Proper condensates and off-diagonal long range order

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Abstract. Within the framework of the algebra of canonical commutation relations in Euclidean space, a long range order between particles in bounded regions is established in states with a sufficiently large particle number. It occurs whenever homogeneous proper (infinite) condensates form locally in the states in the limit of infinite densities. The condensates are described by eigenstates of the momentum operator, covering also those cases, where they are streaming with a constant velocity. The arguments given are model independent and lead to a new criterion for the occurrence of condensates. It makes use of a novel approach to the identification of condensates, based on a characterization of regular and singular wave functions.

Keywords Bose-Einstein condensation · Off-diagonal long range order

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1 Introduction

An important tool for the experimental detection of Bose-Einstein condensates are interference measurements on trapped gases. They are sensitive to the appearance of coherent configurations of particles which all have the same momentum, irrespective of their distance, cf. [1]. On the theoretical side, this phenomenon manifests itself in the absence of decay properties of correlation functions, generally referred to as off-diagonal long-range order (ODLRO). It leads to peak values of the respective Fourier transforms for these coincident momenta, cf. for example [6].

In this note we take a fresh look at this topic, starting from a novel characterization of condensates [2]. Instead of following the Onsager-Penrose approach, where one characterizes condensates by the largest eigenvalues and corresponding eigenfunctions of one-particle density matrices, we focus on the spaces of regular wave functions, which remain finitely occupied in the limit of
infinite particle numbers. Given any open, bounded region $O \subset \mathbb{R}^d$, a proper (infinite) condensate in that region, appearing in the limit of infinite particle densities, is identified with the orthogonal complement of the resulting regular functions with support in $O$. The functions in this orthogonal complement are said to be singular. This approach has the advantage that condensates, appearing in a finite system, can be identified in a clear-cut manner, which does not depend on its global shape or specific number of particles.

Making use of these notions, we will establish in Fock-states on the algebra of canonical commutation relations the appearance of ODLRO in bounded regions if the particle density is sufficiently high. This happens whenever homogeneous proper condensates are formed in the limit of infinite densities. It turns out that these proper condensates can be described by eigenstates of the momentum operator, possibly with a momentum different from zero. Hence, our results cover also the situation where the condensate propagates with a constant velocity.

The notation and concepts used in this paper, in particular the notion of proper condensates and their manifestations, are briefly recalled in Sec. 2. Our main result, concerning the appearance of off-diagonal long range order, is established in Sec. 3. The paper concludes with a brief summary and a new criterion for the occurrence of homogeneous proper condensates. In an appendix, we provide examples, showing that such condensates can appear under conditions which are weaker than the Onsager-Penrose criterion for Bose-Einstein condensation.

## 2 Proper condensates

Let $\mathcal{F} = \bigoplus_n \mathcal{F}_n$ be the bosonic Fock space, viz., the direct sum of $n$-particle spaces $\mathcal{F}_n$ that are defined by the $n$-fold symmetrized tensor products of the single particle space $\mathcal{F}_1 \cong L^2(\mathbb{R}^d)$, $n \in \mathbb{N}_0$. We interpret the elements $f, g \in L^2(\mathbb{R}^d)$ as single particle wave functions on the $d$-dimensional position space $\mathbb{R}^d$. Their canonical scalar product is denoted by $\langle f, g \rangle$. On $\mathcal{F}$, annihilation operators $a(f)$ and creation operators $a^*(g)$ are densely defined. They are antilinear and linear in their entries, respectively, and satisfy the commutation relations

$$[a(f), a^*(g)] = \langle f, g \rangle 1, \quad f, g \in L^2(\mathbb{R}^d),$$

all other commutators being equal to 0.

We will consider sequences of states $\omega$, which can be represented by density matrices $\rho$ on $\mathcal{F}$,

$$\omega(A) = \text{Tr} \rho A, \quad A \in \mathcal{B}(\mathcal{F}).$$
Since these sequences have limits which are no longer representable in this manner, it is meaningful to restrict the states to suitable subalgebras of the algebra $\mathcal{B}(\mathcal{F})$, i.e. the algebra of bounded operators on $\mathcal{F}$. A standard choice is the Weyl algebra, another convenient choice is the resolvent algebra, invented in [3] and used for the analysis of condensates in [1,2]. We need not delve into these issues here and can restrict our attention to the so-called single particle density matrices, given by

$$f, g \mapsto \omega(a^*(f)a(g)),$$ 

$$f, g \in L^2(\mathbb{R}^d). \quad (2.3)$$

It is assumed in the following that $\omega(a^*(f)a(f)) < \infty$ for all $f \in L^2(\mathbb{R}^d)$, which is the case if the state $\omega$ contains a finite (mean) number of particles.

We fix in the following an open, bounded region $O \subset \mathbb{R}^d$, which is thought of as being of macroscopic size, i.e. big compared to typical microscopic length scales. The subspace of functions with support in that region is denoted by $L^2(O)$. Given any sequence of states, we define a corresponding regular subspace of $L^2(O)$ as follows.

**Definition I:** Let $\omega_\sigma, \sigma > 0$, be a sequence of states with properties described above. The corresponding regular subspace $R(O) \subset L^2(O)$ consists of all functions $f \in L^2(O)$ satisfying

$$\limsup_{\sigma \to \infty} \omega_\sigma(a^*(f)a(f)) < \infty.$$

$$\quad (2.4)$$

Its complement $L^2(O) \setminus R(O)$ consists of singular wave functions, which are infinitely occupied in the limit.

There are many reasons why single particle wave functions with support in a bounded region can be infinitely occupied in the limit states, whence are singular. For example, this may be due to high energy effects, as is the case for equilibrium states approaching infinite temperatures. There all wave functions are non-regular in the limit. Yet these cases are of no interest in the present context. We rely here on a more specific characterization of sequences of states that eventually exhibit a proper condensate. In these states there appear, besides clouds of particles with a regular wave function, increasing numbers of particles which all occupy the same singular wave function $s$, cf. [1,2].

**Definition II:** Let $\omega_\sigma, \sigma > 0$, be a sequence of states with properties as in Definition I. The limit of the sequence contains a proper (infinite) condensate in $O$ whenever $R(O)$ is closed and has a one-dimensional orthogonal complement in $L^2(O)$, consisting of the ray spanned by some singular function $s$. This function characterizes a condensate that appears for sufficiently large values of $\sigma$. 

3
Remark: In [2] the possibility was also discussed that the orthogonal complement of $R(O)$ has a finite dimension, different from one. We restrict our attention here to the preceding important case, known to appear in many models, cf. for example [1]. Relevant examples are also recalled in Sec. 4.

Let $\omega_\sigma, \sigma > 0$, be a sequence of states with the properties described in Definition II and let $s \in L^2(O)$ be the (up to a phase unique) normalized function in the orthogonal complement of $R(O)$. Putting

$$\sigma \mapsto n_C(\sigma) = \omega_\sigma(a^*(s)a(s)),$$

this sequence is unbounded in the limit of large $\sigma$. For the corresponding divergent subsequences, it defines the number of particles in $O$, forming a proper condensate in the limit.

Lemma 2.1. Let $\omega_\sigma, \sigma > 0$, be a sequence of states with properties specified in Definition II. The renormalized one-particle density matrices

$$f, g \mapsto n_C(\sigma)^{-1}\omega_\sigma(a^*(f)a(g)), \quad f, g \in L^2(O),$$

converge for suitable subsequences of $\sigma$ in norm to the one-dimensional projection onto the (normalized) singular wave function $s$,

$$\lim_{\sigma} n_C(\sigma)^{-1}\omega_\sigma(a^*(f)a(g)) = \langle s, f \rangle \langle g, s \rangle, \quad f, g \in L^2(O).$$

Proof. Since $R(O)$ is closed, it follows from the uniform boundedness principle [7] that there is some constant $n_R$ such that, uniformly with regard to $\sigma$,

$$\omega_\sigma(a^*(f)a(f)) \leq n_R \|f\|^2, \quad f \in R(O).$$

Now, decomposing

$$f = f_\bot + \langle s, f \rangle s, \quad f \in L^2(O),$$

whence $f_\bot \in R(O)$, one obtains

$$|\omega_\sigma(a^*(f)a(f)) - n_C(\sigma)|\langle f, s \rangle|^2|$$

$$\leq n_R \|f_\bot\|^2 + 2(n_R n_C(\sigma))^{1/2} \|f_\bot\| \|\langle s, f \rangle\|$$

$$\leq (n_R + 2(n_R n_C(\sigma))^{1/2}) \|f\|^2.$$

Thus, picking any subsequence of $\sigma$ for which $n_C(\sigma)$ diverges, the corresponding sequence of renormalized one-particle density matrices converges, as stated. \qed
The preceding lemma shows that the existence of proper condensates in $O$ manifests itself in a clear-cut manner already in the approximating sequence of Fock-states. We emphasize that this does not necessarily imply that the number of particles in these states with wave function $s$ is of macroscopic order, i.e., it need not be proportional to the total (expected) number of particles in $O$. It merely must exceed for large $\sigma$ the maximal possible number $n_R$ of particles occupying some regular wave function. As is shown in the subsequent section, this feature already implies the existence of ODLRO in locally homogeneous states.

3 Off-diagonal long range order

The appearance of ODLRO in states containing condensates is commonly proven by proceeding to the thermodynamic limit of Gibbs-von Neumann ensembles. This is done either by unfolding a trapping potential and adjusting the number of particles or by considering systems with constant density in infinitely growing boxes. We will show here that ODLRO can also be established in fixed bounded regions for sequences of Fock-states, containing an increasing number of particles which form a homogeneous proper condensate in the limit. As we shall discuss in Sec. 4, this result covers the preceding cases.

Proceeding to the details, we recall that the region $O$, which was fixed above, is open and bounded. We will consider open subregions $O_0 \subset O$ whose closure is contained in $O$ and write in this case $O_0 \in O$. Thus, for sufficiently small translations $x \in \mathbb{R}^d$, one has also $O_0 + x \in O$. Denoting by $P$ the momentum operator on $L^2(\mathbb{R}^d)$, this implies $e^{ixP}L^2(O_0) \subset L^2(O)$ for such translations.

Definition III: Let $\omega_\sigma$, $\sigma > 0$, be a sequence of states as in Lemma 2.1. This sequence describes a homogeneous proper condensate in $O$ in the limit if

$$\lim_{\sigma} n_C(\sigma)^{-1}\omega_\sigma(a^*(e^{ixP}f)a(e^{ixP}g)) = \langle s, f \rangle \langle g, s \rangle (3.1)$$

for all $f, g \in L^2(O_0)$, $O_0 \in O$, and translations $x \in \mathbb{R}^d$ such that $O_0 + x \in O$.

It is apparent from Definition I that the regular functions $R(O_0)$ with support in $O_0 \in O$ are contained in $R(O)$. As a matter of fact, the assignment $O_0 \mapsto R(O_0)$ defines a net on the subsets $O_0 \in O$. It follows from Definition III that nets resulting from the corresponding states are also stable under small translations. For, the orthogonal complement of $R(O)$ in $L^2(O)$ coincides with the ray of $s$, which implies for sufficiently small $x$

$$|\langle s, e^{ixP}f \rangle|^2 = |\langle s, f \rangle|^2 = 0, \quad f \in R(O_0). (3.2)$$
Thus, $e^{i x P} R(O_0) \subset \{ s \}^\perp \cap L^2(O_1) = R(O_1)$, provided $O_0 + x \subset O_1 \subset O$. With this information, we can determine now the possible form of the singular function $s$.

**Lemma 3.1.** Let $\omega_\sigma, \sigma > 0$, be a sequence of states that describes a homogeneous proper condensate in $O$ in the limit. The corresponding singular wave function $s$ has the form

$$x \mapsto s(x) = \begin{cases} |O|^{-1/2} e^{i x p} & \text{if } x \in O \\ 0 & \text{if } x \in \mathbb{R}^d \setminus O, \end{cases} \quad (3.3)$$

where $p \in \mathbb{R}^d$ and $|O|$ is the volume of $O$.

**Proof.** Given $O_0 \Subset O$, the orthogonal complement of $R(O_0)$ in $L^2(O_0)$ is the ray of $s_0$, which coincides with the normalized restriction $s|O_0$. (Since $O_0$ is open, it follows after a moments reflection that this restriction is different from 0.) Thus $f - \langle s_0, f \rangle_{s_0} \in R(O_0)$ for any $f \in L^2(O_0)$. We choose now regions $O_0 \Subset O_1 \Subset O$ with corresponding singular functions $s_0$ and $s_1$. Then, for sufficiently small $x, y$ such that $O_0 + x \Subset O_1$ and $O_1 + y \Subset O$, we have

$$\langle s, e^{i(x+y) P} f \rangle = \langle s, e^{i y P} s_1 \rangle \langle s_1, e^{i x P} f \rangle = \langle s, e^{i y P} s_1 \rangle \langle s, e^{i x P} f \rangle, \quad f \in L^2(O_0). \quad (3.4)$$

Since the matrix elements of the unitary translation operators are continuous, it follows from this equality that there is some $k \in \mathbb{C}^d$ such that for small $x$

$$x \mapsto \langle s, e^{i x P} f \rangle = \langle s, f \rangle e^{i x k}, \quad f \in L^2(O_0). \quad (3.5)$$

Equation (3.2) then implies that $k = ip$ for some $p \in \mathbb{R}^d$. Since the region $O_0 \Subset O$ can be arbitrarily chosen, this completes the proof.

The proof that sequences of states, describing a homogeneous proper condensate in $O$ in the limit, exhibit ODLRO is now straightforward. To fix ideas, we choose a length $L_0$ of microscopic (e.g. atomic) size and consider balls $O_0 \Subset O$, centered at the origin of $\mathbb{R}^d$, with diameters $L_0$ and $L \gg L_0$, respectively. Picking any normalized function $f \in L^2(O_0)$, we make use of Lemma 3.1, which yields $|\langle s, e^{i x P} f \rangle| \leq (|O_0|/|O|)^{1/2}$ for $|x| < (L - L_0)/2$. Relation (2.10) then implies for condensate densities $n_C(\sigma)/|O| > n_R/|O_0|$ that

$$\omega_\sigma(\alpha^*(e^{i x P} f) a(e^{i y P} f)) = (n_C(\sigma)/|O|) e^{i(x-y) P} (2\pi)^d |\tilde{f}(p)|^2, \quad (3.6)$$

disregarding contributions of order $(n_R n_C(\sigma))|O_0|/|O|)^{1/2}$; the tilde $\tilde{\phantom{a}}$ denotes Fourier transforms. Thus, for sufficiently large condensate densities $n_C(\sigma)/|O|$,
the correlations between almost all particles in the state have in leading order constant, non-vanishing amplitudes at distances up to \((L - L_0)\). Hence ODLRO prevails in the approximating Fock-states.

Thinking of interference experiments, it is also of interest to determine the Fourier transforms of the correlation functions. To this end we consider the localized plane waves \(x \mapsto e_k(x), \; k \in \mathbb{R}^d\), which are defined as in equation (3.3), putting \(p = k\). Relations (2.7) and (2.10) then imply that for \(n_C(\sigma) > n_R\)

\[
\omega_\sigma(a^*(e_k)a(e_k)) = n_C(\sigma) s^2(L|k - p|/2)^{-2s} \left( \int_0^{L|k - p|/2} dr r^{s-2} \sin(r) \right)^2, \quad (3.7)
\]

disregarding contributions of order \((n_R n_C(\sigma))^{1/2}\). Thus, for \(k = p\), the corresponding number of particles coincides with the number \(n_C(\sigma)\) of particles in the condensate. If \(L|k - p| > 2\), a straightforward estimate shows that the corresponding number is smaller than \(4n_C(\sigma)(L|k - p|)^{-2}\). Given the magnitude of \(L\), it follows that the momentum distribution of the particles in \(O\) has a pronounced peak at the momentum \(p\) of the particles in the condensate. We summarize these results in the following theorem.

**Theorem 3.2.** Let \(O_0 \subset O \subset \mathbb{R}^d\) be concentric balls of diameter \(L_0\) and \(L\), respectively, and let \(\omega_\sigma, \; \sigma > 0\), be a sequence of Fock-states that describes a homogeneous proper condensate in \(O\) in the limit. For values of \(\sigma\) such that \(n_C(\sigma)/|O| > n_R/|O_0|\), there appear in \(\omega_\sigma\) undamped correlations between particles localized in distant balls \(O_0 + x, O_0 + y \subset O\) (ODLRO) at distances \(|x - y| < L - L_0\), cf. equation (3.6). If \(n_C(\sigma) > n_R\), the momentum distribution of the particles in \(O\) in the state \(\omega_\sigma\) has a peak at the joint momentum of the particles forming the condensate, cf. equation (3.7).

We emphasize, that these characteristic properties of condensates appear locally in Fock-states with a finite particle number, provided the density of the local condensate complies with the given constraints.

4 Conclusions

In the present article we have established the existence of long range correlations in bosonic systems of a limited number of particles in a bounded region. The only input used was the assumption that the systems can in principle be enlarged in a manner that leads to the formation of homogeneous proper condensates. That is, there exists a closed subspace of regular wave functions of co-dimension one, having support in the region, whose occupation numbers remain finite, whereas their one-dimensional orthogonal complement can be occupied by an unlimited number of particles.
This input comprises the qualitative features of condensation phenomena, found in experiments with trapped Bose gases. We did not need to assume that the systems are in equilibrium or to specify any dynamics. It was also not necessary to assume that the condensate wave functions are macroscopically occupied, i.e. that the corresponding number of particles is of the same order of magnitude as the total number of particles. It only matters that the number of particles in the condensate substantially exceeds the maximal possible number of particles occupying some regular wave function. If this is given, the existence of the condensate manifests itself in a pronounced peak of the momentum distribution of the particles in the state, which is localized at the common momentum of the particles in the condensate.

Our arguments are based only on kinematic properties of systems of Bosons. Yet the question of whether proper condensates appear depends of course on the dynamics. Simple examples are equilibrium states of non-interacting Bosons in a fixed box in any number of dimensions $d$, where homogeneous proper condensates are formed in the limit of infinite particle numbers. More interesting are systems of non-interacting Bosons, which are confined by some smooth trapping potential. There one must simultaneously increase the number of particles and unfold the trapping potential. The resulting states are in general not homogeneous, providing examples where the spatial translations are spontaneously broken in the limit. Nevertheless, homogeneous proper condensates appear for large particle numbers. They occupy increasing neighborhoods of the minimum of the trapping potential, cf. for example [1, 2].

The proof that homogeneous proper condensates exist in interacting systems is more difficult. Such systems are frequently analyzed by relying on approximations of mean field type. There the existence of proper condensates can be extracted from the literature, cf. for example [3] and references quoted there. A major challenge, however, is a proof in case of genuine two-body interactions. In view of the present results, it amounts to a comparison of the occupation numbers of the largest two eigenvalues of localized one-particle density matrices; it is not necessary to obtain control on the full spectrum. As a matter of fact, one can rely on the following criterion, where we restrict our attention to the case of condensates having vanishing momentum, such as in rotational invariant states.

**Criterion:** Let $\omega_\sigma$, $\sigma > 0$, be a sequence of Fock-states, let $O$ be an open bounded region, and let $R(O)$ be the (closed) subspace of functions $f \in L^2(O)$ satisfying $\int d\mathbf{x} f(\mathbf{x}) = 0$. The sequence describes in the limit a homogeneous proper condensate in $O$ with zero momentum if and only if

$$\limsup_\sigma \omega_\sigma(\mathbf{a}^*(f)\mathbf{a}(f)) < \infty, \quad f \in R(O),$$

(4.1)
and, for some (hence any) function \( s \in L^2(O) \) with \( \int d\mathbf{x} s(\mathbf{x}) \neq 0 \), one has

\[
\limsup_{\sigma} \omega_{\sigma}(a^*(s)a(s)) = \infty. \tag{4.2}
\]

**Remark:** Making use of relation (2.11), there are less stringent, quantitative versions of this criterion, which likewise entail the properties of the approximating Fock-states, presented in Theorem 3.2.

To summarize, the concept of proper condensates provides a meaningful picture of condensation and its features, even if phase transition points (e.g. temperatures) are not sharply defined. The concept also allows to analyze inhomogeneities in the spatial structures of coexisting phases, cf. [2]. Thus, our results provide a fresh look at the longstanding problem to establish the existence of Bose-Einstein condensates in the presence of genuine interactions.

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**Conflict of interest**

There are no relevant financial or non-financial competing interests to disclose.

**Data availability**

Data sharing is not applicable to this article as no new data were created or analyzed in this study.

**Appendix: Illustrative examples**

In this appendix we present some examples of sequences of states that describe homogeneous proper condensates in the limit, but do not comply with the Onsager-Penrose criterion for Bose-Einstein condensation. These examples are merely of a mathematical nature. But they show that our concept of proper condensation differs markedly from the Onsager-Penrose approach. Even though our condition is less stringent, its implications with regard to observable effects of condensation are quite similar. For example, there appear characteristic peaks in the momentum distributions of particles in a gas containing such a condensate.
We fix in the following some open, bounded region $O \subset \mathbb{R}^s$. Let $e_k \in L^2(O)$, $k \in \mathbb{N}_0$, be an orthonormal basis, where we choose for $e_0$ the constant function in $O$. Picking some $0 < \varepsilon < 1$, we define for numbers $n > 1$ the quantities $n_C(n) \doteq n^\varepsilon$ and $\varepsilon_n \doteq \ln((1 + n - n_c(n))/(n - n_C(n)) > 0$. It entails

$$n_c(n) + \sum_{k=1}^{\infty} e^{-\varepsilon_n k} = n_c(n) + e^{-\varepsilon_n} (1 - e^{-\varepsilon_n})^{-1} = n. \quad \text{(A.1)}$$

We then define for $n > 1$ a sequence of gauge invariant quasifree states $\omega_n$ on the algebra of canonical commutation relations, putting

$$\omega_n(a^*(e_k)a(e_l)) = \delta_{k,l} \begin{cases} n_C(n) & \text{if } k = 0 \\ e^{-\varepsilon_n k} & \text{if } k \geq 1. \end{cases} \quad \text{(A.2)}$$

These states may be arbitrarily extended to the full algebra, for example as product states on the given region $O$ and its complement $\mathbb{R}^s \setminus O$. It follows from this definition that

$$\omega_n(a^*(e_0)a(e_0)) = n_C(n), \quad \sum_{k=0}^{\infty} \omega_n(a^*(e_k)a(e_k)) = n. \quad \text{(A.3)}$$

The (mean) number of particles in this sequence with wave function in the condensate state $e_0$ increases with $n$ like $n^\varepsilon$, whereas the maximal occupation number of particles in $O$ with wave function in the orthogonal complement of $e_0$ is bounded by 1. Since the total (mean) number of particles in $O$ in the states is equal to $n$, the condensate is not macroscopically occupied. But the sequence describes a homogeneous proper condensate in $O$ in the limit with all of its consequences, discussed in the main text.

For given orthonormal basis, one can also define Hamiltonians on $L^2(O)$ with corresponding eigenstates and arbitrary discrete spectrum. The states $\omega_n$ are stationary under the action of the corresponding dynamics. Given $n > 1$ and a temperature $T$, there are also Hamiltonians $H_n$ on $L^2(O)$ such that the states $\omega_n$ satisfy the KMS condition for the corresponding dynamics and given temperature. They act on the orthonormal basis $e_k$, $k \in \mathbb{N}_0$, according to

$$H_n e_k = Te_k \begin{cases} \ln(1 + n_C(n)^{-1}) & \text{if } k = 0 \\ \ln(1 + e^{\varepsilon_n k}) & \text{if } k \geq 1. \end{cases} \quad \text{(A.4)}$$

One can extend these Hamiltonians to wave functions with arbitrary support by adding to them operators which commute and act trivially on the wave functions with support in $O$. There exist also more refined examples of this kind.
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