Proper condensates

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In this article a novel characterization of Bose-Einstein condensates is proposed. Instead of relying on occupation numbers of a few dominant modes, which become macroscopic in the limit of infinite particle numbers, it focuses on the regular excitations whose numbers stay bounded in this limit. In this manner, subspaces of global, respectively local regular wave functions are identified. Their orthogonal complements determine the wave functions of particles forming proper (infinite) condensates in the limit. In contrast to the concept of macroscopic occupation numbers, which does not sharply fix the wave functions of condensates in the limit states, the notion of proper condensates is unambiguously defined. It is outlined, how this concept can be used in the analysis of condensates in models. The method is illustrated by the example of trapped non-interacting ground states and their multifarious thermodynamic limits, differing by the structure of condensates accompanying the Fock vacuum. The concept of proper condensates is also compared with the Onsager-Penrose criterion, based on the analysis of eigenvalues of one-particle density matrices. It is shown that the concept of regular wave functions is useful there as well for the identification of wave functions forming proper condensates.

1. INTRODUCTION

We propose in this article a novel characterization of Bose-Einstein condensates. It differs from various previous approaches, based on concepts such as the spectrum of one-particle density matrices in approximating states, the spontaneous breakdown of gauge symmetries in the thermodynamic limit, or the appearance of long range order, cf. for example.\cite{6,8} The latter concepts focus on global properties of the underlying systems. On the other hand, condensates are prepared in realistic experiments in bounded regions with a limited number of particles.

The primary problem appearing in the formulation of a corresponding local criterion for condensation is due to the fact that the states of interest, having a finite particle number, can be described in the Fock representation (they are locally normal). So a sharp criterion that characterizes condensates locally seems to be out of reach. In order to overcome this difficulty, we consider the idealization of an unlimited number of particles occupying regions, which are suitably adjusted to the particle numbers. If the resulting states separate in the limit in an unambiguous manner into an infinite number of particles, occupying a few states, and a regular component consisting of finite numbers of particles occupying each of the remaining states, we speak of proper condensation. As we shall see, the determination of the regular components is crucial for the identification of the wave functions of the condensate. The idealizations underlying our approach are out of experimental reach,
but they allow it on the theoretical side to determine in a clear-cut manner the wave functions of particles forming condensates. Once this has been accomplished, one can return to the states with a large, but finite particle number and study the onset of proper condensation, depending on data such as the temperature, the shape of trapping potentials, etc.

We are interested in states containing a finite number of particles in $s$-dimensional space $\mathbb{R}^s$, which are confined by a trapping potential. Since we need to proceed to limits involving an infinite number of particles, including the passage to appropriate thermodynamic limits, it is convenient to describe the states by positive linear functionals on a specific algebra of bounded operators, the resolvent algebra $\mathcal{A}(\mathbb{R}^s)$ introduced in\textsuperscript{4}. It is superior to the Weyl algebra since contributions due to infinite accumulations of particles are effectively suppressed, whereas on the Weyl algebra they lead to singular states which often defy a meaningful physical interpretation.

The resolvent algebra contains a subalgebra $\mathfrak{A}(\mathbb{R}^s)$ of observables which do not change particle numbers\textsuperscript{3}. Observables which are localized in open bounded or unbounded regions $O \subset \mathbb{R}^s$ are described by subalgebras $\mathfrak{A}(O) \subset \mathfrak{A}(\mathbb{R}^s)$. What matters here is the fact that these algebras contain the resolvents of corresponding particle number operators, $\mu \mapsto (\mu I + a^*(f)a(f))^{-1}$, for $f \in L^2(O)$ and $\mu > 0$, where $a^*(f), a(f)$ are creation and annihilation operators. Our criterion, characterizing states containing proper condensates, is based on these operators.

In the subsequent section we define the notion of proper condensates, exhibit some of its features, and indicate how it can be used in applications. In Sect. 3 we illustrate the method by an analysis of the thermodynamic limits of non-interacting bosons that occupy the ground states in regular trapping potentials. Depending on how this limit is reached, the resulting Fock vacuum is accompanied by different arrangements of condensates. Sect. 4 contains a study of the relation between the notion of proper condensates and the concept of macroscopic occupation numbers, invented by Onsager and Penrose\textsuperscript{7}, which is based on the analysis of one-particle density matrices. Our article concludes with an outlook on further applications of our framework. In an appendix some general properties of the occupation numbers of one-particle density matrices are exhibited.

2. IDENTIFICATION OF PROPER CONDENSATES

We consider arbitrary states on the algebra of observable $\mathfrak{A}(\mathbb{R}^s)$, i.e., positive, linear and normalized functional $\omega : \mathfrak{A}(\mathbb{R}^s) \to \mathbb{C}$. Let us recall that any such state gives rise by the GNS-construction to a representation, where the state is represented by some unit vector in a Hilbert space and the elements of the algebra by concrete bounded operators acting on this space\textsuperscript{5}. The restrictions of the functional to the local algebras, $\omega \upharpoonright \mathfrak{A}(O)$, sometimes called partial states, contain the information which one obtains about $\omega$ by observations in a given region $O \subset \mathbb{R}^s$.

Our criterion, characterizing states containing a proper condensate, deals with primary states. These are states where the weak closures of the algebra of observables in the respective GNS-representations have a trivial center. In applications, interesting examples are pure states and pure phases in case of thermal systems.

**Definition:** Let $O \subset \mathbb{R}^s$ be any (bounded or unbounded) region. A primary state $\omega$ on $\mathfrak{A}(\mathbb{R}^s)$
contains a \textit{proper condensate} in $O$ if there exists some function $f \in L^2(O)$ such that
\[ \omega((\mu 1 + a^*(f)a(f))^{-1}) = 0, \quad \mu > 0. \] (2.1)

**Remark:** All $C_0$-functions, \textit{i.e.} continuous functions vanishing at infinity, of $a^*(f)a(f)$ then vanish in the GNS representation induced by $\omega$, so the single particle state $f$ is infinitely occupied in all states of the corresponding GNS-representation; cf. also the subsequent proposition.

Mixed states, having primary components in their central decomposition that contain proper condensates, can be characterized as follows.

**Proposition 2.1.** Let $\omega$ be a state on $A(\mathbb{R}^d)$. Its central decomposition contains a non-negligible set of primary states with a proper condensate in $O$ iff there is some $f \in L^2(O)$ such that
\[ \limsup_{\mu \to \infty} \mu \omega((\mu 1 + a^*(f)a(f))^{-1}) < 1. \] (2.2)

There is a central projection $Z$ in the weak closure of $A(\mathbb{R}^d)$ in the corresponding GNS-representation such that $\omega(Z)$ indicates the fraction of proper condensate in $O$.

**Proof.** We choose $\mu = \varepsilon^{-1}, \varepsilon > 0$, and put $A_\varepsilon \doteq (1 + \varepsilon a^*(f)a(f))^{-1}$. In order to exhibit the properties of these operators in the limit of small $\varepsilon$, it is convenient to proceed to the (faithful) representation of the full resolvent algebra $R(\mathbb{R}^d)$ on Fock space $\mathcal{F}$. It is generated by the resolvents $R(\lambda, g) \doteq (i\lambda 1 + \phi(g))^{-1}$, where $\phi(g) = 2^{-1/2}(a^*(g) + a(g))$, $g \in L^2(\mathbb{R}^d)$, and $\lambda \in \mathbb{R}\setminus\{0\}$.

It follows by a straightforward computation that the sequence $\varepsilon \mapsto A_\varepsilon$ commutes in norm with all elements of $R(\mathbb{R}^d)$ in the limit of small $\varepsilon$, \textit{i.e.} it is a central sequence. We briefly sketch the argument. Given $g \in L^2(\mathbb{R}^d)$ and $\lambda \in \mathbb{R}\setminus\{0\}$, one has
\[ [R(\lambda, g), A_\varepsilon] = R(\lambda, g)[\phi(g), A_\varepsilon]R(\lambda, g) = R(\lambda, g)[\phi(Pg), A_\varepsilon]R(\lambda, g), \] (2.3)
where $P_\varepsilon$ is the projection onto the ray of $f$. The intertwining relations between $a^*(f)$, $a(f)$, and functions of $a^*(f)a(f)$ imply $\|\phi(f), A_\varepsilon\| \leq (2\varepsilon)^{1/2}$. Thus one arrives at the bound
\[ \|R(\lambda, g), A_\varepsilon\| \leq (2\varepsilon)^{1/2}\lambda^{-2} \|g\|, \] (2.4)
from which the assertion follows.

Turning to the GNS representation induced by the given state $\omega$, the (for decreasing $\varepsilon$) monotonically increasing sequence $\varepsilon \mapsto A_\varepsilon \in A(\mathbb{R}^d)$ converges in the limit of small $\varepsilon$ in the strong operator topology to some operator $P$ in the weak closure of $A(\mathbb{R}^d)$. According to the preceding step, it is an element of its center. Moreover, putting $A_\varepsilon(\mu) \doteq (\mu 1 + \varepsilon a^*(f)a(f))^{-1}$, one obtains
\[ \lim_{\varepsilon \to 0} A_\varepsilon(\mu) = (1/\mu)P \] for any $\mu > 0$. It then follows from the strong operator convergence of these resolvents and the resolvent equality $A_\varepsilon(\mu) - A_\varepsilon(v) = (\mu - \mu)A_\varepsilon(\mu)A_\varepsilon(v)$ that $P$ is a projection. Thus in a factorial representation it is equal to either $0$ or $1$. In view of assumption (2.1), the central decomposition of $\omega$ contains a non-negligible set of primary components in which this projection is equal to $0$. The central projection $Z = (1 - P)$ indicates the fraction of primary states in the decomposition of $\omega$, where this occurs. Since $0 \leq A_{\varepsilon_1} \leq A_{\varepsilon_2}$ if $\varepsilon_1 \geq \varepsilon_2$, it follows that all resolvents $A_\varepsilon, \varepsilon > 0$, also vanish in these states. But then all $C_0$-functions of $a^*(f)a(f)$ vanish according to standard arguments (Stone-Weierstraß approximation). The converse statement is trivial. \qed
It is important to notice that the preceding characterization of states exhibiting a proper condensate in some region does not yet fix the wave functions of the particles forming it. As a matter of fact, if \( h \in L^2(\mathbb{R}^t) \) is orthogonal to the function \( f \) in the proposition and \( \omega(a^*(h)a(h)) < \infty \), one finds by a straightforward estimate that one obtains for the resolvent \( \mu \mapsto (\mu 1 + a^*(f + h)a(f + h))^{-1} \) the same upper bound as for \( f \) in relation (2.2). So there exists an abundance of wave functions which are infinitely occupied in the presence of a proper condensate. This is not surprising since counting the number of particles with a wave function having some overlap with the proper condensate, no matter how small, must be expected to lead to an infinite result.

In view of this situation it is more meaningful to determine the particles which do not have any overlap with a proper condensate.

**Definition:** Let \( \omega \) be a state on \( \mathcal{A}(\mathbb{R}^t) \). A function \( f \in L^2(\mathbb{R}^t) \) is said to be regular if

\[
\lim_{\mu \to \infty} \mu \omega((\mu 1 + a^*(f)a(f))^{-1}) = 1.
\]

(2.5)

The set of all regular functions is denoted by \( \mathcal{R}(\mathbb{R}^t) \) and the regular functions having support in some region \( O \subset \mathbb{R}^t \) are denoted by \( \mathcal{R}(O) \).

The structure of the set of regular functions is clarified in the subsequent lemma.

**Lemma 2.2.** Let \( \omega \) be a state on \( \mathcal{A}(\mathbb{R}^t) \). The corresponding set \( \mathcal{R}(\mathbb{R}^t) \) of regular functions is a complex subspace of \( L^2(\mathbb{R}^t) \).

**Proof.** It is apparent that \( \mathcal{R}(\mathbb{R}^t) \) is stable under multiplication with complex numbers. In order to see that it is stable under taking sums, we proceed as in the proof of the preceding proposition. Let \( A_\delta(f) \triangleq (1 + \delta a^*(f)a(f))^{-1} \) for \( f \in \mathcal{R}(\mathbb{R}^t) \) and \( \delta > 0 \). These operators are monotonically increasing for decreasing \( \delta \) and converge in the limit of small \( \delta \) to the unit operator \( 1 \) in the strong operator topology fixed by the underlying state. We then consider the operators

\[
A_{\varepsilon_1}(f_1)(1 - A_{\varepsilon_2}(f_1 + f_2))A_{\varepsilon_2}(f_2) \\
= \varepsilon A_{\varepsilon_1}(f_1)A_{\varepsilon_2}(f_1 + f_2)a^*(f_1 + f_2)a(f_1 + f_2)A_{\varepsilon_2}(f_2).
\]

(2.6)

Commuting the creation and annihilation operators containing the function \( f_1 \) through the middle term to \( A_{\varepsilon_1}(f_1) \) and keeping the operators containing \( f_2 \) next to \( A_{\varepsilon_2}(f_2) \), one obtains an upper bound on the norm of these operators. It yields for fixed \( \varepsilon_1 > 0 \) and \( \varepsilon_2 > 0 \) after a straightforward computation

\[
\lim_{\varepsilon \searrow 0} \|A_{\varepsilon_1}(f_1)(1 - A_{\varepsilon_2}(f_1 + f_2))A_{\varepsilon_2}\| = 0.
\]

(2.7)

Since \( \|A_{\delta}(f)\| \leq 1 \), it then follows by a three-epsilon argument for \( f_1, f_2 \in \mathcal{R}(\mathbb{R}^t) \) that

\[
\lim_{\varepsilon \searrow 0} \omega(1 - A_{\varepsilon}(f_1 + f_2)) = 0,
\]

(2.8)

proving the statement. \( \square \)

The appearance of proper condensates was studied in non-interacting theories. For equilibrium states in a fixed trapping potential they appear in the limit of infinite particle numbers (maximal chemical potential). In these cases the regular spaces \( \mathcal{R}(\mathbb{R}^t) \) are closed subspaces of \( L^2(\mathbb{R}^t) \). Their
singular orthogonal complement $\mathcal{F}(\mathbb{R}^d)$ describes the wave functions of the particles appearing in proper condensates in the limit states.

Proceeding first to the thermodynamic limit by unfolding the trapping potential and going subsequently to the limit of maximal chemical potential, it turns out that the regular spaces $\mathcal{B}(\mathbb{R}^d)$ are dense in $L^2(\mathbb{R}^d)$, but not closed. This observation has an easy explanation: in the thermodynamic limit the constituents of proper condensates can no longer be described by normalizable wave functions, they become improper states, characterized by constant functions, polynomials etc. The elements of the subspaces $\mathcal{B}(\mathbb{R}^d)$ then serve as test functions. Regardless of this fact, the restrictions of the improper states to bounded regions $O$ are normalizable. As a consequence, the local regular spaces $\mathcal{A}(O)$ are closed. In one and two dimensions they have orthogonal complements $\mathcal{F}(O)$ in $L^2(O)$, describing proper condensates. In higher dimensions such non-trivial orthogonal complements appear in the limit of infinite particle densities. Examples, illustrating these facts, were presented in 1.

It seems worthwhile to extend this analysis to combined approximations, where the approach to the thermodynamic limit and the increase of particle numbers are coupled. In order to illustrate the present concepts, we perform such an analysis in the subsequent section for non-interacting bosons in regular trapping potentials. These potentials are unfolded quite arbitrarily in order to occupy an increasing number of particles, thereby approaching different kinds of thermodynamic limits. It turns out that by unfolding the trapping potential too tardily, proper condensates appear if one rapidly increases the particle number. On the other hand, a swift unfolding of the trapping potential leads exclusively to regular excitations. In this manner one can exhibit distinct local wave functions $\mathcal{F}(O)$ of proper condensates and study in suitable approximations the onset of condensation.

A major challenge, however, is the treatment of theories describing interactions. We do not tackle this demanding issue here and only summarize the general strategy for the verification of the appearance of proper condensates in models, which is suggested by our results. Thinking of such applications, let $\omega_n$ be a sequence of states, which is labeled by the particle number $n \in \mathbb{N}$. In order to exhibit the relevant structures, one must proceed to the limit of this sequence. The sequence may not converge, but since we are dealing with an algebra of bounded operators, it always has limit points according to standard compactness arguments. As a matter of fact, one does not need information about the limits on the full algebra. It suffices to determine the expectation values of resolvents of particle number operators. Their analysis consists of the following steps.

**Step 1:** Determine for the given sequence of states in the limit of large $n \in \mathbb{N}$ the regular space $\mathcal{B}(\mathbb{R}^d)$. If it coincides with $L^2(\mathbb{R}^d)$, there is no sign for proper condensation. If it is closed and has a non-trivial orthogonal complement $\mathcal{F}(\mathbb{R}^d)$, the latter space describes the wave functions of a proper condensate. If $\mathcal{B}(\mathbb{R}^d)$ is dense, but not closed, proceed to the local regular spaces $\mathcal{A}(O)$. They are expected to be closed. If they have an orthogonal complement $\mathcal{F}(O)$, it describes locally a proper condensate.

**Step 2:** Proceed to the analysis of the structure of condensates appearing in the states with a finite particle number. In cases of interest, the spaces $\mathcal{F}(O)$ are expected to be finite dimensional. The corresponding subalgebras of observables $\mathfrak{A}(\mathcal{F}(O))$, involving resolvents of operators with functions in $\mathcal{F}(O)$, then have a simple structure. In particular, the operators $N_{\mathcal{F}(O)}$, determining the number
of condensate particles in $O$, are affiliated with $\mathfrak{A}_\mathcal{O}(O)$. Moreover, the restrictions of $\mathfrak{A}_\mathcal{O}(O)$ to states with a finite particle number are isomorphic to matrix algebras. Thus, for any given total particle number $n \in \mathbb{N}$, one can accurately determine and manipulate the properties of the condensate fraction, such as its particle content. This does not affect properties of the regular excitations, described by the regular algebra of observables $\mathfrak{A}_\mathcal{O}(O)$, which is assigned to the regular functions $\mathcal{R}(O)$ and commutes with $\mathfrak{A}_\mathcal{O}(O)$. This feature resembles the empirical fact that for given material content of a system, it is frequently possible to split it quite arbitrarily into different phases.

Step 3: Study the onset of proper condensation. According to folklore, there do not exist phase transitions in finite systems. But, having identified the condensate spaces $\mathcal{O}(O)$ appearing in the limit of infinite particle numbers, one can analyze the emergence of proper condensates in a given sequence of states. This is accomplished by computing the expectation values of the number operators $N_{\mathcal{O}(O)}(O)$ for the proper condensate, $n \mapsto \omega_n(N_{\mathcal{O}(O)})$, and comparing it with the total number of particles in $O$, given by $n \mapsto \omega_n(N(O))$. Particularly interesting are the cases where the difference between these data remains bounded in the limit,

$$\lim sup_n \omega_n(N(O) - N_{\mathcal{O}(O)}) = m_{\mathcal{O}(O)} < \infty.$$  \hspace{1cm} (2.9)

This happens either if the total number of particles in $O$ stays bounded, or if the regular components, described by $\mathcal{R}(O)$, are saturated in the limit. One can then define the onset of proper condensation in $O$ by the number $n_c(O)$ of particles in the condensate which surpass this limit,

$$\omega_n(N_{\mathcal{O}(O)}) \geq m_{\mathcal{O}(O)}, \quad n \geq n_c(O).$$  \hspace{1cm} (2.10)

In equilibrium states one may then use this condition in order to study its relation with other data, such as the temperature of the states.

3. APPLICATION OF THE FRAMEWORK TO NON-INTERACTING GROUND STATES

In order to illustrate the concept of proper condensation and its usage in the interpretation of a theory, we consider the simple example of non-interacting, trapped bosons in the ground state and passages to the thermodynamic limit. As already mentioned, there exist various approximations of this limit which differ by the spaces of wave functions, describing the resulting proper condensates. Depending on the approximation, one can exhibit in states with a finite particle number more or less detailed spatial patterns of the proper condensates, establish the existence of coexisting phases, and encounter critical densities of the regular fractions.

To keep the discussion simple, we assume that the one-particle Hamiltonian on the space of wave functions $L^2(\mathbb{R}^s)$ is of the form $H_1 = P^2 + V(Q)$, where $P, Q$ are the momentum and position operators and $V$ is some real analytic trapping potential, tending sufficiently rapidly to infinity at large distances. (As a matter of fact, less stringent smoothness properties of the potential would be sufficient.) The normalized ground state wave function $x \mapsto g_1(x) \in L^2(\mathbb{R}^s)$ of the single particle states is then also real analytic (Ch. 3.4). The ground state of the corresponding non-interacting system of $n$ particles in the trapping potential is given by

$$\Omega_n = (n!)^{-1/2} a^*(g_1)^n \Omega_0,$$  \hspace{1cm} (3.1)
where $a^*$ denotes the canonical creation operators and $\Omega_0$ the Fock vacuum vector.

We will proceed to the thermodynamic limit by unfolding the trapping potential, which yields for $\lambda > 0$ the scaled Hamiltonians $H_\lambda = P^2 + \lambda^2 V(\lambda Q)$. The corresponding scaled and normalized ground states are $x \mapsto g_\lambda(x) = \lambda^{n/2}g_1(\lambda x)$ and the scaled $n$-particle states are

$$\Omega_{n,\lambda} = (n!)^{-1/2}a^*(g_\lambda)\Omega_0, \quad n \in \mathbb{N}, \lambda > 0. \quad (3.2)$$

In the passage to the thermodynamic limit we need to couple the particle number $n$ and the scaling parameter $\lambda$, $n \mapsto \lambda(n)$, which will be accomplished in different ways.

A. Regular and singular wave functions

We determine now the spaces of regular wave functions $\mathcal{A}(\mathbb{R}^d)$, describing finitely occupied states, and of singular wave functions $\mathcal{S}(\mathbb{R}^d)$, describing proper condensates in the thermodynamic limit. They are identified by computing in a given sequence of states the expectation values of resolvents of the particle number operators $a^*(f)a(f)$, $f \in L^2(\mathbb{R}^d)$, and proceeding to the limit of infinite particle numbers. It follows from the subsequent lemma that the relevant information is encoded in the transition probabilities between $f$ and the ground states, multiplied by the particle number, viz.

$$n |\langle g_{\lambda(n)}, f \rangle|^2.$$

**Lemma 3.1.** Let $g_n \in L^2(\mathbb{R}^d)$ be a sequence of normalized wave functions and let $\omega_n$ be the $n$-particle states, given by the vectors $\Omega_n = (n!)^{-1/2}a^*(g_n)\Omega_0, \quad n \in \mathbb{N}$. If $f \in L^2(\mathbb{R}^d)$ is such that

$$\lim_n n |\langle g_n, f \rangle|^2 = 0,$$

one obtains for all $\mu > 0$

$$\lim_n \omega_n((\mu 1 + a^*(f)a(f))^{-1}) = \mu^{-1}. \quad (3.3)$$

If $f \in L^2(\mathbb{R}^d)$ satisfies $\lim_n n |\langle g_n, f \rangle|^2 = \infty$, then, for all $\mu > 0$,

$$\lim_n \omega_n((\mu 1 + a^*(f)a(f))^{-1}) = 0. \quad (3.4)$$

**Remark:** In the former case, the wave function $f$ is regular and the limit state coincides on the corresponding observables with the Fock vacuum. In the latter case, the wave function $f$ indicates the presence of some proper condensate.

**Proof.** Without loss of generality we may assume that $f$ is normalized, hence $|\langle g_n, f \rangle| \leq 1$. Putting $R_f(\mu) = (\mu 1 + a^*(f)a(f))^{-1}$ and applying arguments given in Proposition 2.1 we have

$$\omega_n(R_f(\mu)) = |\langle \Omega_n, R_f(\mu)\Omega_n \rangle| = (n^{-1/2}a^*(g_n)R_f(\mu)a(g_n)\Omega_n) + (n^{-1/2}R_f(\mu)a(g_n)\Omega_n)$$

$$= |\langle g_n, f \rangle|^2 \omega_{n-1}(R_f(\mu + 1) - R_f(\mu)) + \omega_{n-1}(R_f(\mu))$$

$$= |\langle g_n, f \rangle|^2 \omega_{n-1}(R_f(\mu + 1)) + (1 - |\langle g_n, f \rangle|^2) \omega_{n-1}(R_f(\mu)). \quad (3.5)$$

Making use of $\omega_0(R_f(\mu)) = 1/\mu$, it follows by induction that

$$\omega_n(R_f(\mu)) = \sum_{k=0}^{n} \binom{n}{k} (\mu + k)^{-1} |\langle g_n, f \rangle|^{2k} (1 - |\langle g_n, f \rangle|^2)^{n-k}. \quad (3.6)$$
Now let \( \lim_n |\langle g_n, f \rangle|^2 = 0 \). Then

\[
|\omega_n(R_f(\mu)) - \mu^{-1}| = \sum_{k=1}^{n} (\mu - (\mu + k)^{-1}) (\binom{n}{k} |\langle g_n, f \rangle|^{2k} (1 - |\langle g_n, f \rangle|^2)^{n-k})
\]

\[
= n |\langle g_n, f \rangle|^2 \sum_{l=0}^{n-l} \mu^{-1} \binom{n-l}{l} |\langle g_n, f \rangle|^{2l} (1 - |\langle g_n, f \rangle|^2)^{(n-1)-l}
\]

\[
\leq n |\langle g_n, f \rangle|^2 \mu^{-2} \sum_{l=0}^{n-l} \binom{n-l}{l} |\langle g_n, f \rangle|^{2l} (1 - |\langle g_n, f \rangle|^2)^{(n-1)-l}
\]

\[
= n |\langle g_n, f \rangle|^2 \mu^{-2}.
\] (3.7)

Hence the sequence converges to 0, as stated.

Next, we consider the case that \( \lim_n n |\langle g_n, f \rangle|^2 = \infty \). Thus we may assume that \( |\langle g_n, f \rangle|^2 \neq 0 \) and obtain

\[
\omega_n(R_f(\mu)) = \sum_{k=0}^{n} (\mu + k)^{-1} (\binom{n}{k} |\langle g_n, f \rangle|^{2k} (1 - |\langle g_n, f \rangle|^2)^{n-k})
\]

\[
= \left( (n+1) |\langle g_n, f \rangle|^2 \right)^{-1} \sum_{l=0}^{n+1} (\mu - 1 + l)^{-1} \binom{n+1}{l} |\langle g_n, f \rangle|^{2l} (1 - |\langle g_n, f \rangle|^2)^{(n+1)-l}
\]

\[
\leq \left( (n+1) |\langle g_n, f \rangle|^2 \right)^{-1} (1 + \mu^{-1}) \sum_{l=0}^{n+1} \binom{n+1}{l} |\langle g_n, f \rangle|^{2l} (1 - |\langle g_n, f \rangle|^2)^{(n+1)-l}
\]

\[
= \left( (n+1) |\langle g_n, f \rangle|^2 \right)^{-1} (1 + \mu^{-1}).
\] (3.8)

The expression in the last line converges to 0, completing the proof.

\[\square\]

The wave functions that are regular in the thermodynamic limit can now be determined. Let us recall that it is meaningful to restrict attention in this limit to regular functions with compact support. Because, the proper condensates are globally described by distributions, but their restrictions to bounded regions \( O \) are square integrable functions \( \mathcal{A}_0(O) \), which lie in the orthogonal complements of the regular functions \( \mathcal{R}(O) \). According to the preceding lemma, the transition probabilities of the wave functions \( f \) to the scaled ground states, multiplied by the particle number, contain the relevant information about their interpretation as members of either one of these spaces.

In order to see how this assignment is related to properties of the ground state wave functions, let \( \lambda \mapsto n(\lambda) = c\lambda^{-\kappa} \) for some \( \kappa > 0 \). There exists a corresponding dense set of functions \( f \in L^2(\mathbb{R}^q) \) such that \( \lambda^{-\kappa} |\langle g_{\lambda}, f \rangle|^2 \to 0 \) in the scaling limit \( \lambda \to 0 \). For the proof we make use of the fact that \( g_1 \), being real analytic, can be expanded in a Taylor series about 0. Thus, for any given \( k \in \mathbb{N} \), there exists a polynomial \( x \mapsto P_k(x) \) of degree \( (k-1) \) such that \( |g_1(x) - P_k(x)| \leq c_k |x|^k \) for \( |x| < R_0 \), where \( R_0 \) depends on the analyticity properties of \( g_1 \). This yields for the integrals of the scaled functions over the balls \( B_R = \{ x \in \mathbb{R}^q : |x| < R \} \) and scalings \( 0 < \lambda < R_0/R \)

\[
\int_{B_R} d\lambda d^q |g_1(\lambda x) - P_k(\lambda x)|^2 \leq c_k(R) \lambda^{q+2k}.
\] (3.9)

Now let \( f \in L^2(\mathbb{R}^q) \) be any function with compact support such that its (entire analytic) Fourier transform \( \tilde{f} \) vanishes sufficiently rapidly at the origin. More precisely, \( P_k(\lambda \partial \lambda)(\tilde{f}(p)|_{p=0} = 0 \) for all \( \lambda > 0 \), where \( \partial \lambda \) denotes the gradient in momentum space. Since the linear span of the scaled
polynomials is finite dimensional, such functions exist. As a matter of fact, their linear span is dense in $L^2(\mathbb{R}^d)$. Now, given any such function, it has support in $B_R$ for sufficiently large $R$, so one obtains for small $\lambda$

$$\| \langle g_\lambda, f \rangle \|^2 = \| \langle g_\lambda - P_k \lambda \rangle, f \rangle \|^2 \leq c_k(R) \| f \|^2 \lambda^{s+2k}. \quad (3.10)$$

Let $k \in \mathbb{N}_0$ be the smallest number such that $k > (\kappa - s)/2$. It follows that $\lambda^{-s} \| \langle g_\lambda, f \rangle \|^2 \to 0$ in the limit of small $\lambda$, as stated.

If $\kappa < s$, the above limit is equal to 0 for all functions $f$ with compact support. So the local spaces of regular functions $\mathcal{R}(O)$ do not have an orthogonal complement in $L^2(O)$ for any bounded region $O \subset \mathbb{R}^d$, there appear no proper condensates in the thermodynamic limit. If $\kappa > s$ there arise for any $f$ with compact support the following clear-cut alternatives: either the limit is 0, or it approaches $\infty$.

In the former case, $f$ is a regular member of some space $\mathcal{R}(O)$. It is orthogonal to the homogeneous parts of the approximating polynomial $P_k$, describing a proper condensate, whose square integrable restrictions to bounded regions $O$ form the singular spaces $\mathcal{S}(O)$. In the latter case, the scalar product of $f$ with a condensate wave function is different from 0. It then follows that $\lambda^{-s} \| \langle g_\lambda, f \rangle \|^2$ approaches infinity for small $\lambda$. Note that $f$ may not be a member of a space $\mathcal{S}(O)$, it must merely have some overlap with a singular function. In spite of this feature, one can unambiguously identify the regular and singular wave functions for the given values of $\kappa$.

### B. Coexistence of phases

Whereas in the preceding two cases either the proper condensate or the regular excitations dominate in the thermodynamic limit, the situation is different for $\kappa = s$. It turns out in this intermediate case that the regular excitations can coexist with a condensate in arbitrary portions, viz. they form coexisting phases. So let $n \to \lambda(n) = \sigma n^{-1/s}$ be given, $\sigma > 0$. The resulting states are locally normal in the thermodynamic limit, i.e. their restrictions to any local observable algebra $\mathcal{A}(O)$ can be represented by a density matrix in Fock space, depending on the bounded region $O$. There are no proper condensates in these states; but they appear if one lets $\sigma$ tend to infinity. So, again, one can identify the regular wave functions and the wave functions of the asymptotic proper condensate and disentangle the contributions which are due to the onset of proper condensation from those of the regular excitations.

The strategy of proof is the same as in the preceding lemma. Assuming that the unscaled ground state wave function $g_1$ is different from 0 at the origin, one obtains by a straightforward computation for functions $f \in L^2(\mathbb{R}^d)$ with compact support

$$\nu_f \doteq \lim_n n \| \langle g_{\lambda(n)}, f \rangle \|^2 = \sigma^2 \| g_1(0) \|^2 \int dx f(x)^2. \quad (3.11)$$

Thus if $\sigma$ tends to infinity, this expression diverges, unless the Fourier transform of $f$ vanishes at 0. So the spaces of regular functions $\mathcal{R}(O)$ consist of square integrable functions with support in $O$ and Fourier transforms which vanish at the origin. The condensate spaces $\mathcal{S}(O)$ consist of their orthogonal complements in $L^2(O)$, i.e. the constant functions in $O$. Making use of arguments in the proof of the preceding lemma, we obtain the following result.

**Lemma 3.2.** Let $\sigma > 0$, let $n \to \lambda(n) = \sigma n^{-1/s}$, and let $\omega_{n,\lambda(n)}$ be the states determined by the vectors $\Omega_{n,\lambda(n)}$ in equation (3.2), $n \in \mathbb{N}$. For any compactly supported function $f \in L^2(\mathbb{R}^d)$ and
\( \mu > 0 \), one has
\[
\lim_{n} \omega_{n, \lambda(n)}((\mu 1 + a^* f a(f))^{-1}) = \mu^{-1} \left( 1 - \nu_f e^{-\nu_f} \int_{0}^{1} d\nu \, \mu e^{\nu_f} \nu \right). \tag{3.12}
\]

**Proof.** Making use of relation (3.6) and putting \( \nu_{f,n} \rightarrow n |(g_{k(n)}, f)|^2 \), one obtains
\[
\omega_{n, \lambda(n)}(R_f(\mu)) = (1 - \nu_{f,n}/n)^n \sum_{k=0}^{n} (\mu + k)^{-1} (k!)^{-1} \nu_{f,n}^{k} \prod_{l=0}^{k-1} \left( (1 - l/n)(1 - \nu_{f,n}/n)^{-1} \right). \tag{3.13}
\]
In the limit of large \( n \) one has \( \nu_{f,n} \rightarrow \nu_f \) and \( (1 - \nu_{f,n}/n)^n \rightarrow e^{-\nu_f} \). The product under the sum has the upper bound \( e^{\nu_f} \) and hence is uniformly bounded in \( k \) and \( n \). Thus, by an application of the dominated convergence theorem, one arrives at
\[
\lim_{n \rightarrow \infty} \omega_{n, \lambda(n)}(R_f(\mu)) = e^{-\nu_f} \sum_{k=0}^{\infty} (\mu + k)^{-1} (k!)^{-1} \nu_{f,k}^{k}. \tag{3.14}
\]
This result coincides with the expression given in the statement, as can be established by a routine computation. \( \square \)

It follows from this lemma that the resolvents of the particle number operators \( N(f) = a^*(f) a(f) \) for compactly supported, normalized functions \( f \) are regular in all limit states. This is in accord with the statement that these states are locally normal. It also follows from the lemma that the mean of \( N(f) \) in the limit states is given by \( \omega_n(N(f)) = \nu_f \). Thus it is 0 for regular functions in \( \mathcal{R}(O) \), which indicate the Fock vacuum. For normalized singular functions \( s \in \mathcal{S}(O) \) one obtains \( \omega_n(N(s)) = \nu_s = \sigma^* |g_1(0)|^2 |O| \), which describes a homogeneous condensate with a density determined by \( \sigma \). As already mentioned, it becomes a proper condensate if \( \sigma \) tends to infinity.

### C. Spatial structure of condensates

In case of the special scalings considered in the preceding subsection, the condensates which appeared there were spatially homogeneous. Yet it is an empirical fact that systems with given material content can often be split quite arbitrarily into different phases localized in differing regions, so the corresponding states are inhomogeneous.

We will show now that such more complex structures emerge in the present model if one proceeds to scalings \( n \rightarrow \lambda(n) = \sigma n^{-1/k} \) with \( k > s \). As we have seen, the proper condensates are determined by polynomials \( x \rightarrow P_k(x) \), approximating the wave function of the ground state, where \( k > (k - s)/2 \) denotes the degree of approximation. Because of the scaling involved in the passage to the thermodynamic limit, the homogeneous pieces of this polynomial are of interest. Their restrictions to bounded regions \( O \) form the finite dimensional spaces \( \mathcal{S}(O) \) of singular wave functions, having the regular functions \( \mathcal{R}(O) \) in their orthogonal complement.

We keep the bounded region \( O \) fixed in the following and split the \( n \)-particle space, formed by wave functions with support in this region, into a sum of symmetric tensor products containing regular, respectively singular functions,
\[
\mathcal{F}_n(L^2(O)) = \sum_{l=0}^{n} \mathcal{F}_l(\mathcal{S}(O)) \otimes \mathcal{F}_{n-l}(\mathcal{R}(O)), \tag{3.15}
\]
in an obvious notation. The action of the algebra of condensate observables \( \mathfrak{A}(\mathcal{S}(O)) \), being generated by resolvents with functions in \( \mathcal{S}(O) \), affects only the finite dimensional subspaces \( \mathcal{F}_1(\mathcal{S}(O)) \), the regular subspaces \( \mathcal{F}_{n-1}(\mathcal{R}(O)) \) remain untouched. Thus \( \mathfrak{A}(\mathcal{S}(O)) \) acts like a matrix algebra on \( \mathcal{F}_n(L^2(O)) \). Whence, by a finite number of operations, one can analyze and modify the condensate part of the \( n \)-particle states. In particular, one can discriminate the wave functions of particles in the condensate. Doing this in all regions \( O \), one can thereby unravel their spatial structures.

Furthermore, given any number \( 0 \leq k \leq n \) of particles in the condensate, there is a projection \( P_k \in \mathfrak{A}(\mathcal{S}(O)) \) which projects onto the subspace, \( P_k : \mathcal{F}_n(L^2(O)) \rightarrow \mathcal{F}_k(\mathcal{S}(O)) \otimes \mathcal{F}_{n-k}(\mathcal{R}(O)) \). Applying this projection to the vector \( \Omega_{n,\lambda(n)} \) in equation (3.2), one obtains, apart from some numerical factor,

\[
P_k \Omega_{n,\lambda(n)} = a^*(P_k g_{\lambda(n)})^k a^*((1-P_k)g_{\lambda(n)})^{n-k} \Omega_0.
\]

These vectors define product states \( \omega_{n,k} \) on the algebra \( \mathfrak{A}(\mathcal{S}(O)) \otimes \mathfrak{A}(\mathcal{R}(O)) \),

\[
\omega_{n,k}(AB) = \overline{\omega}_k(A) \overline{\omega}_{n-k}(B), \quad A \in \mathfrak{A}(\mathcal{S}(O)), \quad B \in \mathfrak{A}(\mathcal{R}(O)).
\]

Here \( \overline{\omega}_l \) are the \( l \)-particle states with state vectors \( \overline{\omega}_{l,\lambda(n)} = (l!)^{-1/2}a^*(g_{\lambda(n)})^l \Omega_0 \), \( 0 \leq l \leq n \). Thus, picking any \( 0 \leq k \leq n \), the fraction \( k/n \) of condensate in the resulting states \( \omega_{n,k} \) can be fixed without affecting the total number \( n \) of particles.

So, to summarize, the amount of condensate in the given finite system at zero temperature can be arbitrarily adjusted, just like its spatial patterns, which are determined by the choice of the trapping potential.

### D. Critical densities

In case of scalings for which proper condensates appear in the thermodynamic limit, these outrun eventually the occupation numbers of all other states. Given a space of singular wave functions \( \mathcal{S}(O) \), which has been identified for some particular scaling, it is therefore of interest to analyze the fate of the corresponding regular excitations by changing the scaling and studying the number of particles with wave functions in \( \mathcal{R}(O) \cong \mathcal{S}(O)_{1} \cap L^2(O) \). These numbers can easily be determined.

Let \( N(O), N_{\mathcal{S}}(O), \) and \( N_{\mathcal{R}}(O) \) be, for given region \( O \), the total number operator, the operator counting the particles with wave functions in \( \mathcal{S}(O) \), respectively in the corresponding regular space \( \mathcal{R}(O) \). In order to simplify the discussion, let us assume that \( \mathcal{S}(O) \) is one-dimensional, consisting of multiples of the normalized characteristic function \( \chi_O \) of \( O \). We also note that, without restriction of generality, we may assume that the ground state wave function \( g_1 \) is positive. Putting \( \lambda(n) = \lambda \) for a moment and keeping \( n \) fixed, we have

\[
\omega_{n,\lambda}(N_{\mathcal{R}}(O)) = \omega_{n,\lambda}(N(O)) - \omega_{n,\lambda}(N_{\mathcal{S}}(O)) = n\lambda^2 \left( \int_O dx g_1(\lambda x)^2 - \left( \int_O dx g_1(\lambda x) \chi_O(x) \right)^2 \right).
\]
The expression in the second line is non-negative, analytic for sufficiently small $\lambda$, and it is different from 0. It is also apparent that the two terms in the bracket cancel each other at $\lambda = 0$. Thus there is some number $l \in \mathbb{N}$ and some constant $c(O) > 0$ such that for small $\lambda$ one has in leading order $\omega_{n,\lambda}(N_{\mathcal{O}}(O)) \approx c(O) n^{s+l}$.

It follows that for scalings $n \mapsto \lambda(n) \approx n^{-1/\kappa}$ with $\kappa < s + l$ all excitations in $\mathcal{R}(O)$ disappear in the thermodynamic limit, only the states in $\mathcal{I}(O)$ are occupied, eventually. If $\kappa > s + l$, the number of excitations in $\mathcal{R}(O)$ tends to infinity, indicating the appearance of further modes which contribute to the proper condensate. Of particular interest are the scalings $n \mapsto \lambda(n) = \sigma n^{-1/(s+l)}$. There one arrives at

$$
\lim_{n} \omega_{n,\lambda(n)}(N_{\mathcal{O}}(O)) = c(O) \sigma^{s+l}.
$$

(3.19)

Thus, for these scalings, the particles with wave functions in $\mathcal{R}(O)$ have a critical local density. So the expectation values of the number of condensate particles $n \mapsto \omega_{n,\lambda(n)}(N_{\mathcal{O}}(O))$ with wave functions in $\mathcal{I}(O)$ become dominant if this value is reached, akin to the appearance of a phase transition. So the points illustrated here show that the concept of proper condensates leads to a refined understanding of the onset of condensation.

4. MACROSCOPIC OCCUPATION AND PROPER CONденSATION

We compare now our notion of proper condensates with the concept of macroscopic occupation numbers, proposed by Onsager and Penrose\textsuperscript{7}, which is frequently used in the literature. It also deals with sequences of $n$-particle states $\omega_n$, where one determines for each $n$ the dominant occupation number of single particle states, given by the maximal eigenvalue of the corresponding one-particle density matrices, $n \in \mathbb{N}$. In order to distinguish this concept from our notions, we introduce the following terminology.

**Definition:** Let $\omega_n$ be a sequence of $n$-particle states, $n \in \mathbb{N}$. This sequence describes **growing condensates** if there exist normalized functions $f_n \in L^2(\mathbb{R}^n)$, $n \in \mathbb{N}$, and some constant $0 < \delta \leq 1$ such that

$$
\limsup_{n} \frac{1}{n} \omega_n(a^*(f_n)a(f_n)) \geq \delta.
$$

(4.1)

According to standard terminology, the corresponding single particle states are macroscopically occupied in this case.

Being based in a clear-cut manner on the convenient notion of one-particle density matrices, this characterization of growing condensates has found numerous applications in the analysis of models. Yet, in spite of these successes, it is not fully satisfactory in some respects. First, since the functions $f_n$ vary with $n$, it does not give an answer to the question whether the condensates can be described in the limit of large $n$ by specific wave functions or, more generally, specific improper states. Second, relation (4.1) does not characterize by itself the condensate functions $f_n$. As a matter of fact, adding to $f_n$ any function $h$ for which $\limsup_n \omega_n(a^*(h)a(h)) < \infty$, the resulting functions still comply with this relation. Since it will not always be possible to determine precisely the eigenfunctions of the one-particle density matrices, the structure of the condensates in the limit remains to be even more obscure. Third, one might ask whether the dependence of the expectation values in relation (4.1)
on the particle number \( n \) is really crucial. Taking into account that the universe contains about \( 10^{80} \) atoms, it may still seem meaningful to speak of macroscopic occupation if one replaces the prefactor \((1/n)\) by \((\ln(n)/n)\), say. It turns out, however, that one then opens Pandora’s box. As is shown in the appendix, the set of functions \( f \), satisfying such mildly weaker conditions in a sequence of states exhibiting growing condensates, is huge (it is of second category). In a rough analogy: it is as big as the set of non-rational real numbers compared to the number of rationals.

In view of the results obtained in the preceding sections, it is apparent what is missing in order to solve these conceptual problems: one must determine the wave functions which are regular in the limit. Restricting our attention to the one-particle density matrices, we are led to the following definition.

**Definition:** Let \( \omega_n \) be a sequence of \( n \)-particle states, \( n \in \mathbb{N} \). A function \( f \in L^2(\mathbb{R}^s) \) is said to be one-particle regular if

\[
\limsup_{n} \omega_n(a^*(f)a(f)) < \infty.
\]

(4.2)

The complex subspace of one-particle regular functions is denoted by \( \mathcal{R}(\mathbb{R}^s) \).

Since the number operators, counting particles with given wave function, are unbounded, the space of one-particle regular functions is in general smaller than the full space of regular functions. This is shown in the subsequent lemma. What is of more interest is the observation that if the space \( \mathcal{R}(\mathbb{R}^s) \) is closed and has a finite dimensional orthogonal complement, there exist functions \( f \), not depending on the particle number, for which condition (4.1) is satisfied.

**Lemma 4.1.** Let \( \omega_n \) be a sequence of \( n \)-particle states, \( n \in \mathbb{N} \), and let \( \mathcal{R}(\mathbb{R}^s) \) be the corresponding one-particle regular functions.

(i) \( \mathcal{R}(\mathbb{R}^s) \subset \mathcal{R}(\mathbb{R}^s) \), where \( \mathcal{R}(\mathbb{R}^s) \) is the space of regular functions, defined in the Section 2.

(ii) Let the sequence of states exhibit growing condensates and let the corresponding space \( \mathcal{R}(\mathbb{R}^s) \) be closed and have a finite dimensional orthogonal complement. There is a function \( f \) in this complement, which does not depend on the particle number, for which relation (4.1) is satisfied with some lower bound \( \delta' > 0 \).

**Proof.** (i) The first statement is a consequence of the simple estimate

\[
\omega_n((1-(1 + \varepsilon a^*(f)a(f))^{-1})) = \varepsilon \omega_n(a^*(f)a(f))(1 + \varepsilon a^*(f)a(f))^{-1}) \leq \varepsilon \omega_n(a^*(f)a(f)).
\]

(4.3)

Thus if \( \omega_{n_0} \) is any limit point of the given sequence of states, one has

\[
\omega_{n_0}((1-(1 + \varepsilon a^*(f)a(f))^{-1})) \leq \varepsilon \limsup_{n} \omega_n(a^*(f)a(f)) = \varepsilon c_f, \; f \in \mathcal{R}(\mathbb{R}^s).
\]

(4.4)

So the resolvents of the particle number operators assigned to functions \( f \in \mathcal{R}(\mathbb{R}^s) \) converge in the limit states to the unit operator 1 in the limit of small \( \varepsilon \).

(ii) If the space \( \mathcal{R}(\mathbb{R}^s) \) is a closed subspace of \( L^2(\mathbb{R}^s) \), there exists by the uniform boundedness principle\(^9\) some constant \( c_{\mathcal{R}} \) such that

\[
\omega_n(a^*(f)a(f)) \leq c_{\mathcal{R}} \|f\|^2, \; f \in \mathcal{R}(\mathbb{R}^s), \; n \in \mathbb{N}.
\]

(4.5)
Let $P_\mathfrak{A}$ be the projection onto $\mathfrak{A}(\mathbb{R}^s)$ and let $f_n$, $n \in \mathbb{N}$, be a sequence of functions complying with condition (4.1). One then obtains straightforwardly

$$\omega_n(\alpha^*( (1 - P_\mathfrak{A}) f_n) \alpha((1 - P_\mathfrak{A}) f_n)) \geq \omega_n(\alpha^* f_n \alpha f_n) - 2(c_{\mathfrak{A}} n)^{1/2}, \quad (4.6)$$

hence $\limsup_n (1/n) \omega_n(\alpha^* (1 - P_\mathfrak{A}) f_n \alpha (1 - P_\mathfrak{A}) f_n) \geq \delta$. Since the projection $(1 - P_\mathfrak{A})$ has by assumption finite dimension $d$, it follows that there exists in the compact unit ball of the corresponding subspace some normalized function $f$ such that

$$\limsup_n (1/n) \omega_n(\alpha^* f \alpha f) \geq \delta/d, \quad (4.7)$$

completing the proof.

As was discussed in the preceding sections, the spaces $\mathfrak{A}(\mathbb{R}^s)$ may not be expected to be closed in general if one proceeds to the thermodynamic limit, since then the emerging condensates are to be described by distributions. The method to avoid this problem is to restrict attention to local subspaces $L^2(O) \subset L^2(\mathbb{R}^s)$. Proceeding from the obvious characterization of sequences of states describing locally some growing condensate, one may expect that the resulting local regular spaces $\mathfrak{A}(O)$ are closed in cases of interest and also have finite dimensional orthogonal complements. The preceding results then apply accordingly. We dispense with a discussion of the obvious details.

In our final result, we establish a relation between the notions of growing condensates and of proper condensates in those cases, where one can find a fixed function $f$ for which condition (4.1) is satisfied.

**Proposition 4.2.** Let $\omega_n$ be a sequence of $n$-particle states on the algebra of observables $\mathfrak{A}(\mathbb{R}^s)$ for which condition (4.1) is satisfied for a fixed normalized function $f \in L^2(\mathbb{R}^s)$, not depending on $n \in \mathbb{N}$. There exist limit points $\omega_\infty$ of this sequence, containing in their central decomposition a non-negligible set of primary components with the property that all $C_0$-functions of $\alpha^* f \alpha f$ vanish in the corresponding GNS representation. In other words, they contain a proper condensate.

**Proof.** We make use of the resolvents $A_\varepsilon = (1 + \varepsilon \alpha^* f \alpha f)^{-1}$, $\varepsilon > 0$, considered in Proposition 2.1 and show that the states have weak-* limit points in which the expectation values of these resolvents comply with relation (2.2). The statement then follows from that proposition.

Restricting the number operator $\alpha^* f \alpha f$ to the $n$-particle space $\mathcal{F}_n$, it can be spectrally decomposed into

$$\alpha^* f \alpha f \mid \mathcal{F}_n = \sum_{k=0}^{n} k E_{n,k}, \quad n \in \mathbb{N}. \quad (4.8)$$

By assumption there exists a subsequence $\omega_{n_l}$ such that, disregarding corrections which vanish in the limit of large $n_l$,

$$\sum_{k=0}^{n_l} k \omega_{n_l}(E_{n_l,k}) \geq \delta n_l, \quad l \in \mathbb{N}. \quad (4.9)$$
Denoting by \([x] \in \mathbb{N}_0\) the largest number which is smaller or equal to \(x > 0\), we have

\[
\sum_{k=0}^{n_l} k \omega_n(E_{n_l,k}) \leq \sum_{k=0}^{\lfloor \delta n_l/2 \rfloor} k \omega_n(E_{n_l,k}) + \sum_{k=\lfloor \delta n_l/2 \rfloor}^{n_l} k \omega_n(E_{n_l,k})
\]

\[
\leq \lfloor \delta n_l/2 \rfloor + n_l \sum_{k=\lfloor \delta n_l/2 \rfloor}^{n_l} \omega_n(E_{n_l,k}).
\]  \hspace{1cm} (4.10)

It implies

\[
\sum_{k=\lfloor \delta n_l/2 \rfloor}^{n_l} \omega_n(E_{n_l,k}) \geq \delta/2, \quad l \in \mathbb{N}.
\]  \hspace{1cm} (4.11)

Now let \(\varepsilon > 0\) and let \(D_\varepsilon \doteq (1 - A_\varepsilon) = \varepsilon a^*(f) a(f) (1 + \varepsilon a^*(f) a(f))^{-1}\). Then

\[
\omega_n(D_\varepsilon) = \sum_{k=0}^{n_l} \left(\varepsilon k/(1 + \varepsilon k)\right) \omega_n(E_{n_l,k}) \geq \sum_{k=\lfloor \delta n_l/2 \rfloor}^{n_l} \left(\varepsilon k/(1 + \varepsilon k)\right) \omega_n(E_{n_l,k})
\]

\[
\geq \frac{\varepsilon}{1 + \varepsilon} \left\lfloor \delta n_l/2 \right\rfloor \sum_{k=\lfloor \delta n_l/2 \rfloor}^{n_l} \omega_n(E_{n_l,k}) \geq \frac{\delta \varepsilon \left\lfloor cn_l/2 \right\rfloor}{2(1 + \varepsilon \left\lfloor \delta n_l/2 \right\rfloor)}. \]  \hspace{1cm} (4.12)

It follows that \((1 - \limsup_{\varepsilon \searrow 0} \omega_n(A_\varepsilon)) = \liminf_{\varepsilon} \omega_n(D_\varepsilon) \geq \delta/2 > 0\), independently of the value of \(\varepsilon > 0\). Thus if \(\omega_\infty\) is any weak-* limit point on \(\mathfrak{A} (\mathbb{R}^d)\) of the sequence \(\omega_n\), \(l \in \mathbb{N}\), one has \(\limsup_{\varepsilon \searrow 0} \omega_\infty(A_\varepsilon) \leq (1 - \delta/2) < 1\), completing the proof.

Thus the concepts introduced in the present investigation also add to the understanding of the properties of growing condensates in the limit of large particle numbers.

5. CONCLUSIONS

In the present investigation we have established concepts which allow it to discuss the formation of condensates in an unambiguous manner in states with a finite particle number. The basic idea is to proceed to the theoretical limit of infinite particle numbers and to determine the subspaces of wave functions that describe regular, finitely occupied excitations. This step is necessary in order to clearly identify the wave functions of the proper condensates within the maze of infinitely occupied states which have some overlap with them. In those cases where the spaces of regular functions are closed and have an orthogonal complement, the wave functions in this complement describe the proper condensates, consisting of infinitely many particles in the limit. In view of this feature we refer to those functions as singular. The notion of proper condensate has the status of a superselection rule. As we have seen, the presence of proper condensates can be established by central sequences of observables.

If the regular spaces are not closed, it is an indication that the condensates in the limit states have to be described by improper states. The regular spaces are then dual to these distributions and serve as test functions. One can frequently bypass this feature by proceeding to a local point of view. Restricting the limit states to local observables, the improper states become normalizable, resulting in singular local subspaces of wave functions in the orthogonal complement of the regular ones.
Having identified the relevant regular spaces and their singular complements, one can revert to the states of primary interest, having a finite particle number, and base their analysis on these notions. The algebras of observables which are sensitive to the condensate are assigned to the spaces of singular functions, which are finite dimensional whenever the proper condensates occupy only a limited number of modes. Their restrictions to states with a finite particle number are then isomorphic to matrix algebras, allowing for a convenient analysis and manipulation of the condensate fraction. In particular, the number of particles in the condensate can be changed arbitrarily in these cases without changing the total number of particles in the system or affecting the regular observables. Moreover, one can characterize the onset of proper condensation in given sequences of states by computing the expectation values of the (local) particle number operators for the singular excitations and comparing them with those of the full (local) particle number operators.

We did not discuss here the possibility that the orthogonal complements of the regular functions have infinite dimension. Indeed this is expected to happen in interacting systems if one squeezes the particles into narrow trapping potentials. Then also highly excited states become infinitely occupied. In our opinion these cases are only of secondary interest, similarly to the case of infinite temperatures, where all levels are infinitely occupied and no regular functions survive. We expect that these less transparent forms of condensation can be avoided by choosing appropriate sequences of trapping potentials, where one may be able to establish the onset of proper condensation into a limited number of states.

The notion of proper condensates has already appeared in an analysis of non-interacting systems in arbitrary trapping potentials given in\(^1\). There the idea of focusing on subspaces of regular excitations was systematically pursued in order to identify the singular wave functions in their complement, describing proper condensates. In the present investigation, we have seen that this idea is meaningful more generally. We expect that it will also be useful in interacting theories, where one has less a priori information about possible candidates for the condensate functions. As we have seen, the direct approach for the determination of functions describing proper condensates is difficult. Whenever there are growing condensates in a sequence of states, there exists a maze of other functions (to be precise: of second category) which are also infinitely occupied in the limit of large particle numbers. In contrast, the set of regular functions tends to become smaller in this limit. As a matter of fact, if proper condensates appear, the regular functions are generically meager (of first category), as is obvious if they have a non-trivial orthogonal complement. This feature will hopefully be useful for alternative existence proofs of proper condensates in the presence of interaction.

DEDICATION
This article is dedicated to Helmut Reeh on the occasion of his 90th birthday.

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APPENDIX

We discuss in this appendix some aspects of the direct approach to the determination of condensate wave functions, based on the analysis of one-particle density matrices. As we will see, the concept of growing condensates is quite subtle and depends crucially on the fact that one deals with the exact eigenfunctions of these matrices, assigned to their largest eigenvalues. If one slightly relaxes this condition and only requires that there are one-particle functions which are (almost) macroscopically occupied, there exists an abundance of examples. So this approach does not allow to determine in a precise manner the wave functions of particles in a proper condensate. This observation suggests that concentrating on their complement, the regular functions, may also be meaningful there.

Turning to the analysis, let $\mathcal{H}_2(\mathcal{F})$ be the space of Hilbert-Schmidt operators on the standard bosonic Fock space $\mathcal{F}$ and let $\omega_n$ be a sequence of $n$-particle states, described by density matrices $\rho_n$ on the subspaces $\mathcal{F}_n$, $n \in \mathbb{N}$. We consider the (real) linear maps $T_n : L^2(\mathbb{R}^s) \to \mathcal{H}_2(\mathcal{F})$, $n \in \mathbb{N}$, given by

$$T_n(f) = a(f) \rho_n^{1/2}, \quad f \in L^2(\mathbb{R}^s). \quad (A.1)$$

Clearly,

$$\|T_n(g)\|_{\mathcal{H}_2(\mathcal{F})}^2 = \omega_n(a^*(g)a(g)) \leq n\|g\|^2, \quad g \in L^2(\mathbb{R}^s), \quad (A.2)$$

so these maps are bounded. The following result is then an immediate consequence of a theorem by Banach (II.4).

**Observation 1:** The linear space of functions $\mathcal{R}(\mathbb{R}^s) \subset L^2(\mathbb{R}^s)$ satisfying

$$\limsup_n \|T_n(f)\|_{\mathcal{H}_2(\mathcal{F})} < \infty, \quad f \in \mathcal{R}(\mathbb{R}^s), \quad (A.3)$$

either coincides with all of $L^2(\mathbb{R}^s)$, or it is meager (a countable union of nowhere dense sets) in $L^2(\mathbb{R}^s)$.

In view of condition (4.1), the latter alternative obtains in the presence of growing condensates. So the set of one-particle regular functions is small. In order to obtain some further insights into the structure of their singular complement, let us slightly relax condition (4.1) by replacing the factor $(1/n)$ by $(\chi(n)/n)$, where $\chi$ is a function tending arbitrarily slowly to $\infty$ in the limit of large $n$. Functions $f \in L^2(\mathbb{R}^s)$ for which the resulting condition is satisfied are said to be almost macroscopically occupied. As a matter of fact, one can arbitrarily choose a countable number of functions $\chi_m, m \in \mathbb{N}$, with decrecent increase and there still exists an abundance of functions $f \in L^2(\mathbb{R}^s)$ complying with the resulting conditions. This observation is based on a result of Banach-Steinhaus (condensation of singularities (II.4)).

**Observation 2:** Let $\omega_n$, $n \in \mathbb{N}$, be a sequence of states, exhibiting growing condensates, and let $\chi_m$, $m \in \mathbb{N}$, be a sequence of functions which are arbitrarily slowly tending to $\infty$. There exists a subset of functions $\mathcal{L}(\mathbb{R}^s)$ of second category in the complement of the one-particle regular functions $\mathcal{R}(\mathbb{R}^s)$ such that

$$\limsup_n (\chi_m(n)/n) \omega_n(a^*(f)a(f)) = \infty, \quad f \in \mathcal{L}(\mathbb{R}^s), \quad m \in \mathbb{N}. \quad (A.4)$$
We briefly sketch the proof of this statement. Let $T_n, n \in \mathbb{N}$, be the maps defined in (A.1). We then consider the double sequence $T_{m,n} \doteq (\chi_m(n)/n)^{1/2} T_n$ for $m, n \in \mathbb{N}$. According to the preceding argument, these maps are bounded, $\|T_{m,n}\| \leq \chi_m(n)^{1/2}$. Since the given sequence of states contains growing condensates, there exist functions $f_n, n \in \mathbb{N}$, such that for some subsequence of states

$$\omega_{n_k}(a^* (f_{n_k}) a(f_{n_k})) \geq (\delta/2) n_k, \quad k \in \mathbb{N}.$$  \hfill (A.5)

This implies, for any given $m \in \mathbb{N}$, that $\limsup_k \|T_{m,n_k} (f_{n_k})\|_{H^2(F)} = \infty$ in view of the divergence of $\chi_m(n)$ in the limit of large $n$. It follows that the set of functions $M_m, m \in \mathbb{N}$, for which $\limsup_k \|T_{m,n_k} (g)\|_{H^2(F)} < \infty$, $g \in M_m$, is a meager set. Thus the countable union $\bigcup_m M_m \subset L^2(\mathbb{R}^4)$ is also meager, so its complement $\mathbb{Z}(\mathbb{R}^4)$ is of second category.

**Data availability**

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

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