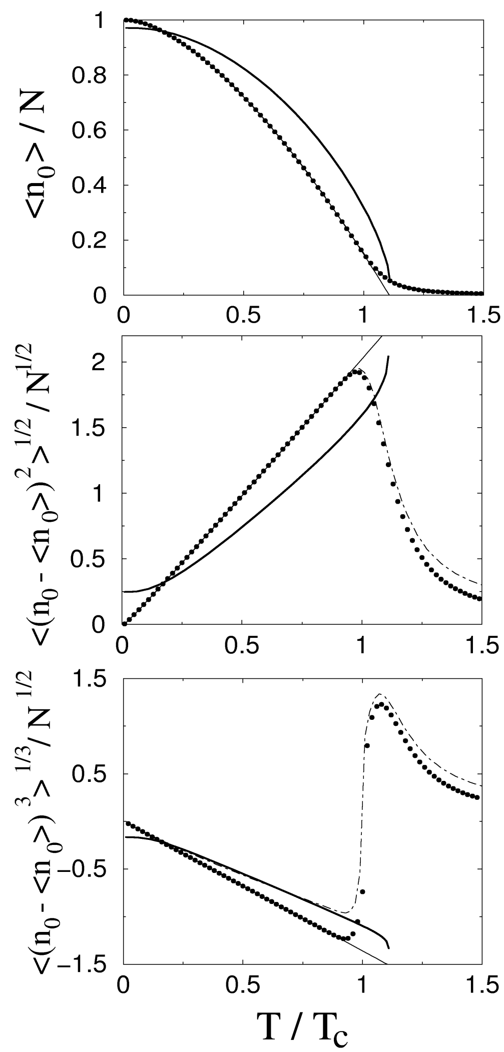

FIG. 1. Relative mean value $\bar{n}_0/N$, variance $\sqrt{\Delta n_0^2/N}$, and third centered moment of the ground-state occupation vs T/T_c for the dilute weakly interacting gas [Eqs. (2), thick solid lines] and for the ideal gas according to Eqs. (1) (thin solid), exact numerical calculations of [15] (dotted) as well as the "nonequilibrium laser theory" analytical Eqs. (6)–(8) (dot-dashed). Thick solid lines differ from others due to interaction, $U_{\mathbf{k}}N^{1/3}/V\varepsilon_1 = 0.05$. Thin solid and dotted lines coincide at low temperatures but differ near T_c due to mesoscopic effects of the finite number of atoms, $N = 1000$, where Eqs. (6)–(8) give a very good account of the problem. Dot-dashed and dotted lines for $\bar{n}_0$ overlie one another.

term in Eq. (2) is resonantly large but the second term is relatively small. In this case, the effective energy spectrum, which can be introduced for the purpose of comparison with the ideal gas formula, is $\varepsilon_{\mathbf{k}}^{\text{eff}} = T \ln[z(A_{\mathbf{k}})] \simeq (1 + A_{\mathbf{k}})\varepsilon_{\mathbf{k}}/2 \simeq \varepsilon_{\mathbf{k}}^2 V/2U_0\bar{n}_0 \simeq \mathbf{k}^2/2M$. That is, the strongly coupled modes in the weakly interacting gas have approximately the same effective energy as that of a free atom.

This remarkable property explains the reduction in BBG fluctuations by a factor of 2 and the anomalous scaling $\propto N^{4/3}$ similar to that of IBG. These facts were considered in [1] to be an "accidental coincidence." We see now that, roughly speaking, this is so because the atoms are coupled in strongly correlated pairs such that the number of independent degrees of freedom contributing to the fluctuations of the total number of excited atoms is only $1/2$ the atom number N. This pair correlation mechanism is a consequence of two-mode squeezing due to Bogoliubov coupling between $\mathbf{k}$ and $-\mathbf{k}$ modes. The fact that an even number of quanta in two coupled modes can be much more probable than an odd number is clearly seen from the explicit formula for the probability distribution of the two-mode occupation in BBG,

$$P_2(n_{\mathbf{k}} + n_{-\mathbf{k}}) = \frac{[z(A_{\mathbf{k}}) - 1][z(-A_{\mathbf{k}}) - 1]}{z(-A_{\mathbf{k}}) - z(A_{\mathbf{k}})} \{[z(A_{\mathbf{k}})]^{-n_{\mathbf{k}}-n_{-\mathbf{k}}-1} - [z(-A_{\mathbf{k}})]^{-n_{\mathbf{k}}-n_{-\mathbf{k}}-1}\}. \tag{5}$$

For an arbitrary trapping potential, Eq. (1) remains precisely the same if $\varepsilon_{\mathbf{k}}^{(0)}$ stands now for a trap energy spectrum. A generalization of Eq. (2) is more subtle. It is very likely that in the general case of an arbitrary power-law d-dimensional trap, $\varepsilon_{\mathbf{l}} = \hbar \sum_{j=1}^{d} \omega_j l_j^\sigma$, $\mathbf{l} = \{l_j\}$, the interaction also results in anomalously large fluctuations in the ground-state occupation and their formal infrared divergence due to the squeezing of excited states via Bogoliubov coupling and renormalization of the energy spectrum. In the case of the isotropic harmonic trap this was demonstrated in [1] for the variance of the ground-state occupation. Hence, the ideal gas model for traps with a low spectral index $\sigma < d/2$ (e.g., for a harmonic trap where $\sigma = 1$), showing Gaussian, normal thermodynamic condensate fluctuations with $\Delta n_0^2 \propto N$ instead of anomalously large fluctuations, is not robust with respect to the introduction of a weak interaction.

At the same time, the ideal-gas model for traps with a high spectral index $\sigma > d/2$ (e.g., for a box where $\sigma = 2$) exhibits non-Gaussian anomalously large fluctuations with $\Delta n_0^2 \propto N^{2\sigma/d} \gg N$ similar to those found for the interacting gas. Fluctuations in the IBG and BBG differ by a factor of the order of 1, which, of course, depends on the trap potential and is equal to $1/2$ in the particular case of the box where $\Delta n_0^2 \propto N^{4/3}$, Eqs. (3) and (4). We conclude that, contrary to the interpretation formulated in [1], similar behavior of the BEC fluctuations in the ideal and interacting gases in a box is *not* accidental but is a general rule for all traps with a high spectral index $\sigma > d/2$, i.e., a relatively low dimension $d < 2\sigma$.

As follows from Eq. (2), the interaction essentially modifies the BEC fluctuations also at very low temperatures, $T \ll \tilde{\varepsilon}_1$ (see Fig. 1). Namely, in BBG a temperature-independent quantum noise, $\tilde{\kappa}_m^{\text{BBG}}(T \to 0) \neq 0$, $m \geq 2$, additional to the IBG noise, $\tilde{\kappa}_m^{\text{IBG}}(T \to 0) = 0$, $m \geq 2$, appears due to quantum fluctuations of the excited atoms which are forced by the interaction to occupy the excited levels even at $T = 0$, so that $\bar{n}_{\mathbf{k}}(T = 0) \neq 0$.

Our canonical-ensemble quasiparticle approach also makes it clear how to extend the Bogoliubov and more advanced diagram methods to the solution of the canonical ensemble BEC problem and ensure conservation of the number of particles. The latter fact cancels the main argument of [2] against [1]. Our work, and, in particular, Eq. (2) for the cumulants, correctly takes into account one of the main effects of the interaction, namely, dressing of the excited atoms by the macroscopic condensate via the Bogoliubov coupling. If one ignores this effect, as was done in [2], the results can be misleading. This explains the sharp disagreement of the ground-state occupation variance obtained in [2] with the predictions of [1] and our results as well. Note also that the statement from [2] that "the phonon spectrum plays a crucial role in the approach of [1]" should not be taken literally since the relative weights of bare modes in the eigenmodes (quasiparticles) is, at least, no less important than eigenenergies themselves. In other words, our derivation of Eq. (2) shows that squeezing of the excited states due to Bogoliubov coupling is crucial for the correct calculation of the BEC fluctuations. Besides, the general conclusion that very long wavelength excitations have an acoustic, "gapless" spectrum (in the thermodynamic limit) is a cornerstone fact of the many-body theory of superfluidity and BEC [9].

The preceding IBG and BBG analysis works well when we are not too near T_c. There two additional effects should be included. The first one is a mesoscopic effect of a finite number N of atoms in a trap which is taken into account by Eqs. (1) and (2) only via a discreteness of the single particle spectrum $\varepsilon_{\mathbf{k}}$ due to a finite-size effect, $L \propto N^{-1/3}$. This finite-size (discreteness) effect produces some shift of the BEC temperature (compared to its thermodynamic-limit value, T_c) which is usually a few percent increase for a box, as is clearly seen in Fig. 1, or a few percent decrease for a harmonic trap. The latter effects were studied by many authors (see review [18]), and our formulas (1), (2), and (6)–(8) agree with their results. For the BBG, i.e., mean-field, model in the vicinity of T_c, the condensate occupation is negligible and the properties of the BBG and IBG are very similar, e.g., T_c remains the same. Furthermore, we now have a good treatment of the IBG with a finite number of atoms from our nonequilibrium approach [3,4] (dot-dashed lines in Fig. 1). In particular, we find analytical results, in very good agreement with exact (numerical) calculations of [15] (dotted lines in Fig. 1), for the equilibrium condensate distribution $\rho_0(n_0)$ and the partition function Z_N:

$$\rho_0(n_0) = \frac{1}{Z_N} \frac{(N - n_0 + \mathcal{H}/\eta - 1)!}{(\mathcal{H}/\eta - 1)!\,(N - n_0)!} \left(\frac{\eta}{1 + \eta}\right)^{N-n_0}, \tag{6}$$

$$Z_N = \sum_{n=0}^{N} \binom{n + \mathcal{H}/\eta - 1}{n} \left(\frac{\eta}{1 + \eta}\right)^n, \tag{7}$$

where $n = N - n_0$ and the $\binom{r}{s} = r!/s!\,(r - s)!$. The results are valid for any trapping potential which controls the parameters $\mathcal{H}$ and η via energy spectrum $\varepsilon_{\mathbf{k}}$ of a trap,

$$\mathcal{H} = \sum_{\mathbf{k}\neq 0} \frac{1}{(e^{\varepsilon_{\mathbf{k}}/T} - 1)}, \qquad \eta\mathcal{H} = \sum_{\mathbf{k}\neq 0} \frac{1}{(e^{\varepsilon_{\mathbf{k}}/T} - 1)^2}. \tag{8}$$

In the thermodynamic limit the temperature range where the mesoscopic effect is pronounced shrinks to the point $T = T_c$. However, the BBG analysis still remains incomplete at $T \sim T_c$ because of another (second) effect: namely, the interaction between quasiparticles is not negligible near T_c. The corresponding higher order effects of the interaction, in particular, a further renormalization of the mode coupling and energy spectrum, can be taken into account via the particle-number-conserving canonical-ensemble quasiparticle approach. The problem can be solved effectively by applying either the traditional methods of statistical physics and their nonequilibrium generalizations [9,17–20] to the canonical-ensemble quasiparticles or the master equation approach that works surprisingly well even without any explicit reduction of the many-particle Hilbert space [3,4]. The many-body effects beyond mean-field theory were studied through the path-integral Monte Carlo simulations [21]. These effects of weak interaction increase the mean condensate occupation and the transition temperature. However, for the parameters of the recent experiments [11], the modifications are less than the mean-field finite-size corrections. Thus, the present analysis is consistent with the current understanding of the mean condensate occupation and yields analytical formulas for all higher moments.

We conclude that the problem of BEC fluctuations in the weakly interacting gas can be clearly formulated and solved by an analysis in the tradition of many-body theory. In particular, the result (2), obtained on the level of the well-known first-order Popov approximation (mean-field theory), can be generalized to the level of the second-order Beliaev-Popov approximation which is considered to be enough for a detailed account of most of the many-body effects [17]. In principle, a condensed state can be defined via the bare trap states as their many-body mixture fixed by the interaction and external conditions like boundary conditions, superfluid flow pattern (“domain” or vortex structure), temperature, number of atoms, etc. Hence, occupation statistics of the ground as well as excited states of a trap is a very informative feature of the BEC and is well defined mathematically. Of course, there are other quantities that characterize BEC fluctuations, e.g., occupations of collective, dressed, or coherent excitations, different phases, and correlation functions.

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