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On Solvable Boson Models

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Abstract: The problem of equilibrium states and/or ground states of exactly solvable homogeneous boson models is stated and explicitly proved as a special case of the general variational problem of statistical mechanics in terms of quasi-free states. We apply the result to a model of superradiant Bose-Einstein condensation and to the Pairing Boson Model.

KEY WORDS: Solvable boson models, Bose-Einstein condensation, canonical commutation relations, equilibrium states, quasi-free states, gauge breaking, entropy densities, variational principles, superradiance, pairing boson model.

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Contents

1	Intr	oduction	2	
2	Qua	si-free Bose systems	4	
	2.1	Heuristics	4	
	2.2	CCR and quasi-free states	5	
	2.3	Equilibrium states	10	
	2.4	Condensate Equations	12	
3	App	olications	13	
	3.1	Superradiant Bose-Einstein Condensation	13	
	3.2	Pairing Boson Model with BCS and Mean-Field Interactions $\ . \ . \ . \ .$	15	
		3.2.1 BCS attraction $u > 0$: coexistence of BEC and boson pairing	15	
		3.2.2 BCS repulsion: $u < 0$ and generalized (type III) Bose condensation .	19	

1 Introduction

Soon after the discovery of superfluidity F. London made a connection between this phenomenon and the almost forgotten Bose-Einstein condensation (BEC) in the free Bose gas [1]. His arguments were essentially based on fact that Helium-4 atoms are bosons, and their superfluidity can be understood in terms of the Bose statistics that they obey. Almost ten years later N.N. Bogoliubov [2] proposed a microscopic theory of the superfluidity of Helium-4 showing that it can be regarded as a consequence of Bose-Einstein condensation in an *interacting* system. The Bogoliubov theory had a serious impact since just a few years before Landau had developed a spectral criterion for superfluidity and according to this criterion the free Bose gas is not a superfluid even in the presence of BEC.

But more than eighty years after the prediction of Bose-Einstein condensation the problem of whether this phenomenon is stable with respect to realistic pair-interaction is still unsolved and seems beyond the reach of the present methods. Either one must use a very special pairpotential or one must truncate the Hamiltonian. The second course was followed by many authors. One such approach is to use a Hamiltonian which is a function of the occupation of the free-gas single particle states [3]. Since all the operators in these models commute, they can be investigated by probabilistic techniques using Laplace's method (*Large Deviations*) [4], [5]. However these models (which include mean-field or imperfect Bose gas) produce a spectrum identical to that of the free Bose gas and therefore does not satisfy the superfluidity criterion. A more plausible model is the so-called Bogoliubov model, also called the weakly imperfect Bose-gas, see [2] and [6]. This model takes into account more interaction terms without losing its exact solvability. The basic ingredients of this model in terms of states on the CCR-algebra of the boson observables, including the problem of the Bogoliubov-Landau spectral behaviour, has been analyzed in [7, 8]. Later the boson *Pairing Model* was introduced as a further refinement of the Bogoliubov model by including of BCS boson interaction [11]. Theoretical work on this model resulted into some intriguing properties like the occurrence of two types of condensation, a boson BCS-type *pair condensation* and the standard *one-particle* condensation, as well the presence of a spectral gap in the elementary excitations spectrum [12] - [16].

The methods that have been used so far for the study of these solvable models have been the Bogoliubov approximating Hamiltonian method [6] and some form of Laplace's method [4], [5]. One should also mention the non-commutative large deviation method developed by [17] for lattice systems and later refined in [18]. This method has not been rigorously extended to Bose systems mainly due to technical problems with unbounded operators. However on a formal level it gives the right variational formulas (see for example [16].) Here we develop a new method based on the *quasi-free* states on the algebra of observables given by the algebra of the canonical commutation relations [19, 20].

All the solvable models referred to above share the property that their equilibrium states and/or ground states, which are states on the algebra of the Canonical Commutation Relations (CCR) are completely determined by the one- and two-point correlation functions. Such states are called quasi-free states. This class of states has been intensively studied in the sixties and seventies. Although quasi-free states are frequently used as the ideal laboratory for performing tests of all kinds, this mathematical analysis turned out to be much too technical to be very practical for its utility in the study of Bose systems in physics, see e.g. [21], [22].

This paper is intended to remedy this failure by giving a presentation of the quasi-free states suitable for the study of space homogeneous systems. In particular we prove the explicit form of the variational principle of statistical mechanics for all solvable boson models. We prove that for these models the set of states over which one minimizes the free-energy density (or grand-canonical pressure) is reducible to the set of homogeneous quasi-free states. The main technical step in this is the explicit formula for the entropy density of a general quasi-free state including the non-gauge symmetric ones.

Though the variational principle when solved fully, in principle contains all the information about the model, in practice it is often difficult to solve. A very useful additional tool is the use of *condensate equations* introduced in [23, 24]. They form an essential part of the study of the variational principle and can be derived without any explicit knowledge of the entropy of the system, Section 2. Moreover, they are always valid as opposed to the Euler-Lagrange equations which are not always satisfied because either the stationary point is a maximum or the minimum does not correspond to any stationary point.

In Section 3 we apply our method to the Pairing Boson Model with Mean-Field and BCS interactions to obtain the variational principle conjectured in [16] (and proved in [25]), supplemented by the *condensate equations*. This model with BCS *attraction* is a very good example of a situation, when the condensate equations can give some conclusions more directly. For instance, from the condensate equations (3.18), (3.19), one immediately concludes

that there is neither pairing nor zero-mode condensation for negative chemical potentials and also that zero-mode condensation implies a non-trivial boson pairing. An unusual property of this model is that for the BCS *repulsion* it is not completely equivalent to the mean-field case: the repulsion does not change the density of corresponding thermodynamic potentials but produces a generalized (type III) condensation à la van den Berg-Lewis-Pulé.

Another application is the model, analyzed in [26], which describes the phenomenon of the recently observed superradiance of the BEC accompanied by a matter-wave grating and amplification.

2 Quasi-free Bose systems

2.1 Heuristics

The concrete and traditional approach to Bose systems in physics is to start with the symmetric Fock Hilbert space of vector states \mathfrak{F} . Consider $L^2(\mathbb{R}^n)$ the space of square integrable functions on \mathbb{R}^n , n is the number of degrees of freedom. One considers the creation and annihilation operators: for any $f, g \in L^2(\mathbb{R}^n)$, the creation operator is given by $a^*(f) = \int dx f(x) a^*(x)$ acting in \mathfrak{F} , the annihilation operator is its adjoint operator a(f), and satisfying the usual canonical commutation relations

$$[a(x), a^*(y)] = \delta(x - y), [a(x), a(y)] = 0, \qquad (2.1)$$

leading to the relations

$$[a(f), a^*(g)] = (f, g), \ [a(f), a(g)] = 0.$$
(2.2)

It is assumed that there exists a particular normalized vector Ω in \mathfrak{F} such that it is annihilated by all a(x) and hence that for all f:

$$a(f)\Omega = 0. \tag{2.3}$$

The symmetric Fock space \mathfrak{F} is then the Hilbert space is the linear span generated by all vectors of the set: $\{a^*(f_1)a^*(f_2)...a^*(f_n)\Omega\}_n$ for all f_i and for all $n \in \mathbb{N}$.

A vector-state ω_{Ψ} of a boson system is an expectation value of the type $\omega(A) = (\Psi, A\Psi)$, where Ψ is a normalized vector of the Fock space and where A is any observable of the boson system. Remark that each observable is a function of the boson creation and annihilation operators. In particular, the physical model is defined through the energy observable, called Hamiltonian. For a two-body interaction v the general model takes the following form in a finite volume $V = |\Lambda|$:

$$H_{\Lambda} = \int_{\Lambda} dx \frac{1}{2m} \nabla a^*(x) \cdot \nabla a(x) + \frac{1}{2V} \int_{\Lambda} dx \int_{\Lambda} dy \, a^*(x) a^*(y) v(x-y) a(x) a(y) \tag{2.4}$$

Stability of the model requires that the Hamiltonian operator acting in the Fock space is bounded from below. In this paper we adopt the following definition: we shall say that a system is *solvable* if the corresponding density of the thermodynamic potential can be expressed explicitly via a finite number of correlation functions. We shall make this definition more exact later. In general the model (2.4) described above is not solvable. The natural way of defining solvability is in terms of the correlation functions.

The state ω is known if one can find all its correlation functions

$$\omega(a^*(f_1)...a^*(f_n)a(g_1)...a(g_m)) \tag{2.5}$$

for all functions f_i, g_j . One should realize that in order to know the state one has to know an infinity of correlation functions, for all $n, m \in \mathbb{N}$. This makes the many-body problem unsolvable in most cases.

In the literature one can find many approximation procedures, where the original state ω is replaced by a state $\tilde{\omega}$ constructed via various *decoupling* procedures such that all higher order correlation functions can be expressed in terms of those of order less than some n + m. It must remarked that on the basis of the Marcinkiewicz theorem [27, 28], many of them are erroneous. Indeed, this theorem tells us that if the decoupling holds for all correlation functions from some n+m on, then the decoupling holds for all correlation of order n+m > 2. This means that the only decoupling, not contradicting the positivity of the state $\tilde{\omega}$, is the one in terms of the one-point function, $\tilde{\omega}(a(f))$ and two-point functions, $\tilde{\omega}(a^*(f)a(g))$, $\tilde{\omega}(a(f)a(g))$, for all f and g. Any state satisfying the decoupling procedure described above is called a "quasi-free state" (qf-state).

In the rest of this section we recall the main features of the boson Gibbs states, in particular the class of space homogeneous quasi-free states which are necessary for the formulation of the variational principle of statistical mechanics for solvable models.

Our main original contribution in this section is a proof of the existence of a canonical automorphism mapping a gauge breaking state in a gauge invariant one. This result will be essential for the explicit computation of the entropy density of the state, which makes possible the explicit formulation the variational principle for our class of solvable boson models.

2.2 CCR and quasi-free states

In order to define the total set of all *quasi-free* states it is convenient to work with the boson field which is defined on \mathfrak{T} a suitable subspace of $L^2(\mathbb{R}^n)$, called a space of *test functions*. This field is defined by the map $b : f \in \mathfrak{T} \mapsto b(f)$, where the linear operator b(f) on Fock space is given by

$$b(f) = a(f) + a^*(f).$$

The Canonical Commutation Relations (CCR) for these fields are now

$$[b(f), b(g)] = 2i\sigma(f, g) , \qquad (2.6)$$

with $\sigma(f,g) = \Im(f,g)$. Note that the fields are real-linear in their argument: $b(\lambda f) = \lambda b(f)$, for $\Im(\lambda) = 0$, but $b(if) = i(-a(f) + a^*(f))$ and $a(f) = \frac{1}{2}((b(f) + ib(if)))$.

It is equivalent to use the field operators as the generators of all observables instead of creation and annihilation operators. To avoid using unbounded operators we use the Weyl operators as the generators of the algebra of observables \mathfrak{A} of the system. These are given by:

$$W(f) = \exp\{ib(f)\},\tag{2.7}$$

for any $f \in \mathfrak{T}$. The CCR are then equivalent to the relations

$$W(f)W(g) = e^{-i\sigma(f,g)}W(f+g).$$
 (2.8)

We shall denote the set of states on \mathfrak{A} by \mathfrak{S} . We recall that a state $\omega \in \mathfrak{S}$, is any normalized linear positive form on \mathfrak{A} .

Very often it is convenient to define states though their *truncated functions* $\omega(b(f_1)b(f_2)\ldots b(f_n))_t$ for $f_1, f_2, \ldots f_n \in \mathfrak{T}$. These functions are defined recursively through the formula

$$\omega(b(f))_t = \omega(b(f)), \qquad \omega(b(f_1)...b(f_n)) = \sum \omega(b(f_k)...)_t...\omega(...b(f_l))_t, \qquad (2.9)$$

where the sum is over all possible partitions of $\{1, ..., n\}$ and where the order within each of the clusters is carried over from the left to the right.

Let ω be an arbitrary state on the Weyl algebra \mathfrak{A} , then for all $f \in \mathfrak{T}$, the expectation values $\omega(W(f))$ are known and can be expressed in terms of the truncated functions (see e.g.[20]),

$$\omega(W(f)) = \omega(e^{i\lambda b(f)}) = \sum_{n=0}^{\infty} \frac{i^n \lambda^n}{n!} \omega(b(f)^n) = \exp\left\{\sum_{n=1}^{\infty} \frac{i^n \lambda^n}{n!} \omega(b(f)^n)_t\right\}.$$
 (2.10)

For the models that we study in this paper we shall see that only the one- and two-point functions play a role. The one-point function is determined by the linear functional ϕ on \mathfrak{T} and the two-point functions by two (unbounded) operators R and S on \mathfrak{T} . These are defined by

$$\phi(f) = \omega(a^*(f)), \tag{2.11}$$

and the truncated two-point functions

$$\langle f, Rg \rangle = \omega(a(f)a^*(g)) - \omega(a(f))\omega(a^*(g)), \quad \langle f, Sg \rangle = \omega(a(f)a(\overline{g})) - \omega(a(f))\omega(a(\overline{g})) \quad (2.12)$$

where \overline{g} stands for the complex conjugate of g. Clearly $\omega(b(f)b(f))$ can be expressed in terms of these two operators and ϕ . Note that the operator R is self-adjoint. We shall denote by $\mathfrak{S}_{\phi,R,S}$ the elements of \mathfrak{S} determined by the triplet ϕ , R and S.

Since *-automorphisms (canonical transformations) leave the CCR invariant, many properties of a state are conserved under these transformations. We shall say that states are *canonically equivalent* if they can be transformed into each other in such a way.

It is easy to see that in general there is a canonical transformation which transforms a state ω into a state ω_0 with $\phi = 0$. For any real linear functional χ on \mathfrak{T} , the transformation τ_{χ} on the boson algebra defined by

$$\tau_{\chi}(W(f)) = e^{i\chi(f)}W(f) \tag{2.13}$$

together with linearity and conservation of products, is a canonical transformation. Clearly this transformation translates the boson field: $\tau_{\chi}b(f) = b(f) + \chi(f)$. Now the composition of a state ω with the transformation τ_{χ} , $\omega_0 = \omega \circ \tau_{\chi}$ is again a state and $\omega_0(b(f)) = \omega(b(f)) + \chi(f)$. Therefore if we choose $\chi(f) = -\omega(b(f)) = -2\Re e \phi(f)$, which is real linear, then the one-point function of ω_0 vanishes. Moreover the reduced two-point functions are left invariant so that operators R and S are unchanged.

It is clear that the positivity of the state ω implies that

$$\omega((a(f) + a^*(\overline{g}))(a(f) + a^*(\overline{g}))^*) \ge 0$$
(2.14)

for all $f, g \in \mathfrak{T}$. Assuming $\phi = 0$ the inequality (2.14) is equivalent to

$$\langle f, Rf \rangle + \langle f, Sg \rangle + \langle g, S^*f \rangle + \langle g, (R-1)g \rangle \ge 0$$
 (2.15)

for all $f, g \in \mathfrak{T}$. Putting f = 0 we see that $R \ge 1$ and putting $g = -R^{1/2}h$ and $f = R^{-1/2}Sh$ gives

$$R(R-1) + S^*S - R^{-1/2}S^*SR^{1/2} - R^{1/2}S^*SR^{-1/2} \ge 0.$$
(2.16)

Notice that if operators R and S commute, then the latter simplifies to

$$T^{2} \equiv R(R-1) - S^{*}S \ge 0.$$
(2.17)

Now we introduce the one-parameter group of gauge transformations. This group of canonical transformations or CCR-automorphisms, $\{\tau_{\lambda} | \lambda \in \mathbb{R}\}$, is defined by

$$\tau_{\lambda}(a^*(f)) = e^{i\lambda}a^*(f), \ \tau_{\lambda}(a(f)) = e^{-i\lambda}a(f).$$
(2.18)

A state ω is called *gauge invariant* if $\omega \circ \tau_{\lambda} = \omega$ for all $\lambda \in \mathbb{R}$ holds. In particular for a state $\omega \in \mathfrak{S}_{\phi,R,S}$ the one- and two-point functions transform under such a gauge transformation as follows:

$$\begin{aligned} (\omega \circ \tau_{\lambda})(a^{*}(f)) &= e^{i\lambda}\omega(a^{*}(f)), \\ (\omega \circ \tau_{\lambda})(a(f)a^{*}(g)) &= \omega(a(f)a^{*}(g)), \\ (\omega \circ \tau_{\lambda})(a(f)a(g)) &= e^{-i2\lambda}(\omega)(a(f)a(g)). \end{aligned}$$

or equivalently (ϕ, R, S) is transformed into $(e^{i\lambda}\phi, R, e^{-i2\lambda}S)$. Therefore a necessary condition for gauge invariance is that $\phi = 0$ and S = 0.

We now prove that any $\omega \in \mathfrak{S}_{\phi,R,S}$ is canonically equivalent to a state $\widetilde{\omega} \in \mathfrak{S}_{\widetilde{R}} \equiv \mathfrak{S}_{0,\widetilde{R},0}$ if R and S commute and $\overline{Rf} = R\overline{f}$ for all $f \in \mathfrak{T}$. We shall see later that these conditions are satisfied for translation invariant states. We determine explicitly the operator \widetilde{R} as a function of R and S. This result is similar to the more restricted result stated in [19], where only the existence of such a map between pure quasi-free states (see definition later) is proved. Here we prove not only the existence of this map but we give its explicit construction.

Theorem 2.1. Let $\omega \in \mathfrak{S}_{\phi,R,S}$ with R and S commuting and $\overline{Rf} = R\overline{f}$ for all $f \in \mathfrak{T}$. Then there exists a canonical transformation τ mapping ω into $\widetilde{\omega} \in \mathfrak{S}_{\widetilde{R}}$ where the operator \widetilde{R} is given, in terms of the operators $R \geq 1$ and $T \geq 0$, by

$$\widetilde{R} = \frac{1}{2} + \left(T^2 + \frac{1}{4}\right)^{\frac{1}{2}}.$$
(2.19)

Proof. Clearly we can assume that $\phi = 0$. By applying a canonical transformation similar to the gauge transformation in (2.18) we can transform operator S into |S|. Then we consider another canonical transformation γ (also called Bogoliubov transformation)

$$\widetilde{a}(f) = \gamma(a(f)) = a(Uf) - a^*(\overline{Vf})$$
(2.20)

where U and V are commuting self-adjoint operators commuting with R and S and satisfying $\overline{Uf} = U\overline{f}, \overline{Vf} = V\overline{f}$ and $U^2 - V^2 = I$. We consider the two equations

$$\langle f, Rg \rangle = \widetilde{\omega}(a(f)a^*(g)) = \omega(\gamma(a(f)a^*(g)))$$
(2.21)

$$0 = \langle f, \tilde{S}g \rangle = \tilde{\omega}(a(f)a(\overline{g})) = \omega(\gamma(a(f)a(\overline{g})))$$
(2.22)

in order to express \hat{R} as a function of R and S or preferably T. One computes explicitly the following equations from the former ones, using the symmetry of R and S.

$$\widetilde{R} = U^2 R + V^2 (R - 1) - 2UVS, \qquad (2.23)$$

$$0 = U^2 S - UV(2R - 1) + V^2 S.$$
(2.24)

From the second relation (2.24) one gets a quadratic equation for the operator $X := UV^{-1}$, which is semi-bounded from below by I. Then solution of this equation has the form:

$$X = \left(R - 1/2 + \left(\left(R - 1/2\right)^2 - S^2\right)^{1/2}\right)S^{-1}.$$
(2.25)

Using the relation (2.17) between the operators S and T, one gets

$$X = \left(R - \frac{1}{2} + \left(\frac{T^2 + \frac{1}{4}}{1}\right)^{1/2}\right) \left(R(R - 1) - \frac{T^2}{1}\right)^{-1/2}.$$
(2.26)

This gives for U and V:

$$U = X(X^2 - 1)^{-1/2}, \quad V = (X^2 - 1)^{-1/2}$$
 (2.27)

which we insert into the first equation (2.23) to obtain \tilde{R} as a function (2.19) of R and T. The canonical transformation τ of the theorem is of course given by the composition of the gauge transformation with the Bogoliubov transformation.

The states we shall be considering will be translation invariant. Space translations are again realized by a group of canonical transformations $\{\tau_x | x \in \mathbb{R}^n\}$ of the algebra of observables \mathfrak{A} given by $\tau_x(a(f)) = a(T_x f)$ where $(T_x f)(y) = f(y - x)$. The translation invariance of a state ω , given by $\omega \circ \tau_x = \omega$ for all $x \in \mathbb{R}^n$, is immediately translated to the operators R, Sby the property that they both commute with the operators T_x for $x \in \mathbb{R}^n$.

Translation invariance implies that $\phi(f) = c\hat{f}(0)$ where \hat{f} denotes the Fourier transform of f and $c = \omega(a^*(0))$. On the other hand it is well-known [30] that if A is such a translation invariant operator, then there exists a function ξ on \mathbb{R}^n whose Fourier transform is a tempered distribution such that for all functions f, $(\widehat{Af})(k) = \xi(k)\widehat{f}(k)$. This is due to the kernel theorem for operator-valued distributions and the convolution theorem for Fourier transforms. In particular, our operators R and S are simple multiplication operators with functions denoted by r(k) and s(k). It is easily checked that for $k \neq 0$, $r(k) = \omega(\widehat{a}(k)\widehat{a}^*(k))$ and $s(k) = \omega(\widehat{a}(k)\widehat{a}(-k)) = s(-k)$ where $\widehat{a}(k)$ is the operator-valued distribution given by the Fourier transform of a(x). For our purposes (see later) we can assume in addition that

r(-k) = r(k). This last property is equivalent to $\overline{Rf} = R\overline{f}$. As R and S are multiplication operators they commute so that (2.17) holds and can be written in terms of r and s:

$$r(k)(r(k) - 1) - |s(k)|^2 \ge 0.$$
(2.28)

It is convenient to introduce a non-negative function t(k), corresponding to the operator T, defined by

$$t(k)^{2} = r(k)(r(k) - 1) - |s(k)|^{2}.$$
(2.29)

The class of translation invariant states $\mathfrak{S}_{\phi,R,S}$ can now be parameterized by the complex number c and the functions $r \ge 1$, $t \ge 0$ and $\alpha(k) = \arg s(k)$.

Now we turn to the *quasi-free* states.

Definition 2.2. A state ω is called a *quasi-free* state (qf-state) if all truncated functions of order n > 2 vanish. This means that a *qf*-state is completely determined by its one- and two-point functions:

$$\omega(W(f)) = \exp\{i\omega(b(f)) - \frac{1}{2}\omega(b(f)b(f))_t\}$$
(2.30)

The set of qf-states will be denoted by \mathfrak{Q} .

Note that a qf-state is completely determined by ϕ , R and S. We denote the qf-state corresponding to ϕ , R and S by $\omega_{\phi,R,S}$. Of course translation invariant qf-states can be parametrized uniquely by the complex number c and the functions $r \ge 1$, $t \ge 0$ and $\alpha(k) = \arg s(k)$. Note also that a qf-state is gauge invariant if and only if $\phi = 0$ and S = 0. The above arguments show that $\omega_{\phi,R,S}$ is canonically equivalent to $\omega_{\tilde{R}} \equiv \omega_{0,\tilde{R},0}$.

We end this section by calculating the entropy for qf-states. For any normal (density matrix) state ω with density matrix ρ the von Neumann entropy is defined by the formula: $S(\omega) = -\text{Tr }\rho \ln \rho$. The entropy is left invariant under any canonical transformation τ (see e.g. [29], Chapters 1 and 9), that is, $S(\omega \circ \tau) = S(\omega)$. Let ω be a translation invariant, locally normal state on the algebra \mathfrak{A} (i.e. its restriction to every bounded region of \mathbb{R}^n is normal). Let $\Lambda \subset \mathbb{R}^n$ be a family of bounded regions increasing to \mathbb{R}^n . Then the entropy density of ω is defined by

$$\mathcal{S}(\omega) = \lim_{\Lambda} \frac{S(\omega_{\Lambda})}{V}, \qquad (2.31)$$

where $V = |\Lambda|$ denotes the volume of Λ , ω_{Λ} is the restriction of ω to Λ and $\lim_{\Lambda} := \lim_{\Lambda \uparrow \mathbb{R}^n}$. For translation invariant qf-states of the type ω_R , \mathcal{S} has been calculated in [31] and is given by

$$S(\omega_R) = \int \nu(\mathrm{d}k) \, \{r(k) \ln r(k) - (r(k) - 1) \ln(r(k) - 1)\}$$
(2.32)

where $\nu(dk) = d^n k/(2\pi)^n$. It is clear from the above argument that the entropy density of $\omega_{\phi,R,S}$ is the same as that for $\omega_{\tilde{R}}$. We state this result in the following proposition.

Proposition 2.3. The entropy density of qf-state with two-point functions defined by R and S is given by

$$\mathcal{S}(\omega_{\phi,R,S}) = \mathcal{S}(\omega_{\widetilde{R}}) = \int \nu(\mathrm{d}k) \left\{ \widetilde{r}(k) \ln \widetilde{r}(k) - (\widetilde{r}(k) - 1) \ln(\widetilde{r}(k) - 1) \right\}$$
(2.33)

where \tilde{r} is given by (2.19):

$$\widetilde{r}(k) = \frac{1}{2} + \left(t^2(k) + \frac{1}{4}\right)^{\frac{1}{2}}.$$
(2.34)

In particular the entropy density is independent of the one-point function ϕ .

2.3 Equilibrium states

An equilibrium state at inverse temperature β of a homogeneous boson system will be defined by the variational principle of statistical mechanics, that is, an equilibrium state is one that minimizes the free energy density.

The free-energy density (or more precisely the grand-canonical pressure) functional is defined on the state space by

$$f(\omega) := \beta \mathcal{E}(\omega) - \mathcal{S}(\omega) , \qquad (2.35)$$

where $\mathcal{S}(\omega)$ is defined in the previous section and $\mathcal{E}(\omega)$ is the energy density. The energy density is determined by the local Hamiltonians of the system under consideration, H_{Λ} , defined for each bounded region of volume V:

$$\mathcal{E}(\omega) = \lim_V rac{1}{V} \omega (H_\Lambda - \mu N_\Lambda) \; ,$$

where μ is the chemical potential and N_{Λ} is the particle number operator. The variational principle of statistical mechanics states that each translation invariant (or periodic) equilibrium state ω_{β} is the minimizer of the free energy density functional, that is, for any state ω :

$$f(\omega_{\beta}) = \inf f(\omega). \tag{2.36}$$

In the definition of \mathcal{E} and \mathcal{S} it was presupposed that the states are locally normal in the sense that ω_{Λ} is a normal state. This is a reasonable assumption since we are basically interested in equilibrium states which are thermodynamic limits of local Gibbs states given locally by their (grand) canonical density matrices $\rho_{\Lambda} = e^{-\beta(H_{\Lambda}-\mu N_{\Lambda})}/\text{Tr} e^{-\beta(H_{\Lambda}-\mu N_{\Lambda})}$.

Let ω be a normal state with density matrix ρ on Fock space \mathfrak{F} , with zero one-point function and with two-point functions given by the operators R and S = 0. Let $\{f_j\}$ be an orthonormal basis of eigenvectors of R with eigenvalues r_j . Consider the operator (trial diagonal Hamiltonian) $H = \sum_j \epsilon_j a_j^* a_j$ with $a_j = a(f_j)$ and $\epsilon_j = \ln(r_j/(r_j - 1))$. Let σ be the density matrix given by $\sigma = e^{-H}/\text{Tr } e^{-H}$. It is clear that the state defined by σ is a qf-state which has two point function

$$\operatorname{Tr} \sigma a(f)a^*(g) = \langle f, Rg \rangle = \operatorname{Tr} \rho a(f)a^*(g).$$
(2.37)

Thus σ is the density matrix for the qf-state ω_R .

We use this construction to prove the entropy inequality

$$S(\omega) \le S(\omega_R). \tag{2.38}$$

Using the Bogoliubov-Klein convexity inequality [20], Lemma 6.2.21, one gets

$$S(\omega_{(R,0)}) - S(\omega) = \operatorname{Tr} \rho \ln \rho - \operatorname{Tr} \sigma \ln \sigma \ge \operatorname{Tr} (\rho - \sigma) \ln \sigma$$
(2.39)

where $\ln \sigma = -\sum_{j} \epsilon_{j} a_{j}^{*} a_{j} - \ln \operatorname{Tr} (\exp -H)$ and hence

$$S(\omega_{\sigma}) - S(\omega) \ge -\sum_{j} \epsilon_{j} (\operatorname{Tr} \rho \, a_{j}^{*} a_{j} - \operatorname{Tr} \sigma \, a_{j}^{*} a_{j}) = 0$$
(2.40)

since the states ρ and σ have the same two-point functions. This proves the inequality (2.38), which is a mathematical expression with the following physical interpretation. The state ω is a state with more non-trivial correlations than its associated qf-state ω_R and therefore it is understandable that the entropy of the state is smaller than or equal than the entropy of its associated qf-state.

Clearly this inequality carries over to the entropy density of locally normal states and using canonical equivalence to locally normal states with non-vanishing ϕ and S. Thus we have for locally normal states in $\mathfrak{S}_{\phi,R,S}$:

$$\mathcal{S}(\omega) \le \mathcal{S}(\omega_{\phi,R,S}) = \mathcal{S}(\omega_{\widetilde{R}}). \tag{2.41}$$

From now on we shall study solvable models, i.e. models with a Hamiltonian whose energy density $\lim_{\Lambda} \omega(H_{\Lambda})/V$ for any translation invariant state ω depends only on the one- and two-point correlation functions of the state. This will be made more precise in Definition 2.5. But, first we impose one last restriction on the states.

Definition 2.4. A translation invariant state ω is called *space-ergodic*, if for any three A, B, C local observables the following holds

$$\lim_{\Lambda} \omega(AB_{\Lambda}C) = \omega(AC)\omega(B)$$

where B_{Λ} the space-average

$$B_{\Lambda} = \frac{1}{V} \int_{\Lambda} dx \, \tau_x(B)$$

Note that for translation invariant states one has that $\omega(B) = \lim_{\Lambda} \omega(B_{\Lambda})$, and therefore the above definition can be written in the form

$$\omega(A(\lim_{\Lambda} B_{\Lambda} - \omega(B)I)C) = 0$$

In other words for a space-ergodic state ω , the *limiting space-average* operator $\overline{B} := \omega - \lim_{\Lambda} B_{\Lambda}$ is proportional to identity I. In the same way one gets $\omega - \lim_{\Lambda} [B_{\Lambda}, A] = 0$ for any local observables A and B. For these reasons the limiting operator \overline{B} is called an *observable at infinity* [20]. Note that \overline{B} is a normal operator since $[\overline{B}, \overline{B^*}] = 0$

As a first application of the ergodicity of states we have

$$\lim_{\Lambda} \omega \left(\frac{a_0^* a_0}{V} \right) = |c|^2 := \rho_0, \qquad (2.42)$$

where ρ_0 is the zero-mode condensate density for boson systems.

Definition 2.5. We shall say that a model is *solvable* if for every ergodic state ω , the energy density $\mathcal{E}(\omega)$ depends only on the *one-point* and *two-point* correlation functions of ω .

Note that if a model is solvable then the energy density $\mathcal{E}(\omega)$ is the same for all $\omega \in \mathfrak{S}_{\phi,R,S}$. We shall denote this common value by $\mathcal{E}(r,t,\alpha,c)$. On the other hand we have shown that for $\omega \in \mathfrak{S}_{\phi,R,S}$, $S(\omega)$ attains its maximum at the qf-state $\omega = \omega_{\phi,R,S}$. Thus we have

$$\inf_{\omega \in \mathfrak{S}_{\phi,R,S}} f(\omega) = f(\omega_{\phi,R,S}) = \beta \mathcal{E}(r,t,\alpha,c) - \int \nu(\mathrm{d}k) \left\{ \widetilde{r}(k) \ln \widetilde{r}(k) - (\widetilde{r}(k)-1) \ln(\widetilde{r}(k)-1) \right\}.$$
(2.43)

Taking the infimum in (2.43) over R, respectively T and ϕ we obtain our main result:

Theorem 2.6. For a solvable boson system the equilibrium state ω_{β} is a qf-state and it is defined by

$$f(\omega_{\beta}) = \inf_{\omega \in \mathfrak{Q}} f(\omega)$$

=
$$\inf_{r,t,\alpha,c} \left\{ \beta \mathcal{E}(r,t,\alpha,c) - \int \nu(\mathrm{d}k) \left\{ \widetilde{r}(k) \ln \widetilde{r}(k) - (\widetilde{r}(k)-1) \ln(\widetilde{r}(k)-1) \right\} \right\}$$

where $\tilde{r}(k)$ is given by (2.34) as a function of r and t.

2.4 Condensate Equations

Next we introduce the notion of *condensate equations* for equilibrium states of general boson system. They constitute essential tools for the study of the equilibrium as well as ground states of boson models. For a full discussion of this topic we refer the reader to [23, 24]. These equations are derived directly from the variational principle of statistical mechanics formulated above. However they have certain advantages over the Euler-Lagrange equations. First of all that they can be derived without any explicit knowledge of the entropy of the system. Secondly, while the Euler-Lagrange equations are not always satisfied because either the stationary point is a maximum or the minimum occurs on the boundary, the condensate equations are always valid.

To this end, consider the following completely-positive semigroups of transformations on the locally normal states in \mathfrak{S} . Let A be any local (quasi-local) observable (with space-average A_{Λ} over region Λ) and let

$$\Gamma_{\Lambda} = \int_{\Lambda} dx \{ [\tau_x(A^*_{\Lambda}), .] \tau_x(A_{\Lambda}) + \tau_x(A^*_{\Lambda}) [., \tau_x(A_{\Lambda})] \}$$

Then for each finite region Λ one can define a semigroup of completely-positive maps on \mathfrak{S} [33] given by

$$\{\gamma_{\lambda,V} = \exp \lambda \Gamma_{\Lambda} | \lambda \ge 0\}.$$

Let ω_{β} be any locally normal state satisfying the variational principle with density matrix ρ_{Λ} . Then using the notation of Definition 2.4, one gets

$$0 \leq \lim_{\lambda \to 0} \frac{1}{\lambda} (f(\lim_{\Lambda} \omega \circ e^{\lambda \Gamma_{\Lambda}}) - f(\omega))$$

$$\leq \lim_{\Lambda} \{\beta \operatorname{Tr} \rho_{\Lambda} A_{\Lambda}^{*}[H_{\Lambda}(\mu), A_{\Lambda}] - \operatorname{Tr} \rho_{\Lambda} A_{\Lambda}^{*} A_{\Lambda} \ln \frac{\operatorname{Tr} \rho_{\Lambda} A_{\Lambda}^{*} A_{\Lambda}}{\operatorname{Tr} \rho_{\Lambda} A_{\Lambda} A_{\Lambda}^{*}} \}$$

The second inequality is a consequence of the bi-convexity of the function: $x, y \to x \ln(x/y)$. Because of the normality of the limiting space-average operator \overline{A} , the second term of the right-hand side of the inequality vanishes and one gets

$$\lim_{\Lambda} \beta \omega_{\beta}(A_{\Lambda}^{*}[H_{\Lambda}(\mu), A_{\Lambda}]) \ge 0$$
(2.44)

and the same inequality with A_{Λ} replaced by A_{Λ}^* .

Using the same argument as above but now working with the group of unitary operators $\{U_t = \exp(itH_{\Lambda}(\mu)) | t \in \mathbb{R}\}$, one gets immediately $\lim_{\Lambda} \omega_{\beta}([H_{\Lambda}(\mu), X]) = 0$ for any observable X. Therefore

$$0 = \lim_{\Lambda} \omega_{\beta}([H_{\Lambda}(\mu), A_{\Lambda}^* A_{\Lambda}]) = \lim_{\Lambda} \{\omega_{\beta}([H_{\Lambda}(\mu), A_{\Lambda}^*] A_{\Lambda}) + \omega_{\beta}(A_{\Lambda}^* [H_{\Lambda}(\mu), A_{\Lambda}])\}.$$
 (2.45)

Using (2.44) and the property that the space-averages commute with all local observables, one gets the general condensate equation:

Theorem 2.7. Let ω_{β} be any limit Gibbs state, satisfying the variational principle for equilibrium states at inverse temperature β , including $\beta = \infty$ which means that ω_{∞} is a ground state, and let A be any local (or quasi-local) observable, then the condensate equation with respect to A is given by

$$\lim_{\Lambda} \omega_{\beta}(A^*_{\Lambda}[H_{\Lambda}(\mu), A_{\Lambda}]) = 0.$$
(2.46)

3 Applications

3.1 Superradiant Bose-Einstein Condensation

This model describes the phenomenon of the recently observed superradiance of the BEC accompanied by a matter-wave grating and amplification. It describes a boson condensate irradiated by laser. This model was introduced and analyzed in [26]. We consider bosons in a cubic box Λ in \mathbb{R}^n with volume $V \equiv |\Lambda|$ and periodic boundary conditions for the corresponding Schrödinger operators. Let Λ^* be the dual set of single particle momenta. For for $k \in \Lambda^*$ let $\phi_k(x) = e^{ikx}/V^{1/2}$ with $x \in \Lambda$, and define the boson creation/anihilation operators $a_k^{\#} \equiv a^{\#}(\phi_k)$. These bosons interact with a laser photon field $\{b_q, b_q^*\}$ with some fixed mode q, where $[b_q, b_q^*] = 1$. For the case of *Rayleigh scattering* the corresponding Hamiltonian has the form:

$$H_{\Lambda}(\mu) = \sum_{k \in \Lambda^*} (\epsilon(k) - \mu) a_k^* a_k + \Omega \, b_q^* b_q + \frac{\lambda}{2V} N_{\Lambda}^2 + \frac{g}{2\sqrt{V}} (a_q^* a_0 b_q + a_0^* a_q b_q^*)$$

where $\Omega, \lambda, g \in \mathbb{R}^+$ and $\epsilon(k) = k^2/2m$. The total system is assumed to be closed and in equilibrium. We consider an equilibrium state ω_β of the total system satisfying the variational principle described in the previous section.

Since the operators a_0/\sqrt{V} , a_q/\sqrt{V} , b_q/\sqrt{V} and N_{Λ}/V are all space averages, by the arguments of Section 2.3 this model is solvable in the sense of Definition 2.5 and the energy

density is given by

$$\mathcal{E}(\rho,\rho_0,\rho_q,\widetilde{\rho}_q,\alpha_0,\alpha_q,\widetilde{\alpha}_q) = \int \nu(\mathrm{d}k) \left(\epsilon(k)-\mu\right)\rho(k) - \mu\rho_0 + (\epsilon(q)-\mu)\rho_q + \Omega\widetilde{\rho}_q + q\sqrt{\rho_0\rho_q\widetilde{\rho}_q}\cos(\alpha_0+\alpha_q+\widetilde{\alpha}_q) + \frac{\lambda}{2}\overline{\rho}^2 \qquad (3.1)$$

where $\rho(k) \equiv r(k) - 1$,

$$\sqrt{\rho_0}e^{\mathrm{i}\alpha_0} \equiv \lim_{\Lambda} \omega_\beta(\frac{a_0}{\sqrt{V}}), \quad \sqrt{\rho_q}e^{-\mathrm{i}\alpha_q} \equiv \lim_{\Lambda} \omega_\beta(\frac{a_q}{\sqrt{V}}), \quad \sqrt{\widetilde{\rho_q}}e^{\mathrm{i}\widetilde{\alpha}_q} \equiv \lim_{\Lambda} \omega_\beta(\frac{b_q}{\sqrt{V}}),$$

and $\overline{\rho} \equiv \int dk \,\rho(k) + \rho_0 + \rho_q$. The entropy is given by (2.32) and depends only on $\rho(k)$. There are *three* relevant condensate densities

$$\rho_0 = \lim_{\Lambda} \omega_\beta(\frac{a_0^* a_0}{V}), \quad \rho_q = \lim_{\Lambda} \omega_\beta(\frac{a_q^* a_q}{V}), \quad \widetilde{\rho}_q = \lim \omega_\beta(\frac{b_q^* b_q}{V})$$

and the last two of them are periodic with period $\kappa = 2\pi/|q|$.

Now we minimise the free-energy (2.35). From (3.1) it is clear the minimum is attained when $\alpha_0 + \alpha_q + \tilde{\alpha}_q = \pi$. The Euler-Lagrange equations, obtained by varying with respect to the other parameters, are:

$$\begin{split} &(\lambda\overline{\rho}-\mu)\rho_0 = \frac{g}{2}\sqrt{\widetilde{\rho}_q\rho_q\rho_0},\\ &(\epsilon(q)+\lambda\overline{\rho}-\mu)\rho_q = \frac{g}{2}\sqrt{\widetilde{\rho}_q\rho_q\rho_0},\\ &\sqrt{\widetilde{\rho}_q}(\sqrt{\widetilde{\rho}_q}-\frac{g}{2\Omega}\sqrt{\rho_q\rho_0}) = 0,\\ &\rho(k) = \frac{1}{e^{\beta(\epsilon(k)+\lambda\overline{\rho}-\mu)}-1}. \end{split}$$

We note that the condensate equations derived from Theorem 2.7 are identical to the first three Euler-Lagrange above, and the therefore these equations must be satisfied.

In order to determine the value of the Bose-Einstein condensation and to see the effect of the irradiation in this model, we have to analyse these four equations. This has already been done in [26]. In fact, if we put $\delta := -\mu + \lambda \overline{\rho}$ as in [26], then these equations yield:

$$\rho_q = \frac{4\Omega}{g^2}\delta , \quad \rho_0 = \frac{4\Omega}{g^2}(\epsilon(q) + \delta) , \quad \widetilde{\rho_q} = \frac{4}{g^2}(\epsilon(q) + \delta)\delta$$
(3.2)

and

$$\overline{\rho} = \frac{4\Omega}{g^2} (\epsilon(q)/2 + \delta) + \rho^{PBG}(-\delta), \qquad (3.3)$$

where $\rho^{PBG}(\mu)$ is particle density in the Perfect Bose-Gas (PBG), that is

$$\rho^{PBG}(\mu) = \int \nu(\mathrm{d}k) \frac{1}{e^{\beta(\epsilon(k)-\mu)} - 1}.$$
(3.4)

Finally we see that the boson part of the equilibrium state ω_{β} is the quasi-free state determined by the 1-point function

$$\omega_{\beta}(a(f)) = \widehat{f}(0)\sqrt{\rho_0}e^{i\alpha_0} + \widehat{f}(0)\sqrt{\rho_q}e^{-i\alpha_q}$$

and by the 2-point truncated function given by

$$r(k) - 1 = \frac{1}{e^{\beta(\epsilon(k) + \lambda \overline{\rho} - \mu)} - 1}$$

with ρ_0, ρ_q and $\overline{\rho}$ determined above.

3.2 Pairing Boson Model with BCS and Mean-Field Interactions

The model was invented in [11] as an attempt to improve the Bogoliubov theory of the weakly imperfect boson gas, see a detailed discussion in [6] and [32]. Using the notation of the previous section the Hamiltonian of the *Pairing Boson Model* (PBH) is then given as in [16, 25] by

$$H_{\Lambda} = T_{\Lambda} - \frac{u}{2V} Q_{\Lambda}^* Q_{\Lambda} + \frac{v}{2V} N_{\Lambda}^2$$
(3.5)

where

$$T_{\Lambda} = \sum_{k \in \Lambda^*} \epsilon(k) a_k^* a_k, \quad Q_{\Lambda} = \sum_{k \in \Lambda^*} \lambda(k) a_k a_{-k}, \quad N_{\Lambda} = \sum_{k \in \Lambda^*} a_k^* a_k.$$
(3.6)

The coupling λ is for simplicity a real L^2 -function on \mathbb{R}^n satisfying $\lambda(-k) = \lambda(k)$, $1 = \lambda(0) \ge |\lambda(k)|$. The coupling constant v is positive and satisfies v - u > 0, implying that the Hamiltonian defines a *superstable* system [25]. For a discussion of the origin of this model see [25] and the references therein.

Again since the operators N_{Λ}/V and Q_{Λ}/V are both space averages, by the arguments of Section 2.3 this model is solvable in the sense of Definition 2.5 and the energy density is given by

$$\mathcal{E}(r,t,\alpha,c) = \int \nu(\mathrm{d}k) \, (\epsilon(k) - \mu)(r(k) - 1) - \mu |c|^2 \qquad (3.7)$$

+ $\frac{v}{2} \left(\int \nu(\mathrm{d}k) \, (r(k) - 1) + |c|^2 \right)^2 - \frac{u}{2} \left| \lambda(0)c^2 + \int \nu(\mathrm{d}k) \, \lambda(k)s(k) \right|^2.$

We have used the relations

$$\omega(a_k^*a_k) = \langle \phi_k, (R-1)\phi_k \rangle + |c|^2 V \delta_{k0}, \quad \omega(a_k a_{-k}) = \langle \phi_k, S\phi_k \rangle + c^2 V \delta_{k0}.$$
(3.8)

With $\rho(k) = r(k) - 1$, $c = \sqrt{\rho_0} e^{i\alpha}$, $\overline{\rho} = \int \nu(dk) \rho(k) + \rho_0$ and $\sigma = \int \nu(dk) \lambda(k) s(k)$, the energy density $\mathcal{E}(r, t, \alpha, c)$ becomes:

$$\mathcal{E}(r,t,\alpha,c) = \int \nu(\mathrm{d}k)\,\epsilon(k)\rho(k) - \mu\overline{\rho} + \frac{v}{2}\overline{\rho}^2 - \frac{u}{2}\left|\rho_0 e^{2i\alpha} + \sigma\right|^2.$$
(3.9)

Since the cases u > 0 and $u \leq 0$ are very different, we shall consider them separately.

3.2.1 BCS attraction u > 0: coexistence of BEC and boson pairing

First we consider u > 0. Clearly, in this case the minimum in (3.9) is attained when $2\alpha = \arg \sigma$. Therefore, instead of (3.9) one can take for further analysis the function $\widetilde{\mathcal{E}}(r,t,c) := \mathcal{E}(r,t,\alpha = (\arg \sigma)/2,c)$, which has the form:

$$\widetilde{\mathcal{E}}(r,t,c) = \int \nu(\mathrm{d}k)\,\epsilon(k)\rho(k) - \mu\overline{\rho} + \frac{v}{2}\overline{\rho}^2 - \frac{u}{2}\left(\rho_0 + |\sigma|\right)^2.$$
(3.10)

The corresponding entropy density $S(\omega)$ is given in (2.33). It is independent of ρ_0 and depends only on $\rho(k)$ and |s(k)|. Then for real $\lambda(k)$, after optimizing with respect to the

$$2\rho(k) + 1 = \frac{f(k)}{E(k)} \coth(\beta E(k)/2), \qquad (3.11)$$

$$s(k) = \frac{u(\rho_0 + |\sigma|)\lambda(k)}{2E(k)} \coth(\beta E(k)/2), \qquad (3.12)$$

$$0 = -\mu + v\overline{\rho} - u(\rho_0 + |\sigma|) , \qquad (3.13)$$

where

$$f(k) = \epsilon(k) - \mu + v\overline{\rho}, \qquad (3.14)$$

and

$$E(k) = \left\{ f^2(k) - u^2 \lambda(k)^2 (\rho_0 + |\sigma|)^2 \right\}^{1/2}.$$
(3.15)

As usual these equations are useful only if they have solutions within the admissible domain of r, t and c which corresponds to the positivity of the state. These three equations coincide respectively with equations (2.8), (2.9) and (2.10) in [16]. The integrated form of the first two equations also coincide with equations (5.1) and (5.2) in [25]:

$$\overline{\rho} = \frac{1}{2} \int_{\mathbb{R}^n} \nu(\mathrm{d}k) \left\{ \frac{f(k)}{E(k)} \operatorname{coth} \frac{1}{2} \beta E(k) - 1 \right\} + \rho_0 , \qquad (3.16)$$

$$(|\sigma| + \rho_0) = \frac{u(|\sigma| + \rho_0)}{2} \int_{\mathbb{R}^n} \nu(\mathrm{d}k) \frac{\lambda(k)^2}{E(k)} \operatorname{coth} \frac{1}{2} \beta E(k) + \rho_0 .$$
(3.17)

On the other hand, we find that the condensate equation (2.46) with respect to $a_0/V^{1/2}$ is

$$\rho_0(-\mu + v\overline{\rho} - u(\rho_0 + |\sigma|)) = 0, \qquad (3.18)$$

cf (3.13), and that with respect to Q_{Λ}/V it takes the form:

$$(\overline{c}^{2} + \overline{\sigma}) \left\{ \int \nu(\mathrm{d}k) \,\lambda(k)(\epsilon(k) - \mu + v\overline{\rho}) \,s(k) + (-\mu + v\overline{\rho}) \,c^{2} - u \left[\int \nu(\mathrm{d}k) \,\lambda(k)^{2}(\rho(k) + 1/2) + \rho_{0} \right] (c^{2} + \sigma) \right\} = 0.$$
(3.19)

Taking into account that $|c|^2 = \rho_0$, one can check that these condensate equations are consistent with the Euler-Lagrange equations (3.11)-(3.13) and/or (3.16)-(3.17).

Remark 3.1. Notice that there is a relation between the condensate equation (3.18) and the Euler-Lagrange equation (3.13). Indeed, by (3.10) the ρ_0 -dependent part of the variational functional has the form

$$\widetilde{\mathcal{E}}_{0}(\rho_{0}) := \frac{1}{2}(v-u)\rho_{0}^{2} - (\mu - v\rho + u|\sigma|)\rho_{0} ,$$

where $\rho := \overline{\rho} - \rho_0$. Since v > u, $\widetilde{\mathcal{E}}_0$ is strictly convex and has a unique minimum at ρ_0^{\min} . For $\mu \leq v\rho - u|\sigma|$ one gets $\rho_0^{\min} = 0$, which is not a stationary point, whereas for $\mu > v\rho - u|\sigma|$ the minimum occurs at the unique *stationary point* $\rho_0^{\min} = (\mu - v\rho + u|\sigma|)/(v - u) > 0$. These of course correspond to the solutions of the Euler-Lagrange equation (3.13), or the condensate equation (3.18).

Remark 3.2. We assumed above that $E(k) \ge 0$. It is clear that E(k) corresponds to the spectrum of the quasi-particles of the model (3.5) and that it should be real and non-negative for all k. We can see this by applying the general and well-known inequality (see e.g. [34], [20] or [23]): $\lim_{V} \omega([X^*, [H_V - \mu N_V, X]]) \ge 0$ holding for each equilibrium state and for each observable X. Let $X = \tilde{a}_k$, where $\tilde{a}_k = u_k a_k - v_k a^*_{-k}$, with

$$u_k^2 = \frac{1}{2} \left(\frac{f(k)}{E(k)} + 1 \right), \quad v_k^2 = \frac{1}{2} \left(\frac{f(k)}{E(k)} - 1 \right).$$
(3.20)

Then one obtains $\lim_{V} \omega([\widetilde{a}_{k}^{*}, [H_{V} - \mu N_{V}, \widetilde{a}_{k}]]) = E(k) \ge 0.$

There are two order parameters in the model (3.5), namely ρ_0 (Bose condensate density) and the function s(k), or the density of condensed BCS-type bosons pairs σ with opposite momenta. By virtue of equations (3.16), (3.17) and (3.13) it is clear that there exists always a trivial solution given by $\rho_0 = s(k) = 0$, i.e. no boson condensation and no boson pairing. The interesting question is about the existence of non-trivial solutions. The variational problem for the Boson pairing model for constant λ has been studied in detail in [16]. It was shown there that the phase diagram is quite complicated and it was only possible to solve the problem for some values of u and v, see Fig. 2 in [16].

The first Euler-Lagrange equation (3.16) implies that for u > 0 (*attraction* in the BCS part of the PBH (3.5)) the existence of Bose-Einstein condensation, $\rho_0 > 0$ for large chemical potentials μ , or the total particle density $\overline{\rho}$. Moreover, it causes (in ergodic states) a boson pairing, $\sigma \neq 0$. This clearly follows from the condensate equations (3.18), (3.19) or the second Euler-Lagrange equation (3.17), since (3.17) is impossible for $\rho_0 > 0$ and $\sigma = 0$. However from the same equation it can be seen that the boson pairing $\sigma \neq 0$ can survive without Bose-Einstein condensation i.e. for $\rho_0 = |c|^2 = 0$. This is proved in the next remark.

Remark 3.3. In this remark we prove that it is possible to have a solution of the condensate equations (3.18), (3.19) with $\rho_0 = 0$ and $\sigma \neq 0$. The proof is based on the analysis in [16]. For simplicity let us take n = 3 and $\lambda(k) = 1$. For $x \ge 0$ we let

$$E(k,x) := \left\{ (\epsilon(k) + x)^2 - x^2 \right\}^{1/2}.$$
(3.21)

and for fixed v > 0

$$I_2(x) = \frac{v}{2} \int_{\mathsf{R}^3} \nu(\mathrm{d}k) \left\{ \frac{\epsilon(k) + x}{E(k, x)} \, \coth \frac{1}{2} \beta E(k, x) - 1 \right\}.$$
 (3.22)

Let ρ_c be the critical density of the Perfect Bose Gas at inverse temperature β :

$$\rho_c := \int_{\mathbb{R}^3} \nu(\mathrm{d}k) \frac{1}{e^{\beta \epsilon(k)} - 1}.$$
(3.23)

Let $\mu_1 = \sup_{x \ge 0} (I_2(x) - x)$. From (3.22) one can check that $I_2(0) = v\rho_c$ and $I'_2(0) = +\infty$, and therefore $\mu_1 > v\rho_c$. Choose $v\rho_c < \mu < \mu_1$ and let \hat{x} be one of the solutions of $\mu = I_2(x) - x$.

Now for $x \ge 0$, let

$$I_1(x) = \frac{v}{2} \int_{\mathbb{R}^3} \nu(\mathrm{d}k) \frac{1}{E(k,x)} \operatorname{coth} \frac{1}{2} \beta E(k,x), \qquad (3.24)$$

$$A(x) = xI_1(x) - I_2(x). (3.25)$$

One can check that A is a strictly concave increasing function of x with $A(0) = -v\rho_c$. Let

$$\alpha := (A(\hat{x}) + \mu)/\hat{x} + 1 = I_1(\hat{x}). \tag{3.26}$$

Note that $A(\hat{x}) + \mu > A(0) + \mu > \mu - v\rho_c > 0$ and therefore $\alpha > 1$. Let the BCS coupling constant $u = v/\alpha$.

We now propose the following solution:

$$\rho_0 = 0, (3.27)$$

$$\rho(k) = \frac{\epsilon(k) + \hat{x}}{2E(k, \hat{x})} \operatorname{coth} \frac{1}{2} \beta E(k, \hat{x}) - \frac{1}{2}, \qquad (3.28)$$

$$s(k) = \frac{\hat{x}}{2E(k,\hat{x})} \operatorname{coth} \frac{1}{2} \beta E(k,\hat{x}).$$
 (3.29)

¿From the definitions above it can be verified that $(s(k))^2 \leq \rho(k)(\rho(k)+1)$. Then using the identities

$$v\overline{\rho} = v \int_{\mathbb{R}^3} \nu(\mathrm{d}k)\rho(k) = I_2(\hat{x}) = \mu + \hat{x},$$

$$u\sigma = \frac{v}{\alpha}\sigma = \frac{1}{\alpha}I_1(\hat{x})\hat{x} = \hat{x},$$

we can check that the condensate equations (3.18), (3.19) are satisfied. Note that (3.27)-(3.29) is also a solution of the Euler-Lagrange (3.11)-(3.13). In fact in [16] we have proved that there is a whole region in the μ - α phase space for which this happens.

Now suppose that $(\tilde{\rho}_0 \neq 0, \tilde{\rho}(k), \tilde{s}(k))$ is another solution of (3.11)-(3.13) for the same values of μ , v and u. Then from (3.13) we can let

$$y := v \int_{\mathbb{R}^3} \nu(\mathrm{d}k)\tilde{\rho}(k) - \mu = u(\tilde{\rho}_0 + |\tilde{\sigma}|) > 0$$
(3.30)

and so from (3.11) and (3.12) we obtain

$$\tilde{\rho}(k) = \frac{\epsilon(k) + y}{2E(k, y)} \operatorname{coth} \frac{1}{2}\beta E(k, y) - \frac{1}{2}s$$
$$\tilde{s}(k) = \frac{y}{2E(k, y)} \operatorname{coth} \frac{1}{2}\beta E(k, y).$$

Integrating these identities we get

$$y + \mu - v\tilde{\rho}_0 = I_2(y),$$

$$\alpha y - v\tilde{\rho}_0 = yI_1(y)$$

and subtracting gives $A(y) = (\alpha - 1)y - \mu$. But from the properties of the function A mentioned above the last equation has only one solution for $\mu > v\rho_c$ and therefore $y = \hat{x}$. Thus the solution coincides with (3.27)-(3.29).

3.2.2 BCS repulsion: u < 0 and generalized (type III) Bose condensation

This unusual "two-stage" phase transitions with one-particle $\rho_0 = |c|^2 \neq 0$ and pair $\sigma \neq 0$ condensations is possible only for *attractive* BCS interaction u > 0. It was was predicted in the physics literature (see for example [11, 15]) and proved in [16, 25]. The case of *repulsion* $(u \leq 0)$ in the BCS part of the PBH (3.5) is *quite different*. The case u = 0, of course, corresponds to the Mean-Field Bose gas.

Remark 3.4. Formally one deduces that (3.17) for $u \leq 0$ implies only trivial solutions $\rho_0 = 0$, $\sigma = 0$, but since the equation gives stationary points of the variational problem, this observation can not be conclusive. On the other hand the condensate equations (3.18), (3.19) give immediate but only partial information that for $\mu < 0$ the Bose condensation ρ_0 and boson pairing σ must be zero. The inequalities of Remark 3.2 do not give more information about those parameters.

The pressure for $u \leq 0$ was obtained rigorously in [16], in fact for a wider class of interactions then we consider here. The nature of the phase transition was studied in [25] where a method of external sources was used to prove the variational principle. Below we give another argument that solves the problem for the BCS repulsion in the PBH model (3.5).

Let us therefore take u < 0. Then clearly

$$\mathcal{E}(r,t,\alpha,c) \ge \int \nu(\mathrm{d}k)\,\epsilon(k)\rho(k) - \mu\overline{\rho} + \frac{v}{2}\overline{\rho}^2.$$
(3.31)

Therefore, since $r \mapsto r \ln r - (r-1) \ln(r-1)$ is increasing and $\tilde{r}(k) \leq r(k)$, we have

$$\mathcal{S}(\omega_{\phi,R,S}) \le \mathcal{S}(\omega_{\widetilde{R}}) \le \mathcal{S}(\omega_R), \tag{3.32}$$

where $\mathcal{S}(\omega_R) = \mathcal{S}(\omega_{\phi,R,S=0}) = \mathcal{S}(\omega_{\phi=0,R,S=0})$ as in (2.32), the free-energy density $f(\omega_\beta)$ is bounded below by the free-energy density $f^{MF}(\beta,\mu)$ of the MF boson model. On the other hand:

$$f(\omega_{\beta}) = \inf_{\rho_{0}, \alpha, r, s} \left\{ \beta \mathcal{E}(r, t, \alpha, c) - \mathcal{S}(\omega_{\phi, R, S}) \right\} \leq \inf_{\rho_{0}=0, s=0} \left\{ \beta \mathcal{E}(r, t, \alpha, c) - \mathcal{S}(\omega_{\phi, R, S}) \right\}$$
$$= \inf_{\rho} \left\{ \beta \left(\int \nu(\mathrm{d}k) \,\epsilon(k) \rho(k) - \mu \rho + \frac{v}{2} \rho^{2} \right) - \mathcal{S}(\omega_{R}) \right\},$$
(3.33)

where $\rho = \int \nu(dk)\rho(k)$. It is well known that the last infimum gives the free-energy density of the MF model (though this infimum is not attained with $\rho_0 = 0$ for $\mu > v\rho_c(\beta)$) and therefore $f(\omega_\beta)$ coincides with the free-energy density $f^{MF}(\beta,\mu)$. Here $\rho_c(\beta)$ is the critical density for the Perfect Bose Gas (3.23). Thus we have the following: In the case of BCS repulsion u < 0 the free energy for the PBH is the same as for the mean-field case:

$$f(\omega_{\beta}) = f^{MF}(\beta, \mu) . \qquad (3.34)$$

Returning to the variational principle this means that the infimum of the free-energy functional in the repulsive case is not attained for $\mu > v\rho_c(\beta)$. Since the critical density $\rho_c(\beta)$ is bounded (for n > 2), we must have BEC in this domain. But now it cannot be a simple accumulation of bosons in the mode k = 0, i.e. $\rho_0 \neq 0$, since it would imply that $c \neq 0$, and by consequence a positive BCS energy in $\mathcal{E}(r, t, \alpha, c)$, see PBH (3.5). The situation which one finds strongly suggests a relation to what is known as generalized condensation. The possibility of such condensation was predicted by Casimir [36] and studied extensively by van den Berg, Lewis and Pulé [37]. One form of generalized condensation is called *type III*; here the condensate is spread over an infinite number of single particle states with energy near the bottom of the spectrum, without any of the states being macroscopically occupied. To make contact with the large deviation and variational techniques developed by van den Berg, Lewis and Pulé, see e.g. [4], [5], note that though the infimum in the right-hand side of (3.33) cannot be reached within the space of regular measures $\rho(k)$ with $\rho_0 = 0$, there is a sequence of regular measures $\{\rho^{(l)}(k)\}_l$ such that $\rho^{(l)}(k) = 0 \, \delta(k) + \rho^{(l)}(k) \to \tilde{\rho}_0 \delta(k) + \tilde{\rho}(k), \ l \to \infty$. Here $\tilde{\rho}_0 > 0$ when $\mu > v \rho_c(\beta)$.

If \mathcal{F} denotes the free-energy density functional in terms of $(\rho_0, \rho(k), s(k))$, then we get:

$$\lim_{l \to \infty} \mathcal{F}(0, \rho^{(l)}(k), s^{(l)}(k) = 0) = \mathcal{F}(\widetilde{\rho}_0, \widetilde{\rho}(k), \widetilde{s}(k)).$$
(3.35)

Mathematically this is because the functional \mathcal{F} is not *lower* semi-continuous on the set of *regular measures*. The physical explanation was given in [25]: In the case u < 0 this model corresponds to the *mean-field* model but with *type III* Bose condensation, i.e. with approximative regular measures that have no atom at k = 0. The fact that repulsive interaction is able to "spread out" the one-mode (*type I*) condensation into the *type III* was also discovered in other models [38], [39].

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