Classicality of atom-atom correlations in weakly interacting condensed Bose gases

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Abstract. Trapped bosonic gases have been shown to exhibit enhanced first-order coherence in various interferometric measurements when cooled below the critical temperature of Bose–Einstein condensation. However, first-order coherence does not reveal many-atom features for which higher-order atomic correlations must be explored. Here the second-order coherence is studied in the context of classicality of atom-atom correlations. To lowest order with respect to the inverse atom number an inequality for the condensate mode is derived that should hold for purely classical atom-atom correlations. A possible violation of this classical inequality is shown to be hardly possible, so that below the critical temperature the atomic gas should be considered as classical.

1. Introduction
The measurement of correlations in bosonic and fermionic gases at ultralow temperatures is presently a topic of large interest. Correlations between atoms, that is, correlations of higher-order than pure interference, have been measured for bosons and fermions, showing bunching and anti-bunching, respectively [1–6]. These correlations are due to bosonic or fermionic nature of the atoms and due to interactions between these. In the case of bosons, where bunching prevails, one may be led to the assumption that then, similar to the case of a light field showing bunching of photons, the atom-atom correlations do not show a quantum but a classical nature. The purpose of this contribution is to confirm this assumption by giving further indications to it.

Atom-atom correlations are commonly associated with the joint probability density of two atoms being at two specified space-time locations [7]. Whereas the association certainly cannot be denied, the correlation function nevertheless cannot be claimed to be proportional to the joint probability, as is inferred commonly. This issue is crucial for restricting first the generality of classifications based on classical Schwarz inequalities applied to intensity-intensity correlation functions, such as in the bunching / anti-bunching distinction for optical fields. Nevertheless, for the purpose of classifying atom-atom correlations as being classical or non-classical [8–10], such a criterion can be applied to atomic fields, assuming the above mentioned approximation can be justified. It can then be shown that for various trap geometries and for temperatures below the critical temperature the Bose gas reveals only classical atom-atom correlations.

The paper is organized as follows: In Sec. 2 the issue of joint probability versus correlation function is presented and a criterion of non-classicality of correlations is introduced. Section 3 then introduces a formulation of a condensed gas, which serves to separate the condensate contribution and to apply the non-classicality condition. Finally, the classicality of the condensate correlations is shown and some
trap geometries are studied to further indicate the purely classical nature of correlations at ultra-low temperatures.

2. Correlation function versus joint probability density
We assume a gas of weakly interacting bosonic atoms confined in a trap of yet unspecified geometry. The atoms are described by the atom-field operator $\hat{\Phi}(r)$ that obeys the bosonic commutation relation

$$\left[\hat{\Phi}(r_1), \hat{\Phi}^\dagger(r_2)\right] = \delta(r_1 - r_2). \tag{1}$$

The first-order coherence function of the atomic gas is

$$G^{(1)}(r_1, r_2) = \langle \hat{\Phi}^\dagger(r_1)\hat{\Phi}(r_2) \rangle, \tag{2}$$

where the expectation value is performed over an arbitrary quantum state of the system of indistinguishable bosonic atoms. It is identical to the single-atom density matrix:

$$\rho(r_2, r_1) = G^{(1)}(r_1, r_2). \tag{3}$$

The density of atoms results from this matrix as its diagonal elements,

$$\rho(r) = \rho(r, r), \tag{4}$$

and the mean atom number is then the integrated density:

$$\bar{N} = \int d^3r \rho(r), \tag{5}$$

with the corresponding atom-number operator being

$$\hat{N} = \int d^3r \hat{\Phi}^\dagger(r)\hat{\Phi}(r). \tag{6}$$

The next-order correlation function is describing correlations between pairs of atoms. It reads in normally ordered form [7]

$$G^{(2)}(r_1, r_2) = \langle \hat{\Phi}^\dagger(r_1)\hat{\Phi}^\dagger(r_2)\hat{\Phi}(r_2)\hat{\Phi}(r_1) \rangle. \tag{7}$$

This function is not normalised to unity. Its norm is obtained as

$$\int d^3r_1 \int d^3r_2 G^{(2)}(r_1, r_2) = \bar{N} \left( \bar{N} + Q_N \right), \tag{8}$$

where $Q_N$ is the Mandel Q parameter associated to the atom-number fluctuations. It is defined as

$$Q_N = \frac{\Delta N^2}{\bar{N}} - 1, \tag{9}$$

where the rms spread of atom-number fluctuations, $\Delta N$, is defined by

$$\Delta N = \sqrt{\langle \hat{N}^2 \rangle - \bar{N}^2}. \tag{10}$$
Thus the correlation function (7) can be normalized to unity, dividing it by Eq. (8). The resulting unit-normalized correlation function is

\[ P^{(2)}(\mathbf{r}_1, \mathbf{r}_2) = \frac{\langle \hat{\Phi}^\dagger(\mathbf{r}_1) \hat{\Phi}^\dagger(\mathbf{r}_2) \hat{\Phi}(\mathbf{r}_2) \hat{\Phi}(\mathbf{r}_1) \rangle}{N(N + Q_N)}. \]  

(11)

Note that this function differs from the usual “normalised” correlation function \( \tilde{g}^{(2)} \) by the presence of \( Q_N \) in its denominator. As this type of correlation function is associated with the joint probability density for observing two atoms at position \( \mathbf{r}_1 \) and \( \mathbf{r}_2 \), its normalised version, Eq. (11), may be identified as this joint probability density.

However, for being a proper joint probability density certain minimal conditions must be obeyed. One of them is that integration of one of the arguments of the joint probability density results in the corresponding single-atom probability density, which is the unit-normalized version of the atomic density (4). That is the condition

\[ \int d^3 r_2 P^{(2)}(\mathbf{r}_1, \mathbf{r}_2) = \int d^3 r_2 P^{(2)}(\mathbf{r}_2, \mathbf{r}_1) = P^{(1)}(\mathbf{r}_1), \]  

(12)

must hold with the single-atom probability being

\[ P^{(1)}(\mathbf{r}) = \frac{\rho(\mathbf{r})}{N}. \]  

(13)

The corresponding integrals of our joint probability, Eq. (11), result however as

\[ \int d^3 r_2 P(\mathbf{r}_1, \mathbf{r}_2) = \int d^3 r_2 P(\mathbf{r}_2, \mathbf{r}_1) = \frac{\langle \hat{\Phi}^\dagger(\mathbf{r}_1) \hat{\Phi}(\mathbf{r}_1) \left( \hat{N} - 1 \right) \rangle}{N(N + Q_N)} \neq P^{(1)}(\mathbf{r}_1). \]  

(14)

Therefore our joint probability density, as defined in Eq. (11), in general does not fulfill the fundamental condition (12). It is therefore only a quasi probability density, similar to the quasi phase-space distributions of the quantized harmonic oscillator.

There are, however, limiting cases where this condition is fulfilled. One of these is the case when the atomic gas finds itself in a many-atom eigenstate of the atom-number operator \( \hat{N} \). Then \( Q_N = -1 \) and the action of \( \hat{N} \) to the rhs in the nominator trivially becomes the eigenvalue \( N \) of the atom-number eigenstate which obeys \( N = \hat{N} \). It is obvious that in this case the rhs of Eq. (14) reduces to the value as given in the condition (12).

In general, however, the many-atom quantum state \( \hat{\rho} \) must be considered as a weighted sum of normalized quantum states \( \hat{\rho}_N \), each being an \( N \)-atom eigenstate of \( \hat{N} \),

\[ \hat{\rho} = \sum_N P_N \hat{\rho}_N, \]  

(15)

where \( P_N \geq 0 \) is the probability to observe \( N \) atoms. For such a state the rhs expression in Eq. (14) becomes

\[ \frac{\langle \hat{\Phi}^\dagger(\mathbf{r}_1) \hat{\Phi}(\mathbf{r}_1) \left( \hat{N} - 1 \right) \rangle}{N(N + Q_N)} = \sum_N P_N(N - 1)\rho_N(\mathbf{r}_1) \frac{1}{N(N + Q_N)}, \]  

(16)

where \( \rho_N(\mathbf{r}) \) is the atomic density for the state with \( N \) atoms, \( \hat{\rho}_N \).

Assuming that within the supposedly narrow distribution \( P_N \) the atom-number dependent densities \( \rho_N(\mathbf{r}) \) can be approximated as being independent of \( N \), Eq. (16) can be further simplified to

\[ \frac{\langle \hat{\Phi}^\dagger(\mathbf{r}_1) \hat{\Phi}(\mathbf{r}_1) \left( \hat{N} - 1 \right) \rangle}{N(N + Q_N)} \approx \frac{\hat{N} - 1}{N + Q_N} P^{(1)}(\mathbf{r}_1) = \left\{ 1 - \frac{Q_N + 1}{Q_N + N} \right\} P^{(1)}(\mathbf{r}_1). \]  

(17)
It reduces to the single-atom probability density only in the limit of very large mean atom number, \( N \gg 1 \), and under the condition that \( Q_N \ll \bar{N} \). In this case the second term in the bracket on the rhs is negligible. Using the definition (9) from these two conditions results the condition for the rms spread of atom-number fluctuations

\[ \Delta N \ll \bar{N}. \] (18)

That means, not only a very large mean atom number is required but also a confined atom-number distribution. Note that as \( \Delta N = \sqrt{\bar{N}} \) defines the shot-noise limit, condition (18) still allows for a moderate excess noise, i.e. a weakly super-Poissonian atom-number statistics.

At this point it becomes clear that already from the point of view of the elementary requirement (12) our quasi joint probability density in general is not a true probability density. However, let us assume in the following that this condition is fulfilled by choosing an atomic gas in a quantum state with exactly \( N \) atoms. Even then \( P^{(2)} \) may not be considered as a true probability density. It still depends on the remaining features of the chosen quantum state whether it is a proper probability or not.

This issue is quite in analogy with the definition of quasi phase-space probability densities for the quantized harmonic oscillator: Some quantum states reveal phase-space distributions very close to being classical, others do not. From this analogy emerges the idea to use this discrimination to characterize now the atom-atom correlations as being classical if and only if the function \( P^{(2)} \) is a proper probability density. Otherwise truly quantum, i.e. non-classical, correlations are identified.

It should be noted that this criterium for classicality is necessary but obviously not sufficient, as we are considering only one specific aspect of it being a proper probability density. However, it may serve as an indication for a mainly classical behaviour.

We assume for the moment that the underlying quantum state is such that \( P^{(2)} \) would be a proper joint probability density. Any proper joint probability obeys the Schwarz inequality: For any true probability densities and any arbitrary function \( f(\mathbf{r}) \)

\[
\int d^3r_1 \int d^3r_2 f(\mathbf{r}_1) f(\mathbf{r}_2) P^{(2)}(\mathbf{r}_1, \mathbf{r}_2) \leq \int d^3r |f(\mathbf{r})|^2 P^{(1)}(\mathbf{r}).
\] (19)

Applying this to our function \( P^{(2)} \) and using its definition (11) this Schwarz inequality can be written for the nontrivial case of \( N > 1 \) atoms as

\[
\int d^3r_1 \int d^3r_2 f(\mathbf{r}_1) f(\mathbf{r}_2) \langle \Phi^\dagger(\mathbf{r}_1) \Phi^\dagger(\mathbf{r}_2) \Phi(\mathbf{r}_2) \Phi(\mathbf{r}_1) \rangle \leq (N - 1) \int d^3r |f(\mathbf{r})|^2 \rho(\mathbf{r}).
\] (20)

For further calculations it will be more convenient to reorder operators and to combine all terms on the lhs. This leads to the equivalent inequality

\[
\mathcal{S}[f] = \int d^3r f^2(\mathbf{r}) \langle \hat{n}(\mathbf{r}) \rangle - \int d^3r_1 \int d^3r_2 f(\mathbf{r}_1) f(\mathbf{r}_2) \langle \hat{n}(\mathbf{r}_1) \hat{n}(\mathbf{r}_2) \rangle \geq 0,
\] (21)

where \( \hat{n}(\mathbf{r}) = \Phi^\dagger(\mathbf{r}) \Phi(\mathbf{r}) / N \) is the unit-normalized atom-density operator. The symbol \( \mathcal{S} \) denotes a functional depending on the choice of the function \( f \). For all functions \( f \) this functional must therefore be non-negative.

3. Bose-Einstein Condensate

To further evaluate the above inequality for the case of a Bose-Einstein condensed gas, the atom-field operator is written as the sum of condensate and phonon-like excitations, as in the approach given in Refs [11–13],

\[
\Phi(\mathbf{r}, t) = \Phi(\mathbf{r}, t) \hat{c}(t) + \delta \Phi(\mathbf{r}, t).
\] (22)

Whereas the appearance of the condensate operator \( \hat{c} \) produces terms of the order of \( \sqrt{N} \), the phonon operator \( \delta \Phi(\mathbf{r}, t) \) is of the order 1, as is the unit-normalized condensate mode \( \Phi(\mathbf{r}, t) \). The condensate
wavefunction \( \Phi(r) \) is defined as the eigenmode of the reduced single-atom density operator with the largest eigenvalue, which is the number of condensed atoms \( \bar{N}_c = \langle \hat{c} \hat{c} \rangle \). From this it follows that condensate and phonon modes are strictly orthogonal to each other and that \( \langle \hat{c} \hat{\Psi}(r) \rangle = 0 \).

Using the above definitions we may now write down the various orders of \( N \) of the Schwarz inequality (21), which result as a series of functionals, denoting a sequence of powers of \( 1/\sqrt{N} \):

\[
S[f] = S^{(0)}[f] + S^{(1)}[f] + \ldots
\]  

(23)

Inserting (22) into (21) one obtains the lowest-order term \([/(1/\sqrt{N})] \) as

\[
S^{(0)}[f] = \int d^3 r f^2(\mathbf{r}) \left( \frac{\langle \hat{c} \hat{c} \rangle}{N} \right)^2 - \int d^3 r_1 \int d^3 r_2 f(\mathbf{r}_1) f(\mathbf{r}_2) \frac{\langle \hat{c} \hat{\Psi}(r) \rangle}{N^2} |\Phi(\mathbf{r}_1)\Phi(\mathbf{r}_2)|^2
\]  

(24)

The next term \( S^{(1)} \) would be of order \( (1/\sqrt{N}) \).

Given the mean number of condensed atoms \( \bar{N}_c = \langle \hat{c} \hat{c} \rangle \), the Mandel Q parameter for the atom-number fluctuations of the condensed fraction may be defined as

\[
Q_c = \frac{\Delta N_c^2}{\bar{N}_c} - 1.
\]  

(25)

Moreover, for notational convenience, the mean and rms spread of the function \( f \) averaged over the condensate mode can be defined as

\[
\bar{f}_\Phi = \int d^3 r \Phi^*(\mathbf{r}) f(\mathbf{r}) \Phi(\mathbf{r}),
\]

(\Delta f_\Phi)^2 = \int d^3 r \Phi^*(\mathbf{r}) f^2(\mathbf{r}) \Phi(\mathbf{r}) - (\bar{f}_\Phi)^2.

(26)

(27)

Using these definitions the lowest-order and thus dominant term (24) is rewritten as

\[
S^{(0)}[f] = \frac{\bar{N}_c}{N} \left\{ (\Delta f_\Phi)^2 + (\bar{f}_\Phi)^2 \left( \frac{N - \bar{N}_c - 1 - Q_c}{N} \right) \right\}.
\]  

(28)

As the next-order term \( S^{(1)} \) is a factor \( 1/\sqrt{N} \ll 1 \) smaller, for sufficiently large atom numbers a violation (non-violation) of the Schwarz inequality by the lowest-order condensate contribution \( S^{(0)} \) is unlikely to be compensated or altered by higher-order terms. It is therefore viable to focus only on the condensate contribution \( S^{(0)} \).

Thus let us consider how \( S^{(0)} \) could possibly violate the Schwarz inequality (21), that reads now

\[
S^{(0)}[f(\mathbf{r})] \geq 0.
\]  

(29)

Using Eq. (28) this inequality can be formulated equivalently as

\[
\left\{ (\Delta f_\Phi) + \frac{N - \bar{N}_c}{N} \right\} \geq Q_c + 1 + \frac{N}{N}.
\]  

(30)

For having proper classical atom-atom correlations, this relation has to be true for all possible functions \( f(\mathbf{r}) \). A violation is most easily obtained when the lhs of Eq. (30) becomes minimal with respect to a variation of the function \( f(\mathbf{r}) \). This is obtained by choosing a constant function \( f(\mathbf{r}) = f_0 \neq 0 \) which produces \( \Delta f_\Phi = 0 \). Then we are left with the inequality

\[
S^{(0)}[f_0] = \frac{f_0^2}{N^2} \left[ \bar{N}_c(N - \bar{N}_c) - \Delta \bar{N}_c^2 \right] \geq 0.
\]  

(31)
Can this expression be negative? To answer this question let us define the number of non-condensed (i.e., excited) atoms, \( \hat{N}_e = N - \bar{N}_c \), and consider the (here vanishing) rms spread of the total atom number,

\[
0 = \Delta N^2 = \Delta N_e^2 + \Delta N_c^2 + 2 \left( \langle \hat{N}_e \hat{N}_c \rangle - \bar{N}_e \bar{N}_c \right),
\]

(32)

From this equation it follows that

\[
\bar{N}_c \bar{N}_e - \Delta N_c^2 = \frac{1}{2} \left( \Delta N_e^2 - \Delta N_c^2 + 2 \langle \hat{N}_e \hat{N}_c \rangle \right),
\]

(33)

and given that \( \Delta N_e^2 = \Delta N_c^2 \) and \( \bar{N}_e = N - \bar{N}_c \) one obtains

\[
\bar{N}_c (N - \bar{N}_c) - \Delta N_c^2 = \langle \hat{N}_e \hat{N}_c \rangle.
\]

(34)

Inserting this expression in Eq. (31) the condensate part of the Schwarz inequality becomes

\[
S^{(0)}[f_0] = f_0^2 \frac{\langle \hat{N}_e \hat{N}_c \rangle}{N^2} \geq 0.
\]

(35)

At this point it becomes clear that a violation cannot be attained under these conditions. The correlation of numbers of condensed and excited atoms, being a correlation between two non-negative numbers, will be always non-negative. Therefore the condensate contribution \( S^{(0)} \) cannot be negative and the atom-atom correlations have to be classified as being classical. This is the main result of this paper. Clearly it was obtained under the condition of the presence of a dominant condensate fraction and of a gas with exactly \( N \) atoms. It therefore does not apply to temperatures near or above the condensation temperature.

From Eq. (35) it is already clear that no violation of the Schwarz inequality can be obtained for a condensed Bose gas in general, that is, including atom-atom interactions. Nevertheless, some straightforward examples for an ideal gas may be illustrative. As a first example we choose an ideal Bose gas in an isotropic 3D harmonic trap. Below the condensation temperature \( T_c \) the number of condensed atoms is in this case

\[
\bar{N}_c = N \left[ 1 - \left( \frac{T}{T_c} \right)^3 \right],
\]

(36)

Furthermore, in the canonical ensemble the fluctuation of this property results as [14]

\[
\Delta N_c^2 = N \frac{\pi^2}{6 \zeta(3)} \left( \frac{T}{T_c} \right)^3,
\]

(37)

where \( \zeta(z) \) is the Riemann zeta function. Therefore, from Eq. (31) the condensate part of the Schwarz inequality is obtained as

\[
S^{(0)}[f_0] = f_0^2 \left[ \left( 1 - \frac{\pi^2}{6 N \zeta(3)} \right) \left( \frac{T}{T_c} \right)^3 \right] \left( \frac{T}{T_c} \right)^3 \geq 0.
\]

(38)

This expression becomes negative only for temperatures

\[
T > T_c \left[ 1 - \frac{\pi^2}{6 N \zeta(3)} \right]^{1/3},
\]

(39)

temperatures, that for \( N \gg 1 \) are outside of the range of validity \((T \sim T_c)\) of our approach. Even for a small atom number \( N \) it is practically impossible, since the required temperatures are very near to the condensation temperature, where the yet neglected excited-atom contribution becomes relevant.
To complement this, let us consider an ideal Bose gas in a 3D box potential where the mean number of condensed atoms becomes
\[ \bar{N}_c = N \left[ 1 - \left( \frac{T}{T_c} \right)^{3/2} \right] , \] (40)
and the corresponding fluctuations are [14]
\[ \Delta N_c^2 = 8A\pi^2 \left( \frac{N}{\zeta(\frac{3}{2})} \right)^{4/3} \left( \frac{T}{T_c} \right)^2 , \] (41)
with \( A = 0.105 \). The condensate contribution to the Schwarz inequality is
\[ S^{(0)}[f_0] = f_0^2 \left[ 1 - \left( \frac{8A\pi^2}{\sqrt{N\zeta(\frac{3}{2})}} \right)^{4/3} \left( \frac{T}{T_c} \right)^{1/2} - \left( \frac{T}{T_c} \right)^{3/2} \right] \left( \frac{T}{T_c} \right)^{3/2} . \] (42)
The bracket on the rhs has no minimum for positive temperatures but decays monotonically from its maximum and positive value at \( T = 0 \) to the negative value
\[ - \left( \frac{8A\pi^2}{\sqrt{N\zeta(\frac{3}{2})}} \right)^{4/3} \] (43)
at temperature \( T = T_c \). As this value is quite small for \( N \gg 1 \), this negativity is negligible, and anyway appears at temperatures very close to \( T_c \), where our treatment is beyond validity. Thus, also in this case negativity cannot be attained.

4. Summary and Conclusions
In summary the presented work indicates that the correlations between pairs of atoms in a Bose-Einstein condensed gas are classical. Of course the used criterium for non-classicality can be disputed and is not perfectly valid, as the atom-atom correlation function is only approximately a joint probability distribution. However, the indicated classicality of correlations is within common reasoning, as a Bose-Einstein condensate is clearly a thermal state of the bosonic gas, although a rather peculiar one: As in photon bunching experiments, one would not expect anti-bunching for a thermal state. The preliminary conclusion is therefore, that to observe non-classical correlations a non-equilibrium, non-thermal state might be necessary.

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