The Condensate Equation for non-homogeneous Bosons

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Abstract:

We consider Boson systems with non-ground state ($q \neq 0$)-condensation. This phenomenon is accompanied with spontaneous breaking of the translation symmetry down to a lattice symmetry as well as of the gauge symmetry. We give a general and rigorous derivation of the condensate equation for these systems. We discuss model applications.

KEY WORDS: Bose- Einstein condensation, q-condensation, homogeneous and non-homogeneous condensation, q-condensate equation.

In memory of John T. Lewis

1 Introduction

For homogeneous systems of bosons, the phenomenon of Bose-Einstein condensation into the *ground state* is fairly well known and extensively studied. In this case, condensation arises if the ground state density ρ_0 is nonzero, i.e. we have

$$\rho_0 = \lim_\Lambda \omega(\frac{a_0^* a_0}{V}) > 0 \tag{1.1}$$

where Λ is a finite subset of $\mathbb{R}^\nu$ with volume V, $\lim_\Lambda$ is a limit of $\Lambda \to \mathbb{R}^\nu$, and $\omega(.)$ denotes the expectation with respect to an equilibrium state ω.

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Moreover the

$$a_{k,\Lambda}^* = \frac{1}{\sqrt{V}} \int_\Lambda dx \, a^*(x) e^{ik.x} \tag{1.2}$$

are the usual boson creation operators for momentum k for the system in a cubic domain $\Lambda \subset \mathbb{R}^\nu$.

Through the recent activity in the domain of condensation in traps (see e.g. [1],[2],[3]), the possibility of condensation in a mode corresponding to a nonzero momentum q has arisen. This requires generalizations and/or adaptations of the properties holding for $q = 0$ to the case $q \neq 0$.

In particular, there is the problem of the rigorous derivation of the so-called *condensate equation* [10],[5],[4].

What is the condensate equation? The challenging problem is to prove that there exists equilibrium state(s) ω showing condensation. In our case, this means to show that the state has the property: for some $q \neq 0$,

$$\rho_q = \lim_\Lambda \omega(\frac{a_{q,\Lambda}^* a_{q,\Lambda}}{V}) > 0 \tag{1.3}$$

i.e. the expectation value of the number operator of the q-condensed particles is proportional to the volume. There are many possible techniques to reach that goal. One can apply correlation inequalities, one uses numerical methods, all kinds of approximations, etc. One particular way of proceeding is to derive first for any equilibrium state a general independent equation for the quantity ρ_q. This equation is called "condensate equation". In many cases is solving or working with this equation an economical way to show the existence of Bose-Einstein condensation.

In this paper we give a rigorous derivation of the q-mode condensate equation

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and discuss its applications.

The systems for which we derive the general formula are realistic Bose systems with two-body interactions in dimension $\nu \geqq 1$. The two-body potential v is supposed to be well-behaved and in particular *superstable* [6]. This condition ensures the existence of local Gibbs states and all n-point correlation functions for any number of creation and annihilation operators [7]. Explicitly we consider the following Hamiltonians. Let $\Lambda^* = \{2\pi n / \sqrt[\nu]{V} | n \in \mathbb{Z}^\nu\}$ be the dual momentum set for the cubic region Λ, then

$$H_\Lambda = \sum_{k \in \Lambda^*} \epsilon_k a_k^* a_k + \frac{1}{2V} \sum_{k_1, k_2, q} \widehat{v}(q) a_{k_1-q}^* a_{k_2+q} a_{k_1} a_{k_2} \qquad (1.4)$$

where the ϵ_k are the one-particle energies (e.g. $\epsilon_k = k^2/2m$) and where we omit the subscripts Λ in the a_k, and with $\widehat{v}(q) = \int dx \, v(x) e^{-iq.x}$, i.e. we assume the potential v absolutely integrable. We are interested in properties of equilibrium states corresponding to the systems (1.4). In what follows the most convenient way to define these states is by means of the correlation inequalities [8]. In particular a state ω on the algebra $\mathcal{A}$ of all polynomials in the creation and annihilation operators is an equilibrium state at inverse temperature β and chemical potential μ if it satisfies the following *energy-entropy balance inequalities*:

$$\lim_\Lambda \beta \omega(X^*[H_\Lambda - \mu N_\Lambda, X]) \geqq \omega(X^*X) \ln \frac{\omega(X^*X)}{\omega(XX^*)} \qquad (1.5)$$

for each observable X in the domain $\mathcal{D}$ of $\lim_V [H_\Lambda - \mu N_\Lambda, .]$. In particular the thermodynamic limit Gibbs states are solutions of (1.5).

Our aim is to consider solutions ω of (1.5) satisfying the q-condensation (1.3) and to derive its condensate equation. Of course there may be condensation into more than one q-vector. There might be condensation into maximum ν independent vectors. In the rest of the paper we derive our results explicitly for a single q-vector. The generalizations are straightforward.

2 The condensate equation

First of all we may assume that the matrix elements

$$\omega(A\delta(B)C) \doteq \lim_{\Lambda} \omega(A[H_\Lambda - \mu N_\Lambda, C]) \qquad (2.1)$$

define operators $\delta(B)$ on the common core $\mathcal{D}$ containing all polynomials in the creation and annihilation operators in the sense of the GNS-representation [7] of the state ω, and that the map $\delta : B \rightarrow \delta(B)$ satisfies the properties of a derivation: $\delta(AB) = \delta(A)B + A\delta(B)$ and $\delta(A)^* = -\delta(A^*)$.

In [9] we introduced the operator α_q

$$\alpha_{q,\Lambda} = \frac{a_q}{\sqrt{V}} \qquad (2.2)$$

$$\alpha_q = s - \lim_{\Lambda} \alpha_{q,\Lambda} \qquad (2.3)$$

where $s-\lim_V$ means the strong operator limit in the ω-state GNS-representation. The existence of the operator is ensured for all states which are invariant under a lattice translation group, by the fact that it is an average of operators.

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Remark that limit Gibbs states are homogeneous. Spontaneous symmetry breaking leads to extremal lattice invariant states (see further on).

This operator has the following remarkable properties, see [9]:

1. The operator commutes with all creation and annihilation operators. It is affiliated to the center of the von Neumann algebra generated by all observables, i.e. generated by all polynomials of creation/annihilation operators, [7].

2. In particular, it is a normal operator: $\alpha_q^* \alpha_q = \alpha_q \alpha_q^*$.

3. Its relation to the condensate density operator is the following: $n_q = \alpha_q^* \alpha_q$, where n_q is the q-density operator of the q-condensate $\rho_q = \omega(n_q) > 0$.

4. The operator has a well defined *polar decomposition*: $\alpha_q = U_q \sqrt{n_q}$ with U_q a unitary operator.

5. From its definition, it readily follows that it is not translation invariant, but periodic in the q-direction:

$$\tau_y(\alpha_q) \equiv \lim_\Lambda 1/\sqrt{V} \int_\Lambda dx\, a(x+y)\, e^{iq.x} \tau_q(\alpha_q) = e^{-iq.y} \alpha_q$$

Now we are able to state the main result.

Theorem 2.1. *Let ω (for notational convenience from now on we leave out the β-index) be any equilibrium state, i.e. satisfying (1.5), then for any polynomial $P(a_k^*, a_k, \alpha_q^*, \alpha_q)$ in the creation and annihilation operators a_k and*

the α_q-operators, and for any polynomial $Q(\alpha_q^*, \alpha_q)$ in the α_q-operators, one has the equation

$$\omega(P(a_k^*, a_k)\delta(Q(\alpha_q^*))) = 0. \tag{2.4}$$

Proof. Take any arbitrary complex number λ and substitutes $X = P^* + \lambda Q$ in (1.5). Using the inequality $a \ln \frac{a}{b} \geq a - b$ for positive real numbers and the fact that the operators P and Q commute one gets

$$\beta(|\lambda|^2\omega(P\delta(P^*)) + \bar{\lambda}\omega(P\delta(Q)) + \lambda\omega(Q^*\delta(P^*)) + \omega(Q^*\delta(Q))) \geq |\lambda|^2\omega(PP^* - P^*P)$$

If we show that the λ-constant term $\omega(Q^*\delta(Q))$ vanishes, then the theorem follows from this inequality by virtue of the vanishing of the linear terms in λ. Now we show that this constant term vanishes.

By taking $\lambda = 0$ in the inequality, one gets $\omega(Q^*\delta(Q)) > 0$. After repeating the argument with Q replaced by Q^*, one gets as well $\omega(Q\delta(Q^*)) \geq 0$.

On the other hand using the time invariance of the state ω one gets

$$0 = \omega(\delta(Q^*Q)) = \omega(\delta(Q^*)Q) + \omega(Q^*\delta(Q))$$

This together with the positivity of both terms yields $\omega(Q^*\delta(Q)) = 0$, finishing the proof of the theorem. $\qquad\qquad\square$

Now we are in a position to get the main result, namely the derivation of the condensate equation for the q-mode. This equation is in general referred to as the Euler equation resulting from the minimization of the free energy density functional with respect to variations of the condensate density. We derive two versions of this equation. The first one is intended for general

limit Gibbs states which are homogeneous states but not necessarily extremal invariant equilibrium states. The second version which we derive is for the extremal equilibrium states which are non-homogeneous but q-periodic and which show spontaneous gauge symmetry breaking.

Theorem 2.2. *Let ω be a general limit Gibbs state, satisfying* (1.5), *then the q-condensate equation is given by*

$$\omega(\alpha_q^* \delta(\alpha_q)) = 0 \tag{2.5}$$

Proof. The formula (2.5) follows immediately from the previous theorem by the substitutions $P = \alpha_q^*$ and $Q = \alpha_q$. $\qquad\qquad\square$

The reader will remark the compact form of our equation (2.5) and could ask for its relation to what is usually understood to be the condensate equation. In other words it remains to show that our result of the theorem, does correspond to the Euler equation of the variational principle for the free energy functional with respect to a variation of the condensate. Let us explain the relation between our equation and this variational problem. The latter one is defined as usual. Consider the real map f, called the free energy density functional, defined on the state space: for any state ρ, $f : \rho \to f(\rho)$ where

$$f(\rho) = \lim_{\Lambda} \frac{1}{V} (\beta \rho(H_\Lambda - \mu N_\Lambda) - S(\rho_\Lambda))$$

with μ the chemical potential and $S(\rho_\Lambda)$ the entropy of the restriction of the state to the finite volume Λ. The variational principle of statistical mechanics implies that each homogeneous (or periodic) equilibrium state ω

minimizes the free energy density functional, i.e. one has for any arbitrary state ρ: $f(\omega) \leqq f(\rho)$. The following inequality, proved for lattice systems but immediately extended to continuous systems, is proved in [8]: for any observable X one has

$$\lim_{\Lambda} \beta\omega(X^*[H_\Lambda - \mu N_\Lambda, X]) - \omega(X^*X)\ln\frac{\omega(X^*X)}{\omega(XX^*)} \geqq \lim_{\lambda \to 0^+} \frac{1}{\lambda}(f(\omega \circ \gamma_\lambda) - f(\omega)) \geqq 0 \tag{2.6}$$

where γ_λ with $\lambda \in \mathbb{R}^+$ is a one parameter semigroup of completely positive map of perturbations of the system given by ($\gamma_\lambda = e^{\lambda\Gamma}$) and where

$$\Gamma(.) = \lim_{\Lambda} \Gamma_\Lambda = \lim_{\Lambda} \int_\Lambda dx\,([\tau_x(X^*), \,.\,]\tau_x(X) + \tau_x(X^*)[\,.\,, \tau_x(X)] \tag{2.7}$$

The notation τ_x is used to denote the translation over the distance x. Remark that for the particular choice $X = \alpha_q$ in (2.6), one gets, on the basis of (2.5), that the left hand side of (2.6) vanishes showing that the equilibrium state ω satisfies the Euler equation of the variational principle for all variations of this particular type. The physical meaning of these variations follows from the direct computation $\gamma_\lambda(\alpha_q) = \lim_\Lambda e^{\lambda\Gamma_\Lambda}(\alpha_{q,\Lambda}) = e^{-\lambda}\alpha_q$, i.e. the γ_λ-operation is nothing but the operation changing the values of the creation and/or the annihilation operators of a condensate particle. In other words these arguments yield also an alternative proof of the existence of the Euler equation of the variational principle leading to the condensate equation. In any case this proves that (2.5) is the condensate equation as it is usually defined.

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Now we proceed to the second formulation of the condensate equation valid only for extremal equilibrium states. Indeed if there is q-condensation for a homogeneous equilibrium state ω, satisfying (1.3), then we proved that there is spontaneous symmetry breaking of the gauge symmetry as well as of the space translation symmetry, the latter one into periodic states in the q-direction, determined by the unit vector e, with period $\kappa = \frac{2\pi}{|q|}$. In other words, we proved in [9] that there exists a set $\{\omega_{te}\}$, with t running in the interval $[0, \kappa]$, of equilibrium states, all satisfying the equilibrium condition (1.5), and all different. For these states also the gauge symmetry is broken only for the q-mode. All these states are extremal equilibrium states satisfying the property that the limit operators α_q are reduced to multiples of the unit operator in the GNS-representation of each state ω_{te}, i.e.

$$\alpha_q = \sqrt{\rho_q} e^{i\phi(t)} \tag{2.8}$$

where $\phi(t)$ is a real phase. Remark that this result yields a rigorous mathematical proof of the so-called Bogoliubov procedure which consists in replacing the average operators α_q by c-numbers, see [10].

Without loss of generality we limit the rest of our discussion to the case of one extremal state where we put the phase $\phi(t) = 0$. Also in the rest of this section we denote any of these extremal states shortly by $\widetilde{\omega}$. Moreover we will not work out explicitly the most general formula covering all cases, because the most general formula depends explicitly on the dimensions of the lattice created by the condensate vectors q which contribute to the condensation.

Corrolary 1. *For any extremal state $\widetilde{\omega}$ the condensate equation reads as*

follows

$$(\mu - \epsilon_q)\rho_q - \hat{v}(0)\rho_q^2 - \rho_q \int dk \, (\hat{v}(0) + \hat{v}(k-q))\widetilde{\omega}(a_k^* a_k)$$

$$-\rho_q \int dk \, (\hat{v}(0) + \hat{v}(k-q))\widetilde{\omega}(a_{k-q}^* a_k) - \sqrt{\rho_q} \lim_\Lambda \frac{1}{V^{\frac{3}{2}}} \sum_{k_1,k_2} \widetilde{\omega}(a_{k_1+k_2-q}^* a_{k_2} a_{k_1}) = 0$$

$$(2.9)$$

Proof. The proof follows directly by an explicit computation from (2.5) using the extremal property of the state $\widetilde{\omega}$ yielding the formulae: for all $n, m, r, s \in \mathbb{N}$ one has the equalities

$$\lim_\Lambda \widetilde{\omega}(a_{k_1}^*...(\frac{a_q^*}{\sqrt{V}})^n...a_{k_r}^* a_{p_1}...(\frac{a_q}{\sqrt{V}})^m...a_{p_s})$$

$$= (\rho_q)^{\frac{n+m}{2}} \widetilde{\omega}(a_{k_1}^*......a_{k_r}^* a_{p_1}...(\frac{a_q}{\sqrt{V}})^m...a_{p_s})$$

$$(2.10)$$

$\square$

3   Discussion

In general the condensate equation is used as a handy way in order to obtain an idea about the existence of condensation and/or the amount of condensation in a physical Boson model system. For example the condensate equation for the free Bose gas in three dimensions yields immediately that if the chemical potential $\mu \neq 0$ then there is no condensation. Given the total density, then it determines also the the amount of condensate if $\mu = 0$. For the so-called imperfect Bose gas, the condensate equation reduces the problem to the free bose gas case. For Bose models with realistic two-body interactions,

the condensate equation is a good way to the construction of bounds and/or approximations for the amount of condensate.

Finally we discuss the use of the condensate equation for a model with a q-condensate as studied above. We consider a Bose gas model irradiated by a laser mode treated in [2]. The Hamiltonian of the model is given by

$$H_\Lambda = \sum_k \epsilon_k a_k^* a_k + \Omega\, b_q^* b_q + \frac{\lambda}{2V} N_\Lambda^2 + \frac{g}{\sqrt{V}}\left(a_q^* a_0 b_q + a_q a_0^* b_q^*\right) \qquad (3.1)$$

The first term is the kinetic energy of the bosons, the second one is the kinetic energy of the photon, the third term is the stabilizing boson mean field term and the last term is the interaction between the laser with frequency Ω and the boson modes. The λ and g are positive coupling constants.

The total Hamiltonian is homogeneous as in (1.4). We suppose that we have the system in an extremal equilibrium state for the bosons as well as for the laser mode which we consider as a collective mode like the boson modes. The symmetry is spontaneously broken to a lattice symmetry in the q-direction. We consider the condensate equations (2.9) for the three modes, a_0, a_q and b_q appearing in the interaction. One gets:

$$(\mu - \epsilon_0 - \lambda\rho)\rho_0 = g\sqrt{\rho_0 \rho_q \widetilde{\rho}_q}$$

$$(\mu - \epsilon_q - \lambda\rho)\rho_q = g\sqrt{\rho_0 \rho_q \widetilde{\rho}_q} \qquad (3.2)$$

$$\widetilde{\rho}_q = \frac{g}{\Omega}\rho_0 \rho_q$$

We denote $\widetilde{\rho}_q = \lim_\Lambda \widetilde{\omega}(\frac{b_q^* b_q}{V})$ the q-mode laser density of the photons and

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here we denote by ρ the total density of the boson particles. A solution of these equations in terms of the chemical μ, which is itself fixed by the density of bosons through the formula $\rho = \lim_\Lambda \widetilde{\omega}(\frac{N_\Lambda}{V})$ is the following

$$\rho_0 = \frac{\Omega}{g^2}(\mu - \epsilon_q - \lambda\rho)$$
$$\rho_q = \frac{\Omega}{g^2}(\mu - \epsilon_0 - \lambda\rho) \qquad (3.3)$$
$$\widetilde{\rho}_q = \frac{1}{g^2}(\mu - \epsilon_q - \lambda\rho)(\mu - \epsilon_0 - \lambda\rho)$$

Looking at the paper [2], where this model is analyzed, the reader should realize the power of the condensate equation for the derivation of these results above. For the final analysis of these equations in terms of the chemical potential we refer nevertheless to the original paper [2].

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