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1997 J. Phys. A: Math. Gen. 30 4895

(http://iopscience.iop.org/0305-4470/30/14/006)

J. Phys. A: Math. Gen. **30** (1997) 4895–4913. Printed in the UK PII: S0305-4470(97)81096-7

Superfluidity III

N Angelescu†§, A Verbeure†‖ and V Zagrebnov‡¶

† Instituut voor Theoretische Fysica, Katholieke Universiteit Leuven, Celestijnenlaan 200 D, B-3001 Leuven, Belgium

‡ Département de Physique, Université de la Méditerranée (Aix-Marseille II) and CPT-Luminy, Case 907, F-13288 Marseille Cedex 9, France

Received 20 January 1997, in final form 28 April 1997

Abstract. The theory of Bogoliubov contains the prescription of replacing the ground-state mode $\frac{a_0}{\sqrt{V}}$ by a constant b. In a previous contribution, we showed that the Bogoliubov model was thermodynamically unstable. We stabilized this model by adding 'forward scattering' terms. In this paper we exploit the fact that it is not compulsary to take b equal to $c = \frac{\langle a_0 \rangle}{\sqrt{V}}$. We show that if $b = c$ the Bogoliubov theory does not have a satisfactory thermodynamics. We prove that it is possible to make a proper choice of the ground-state mode, i.e. b as a function of c, in order to obtain the correct excitation spectrum and thermodynamically a second-order phase transition, as is compulsory for a theory of superfluidity.

1. Introduction

During the 50 years since Bogoliubov [1, 2] isolated the zero momentum condensed state in the weakly imperfect Bose gas and applied his celebrated canonical transformation in an attempt to give a microscopic explanation of superfluidity, relatively little progress has been made in order to make the theory compatible with first principles. Ultimately this would provide a really microscopic understanding of superfluidity. One of the main problems is to show the persistence of the zero momentum Bose condensation, taking place in the free Bose gas, in the presence of a realistic two-body interaction. This is still an open question on the rigorous mathematical level. It is this very condensation which is the basis of the theory of Bogoliubov.

Recent important progress in the rigorous study of the 'diagonal models' [3–6], i.e. truncated versions of the full Hamiltonian which are expressed in terms of the occupation number operators alone, on the one hand, give only partial information about the possible behaviour of the original system and, on the other hand, do not provide the nature of the equilibrium states. These 'diagonal' models are in fact only thermodynamically solvable models and the results [3–6] are related to expectation values of observables, which are functions of the occupation number operators. However, these results are impressive in the sense that they show persistance of the Bose condensate in these non-trivial models. Attempts to extend this result to non-diagonal models, for example to the so-called 'pair Hamiltonian' model [7–11] or to Bogoliubov's original weakly coupled imperfect Bose gas

§ Permanent address: Department of Theoretical Physics, Institute for Atomic Physics, PO Box MG-6, Bucharest, Romania. E-mail address: gangel@roifa.ifa.ro

‖ E-mail address: andré.verbeure@fys.kuleuven.ac.be

¶ E-mail address: zagrebnov@cpt.univ-mrs.fr

0305-4470/97/144895+19$19.50

[12, 13], are either far from complete, or lead to 'unphysical' features, such as a gap in the spectrum of excitations, contradicting the Hugenholtz–Pines–Gavoret–Nozières analysis [14, 15] about the absence of a gap (generally related to the Goldstone theorem) for the full Hamiltonian.

To be precise, a system of identical bosons of mass m in a cubic box $\Lambda \subseteq \mathbb{R}^3$ of volume $V = L^3$, with periodic boundary conditions for the wavefunctions, is described by the full two-body interaction Hamiltonian:

$$H_V = \sum_k \varepsilon_k a_k^* a_k + \frac{1}{2V} \sum_{k;k',q} v(q) a_{k+q}^* a_{k'-q}^* a_{k'} a_k \tag{1.1}$$

where the sum runs over the set

$$\frac{2\pi}{L}\mathbb{Z}^3 \qquad \text{and} \qquad \varepsilon_k = \frac{k^2}{2m}.$$

$a_k^{\#}$ are the boson creation/annihilation operators in the one-particle state $\psi_k(x) = V^{-1/2}\mathrm{e}^{\mathrm{i}kx}$, $x \in \Lambda$; $k \in \Lambda^*$, i.e.

$$a_k = V^{-1/2} \int_\Lambda \mathrm{d}x\, \mathrm{e}^{\mathrm{i}kx} a(x) \qquad [a(x), a^*(y)] = \delta(x - y)$$

and $v(q) = \int_{\mathbb{R}^3} \mathrm{d}x\, \mathrm{e}^{-\mathrm{i}qx}\phi(x)$, ϕ is the periodically extended two-body interaction potential.

There is no hope that the Hamiltonian (1.1) would be exactly solvable, even in the thermodynamic sense, as it is the case for the diagonal models.

A first approach to the problem is to look for a Hartree–Fock approximation of (1.1). Many authors followed this path. This is done in a straightforward way in, see for example, [12]. Considering the variational formulation of the equilibrium state, they restrict the variational procedure to the set of quasifree states and find an upper bound for the free energy. Unfortunately this does not state anything about the real equilibrium states being close to the minimizing quasifree state.

The main idea of Bogoliubov's theory of superfluidity is that switching on the interaction in a condensed free Bose gas does not destroy the Bose condensate which should play a dominant role in the formation of the effective interactions between the particles, i.e. only interactions via the condensate are important. This led Bogoliubov to the following truncated Hamiltonian:

$$H_V^B = \sum_{k\neq 0} \left(\varepsilon_k + (v(0) + v(k))\frac{a_0^* a_0}{V}\right) a_k^* a_k + \frac{1}{2V} \sum_{k\neq 0} v(k)(a_k^* a_{-k}^* a_0 a_0 + a_0^* a_0 a_{-k} a_k) + \frac{1}{2V} v(0)(a_0^* a_0)^2. \tag{1.2}$$

Remark that this is a soluble Hamiltonian [16].

In the diagrammatic language, this means that all direct interactions of the particles with $k \neq 0$, i.e. above the condensate, are disregarded. It should be remarked that the indirect interaction of these excited particles, via the condensate, as well as condensed particles, can be due to the instability of the system (1.2), despite a direct repulsive ($v(0) > 0$) interaction between them. In fact this is the case. In [16] we showed that the pressure $p_V(H_V^B - \mu N_V)$ diverges for chemical potentials $\mu > 0$, while for $\mu \leqslant -\frac{1}{2}\phi(0)$, one obtains the pressure of the ideal Bose gas. Following the standard analysis of the theory of superfluidity [14, 15], the physical region is precisely $\mu > 0$. Hence, there is some work to do in order to remedy this basic deficiency.

The next step in the theory of Bogoliubov is the so-called *Bogoliubov approximation*, which consists of the following. As the operators $a_0^{\#}V^{-1/2}$ almost commute for large

volumes, they are replaced by c-numbers to be determined either from a variational principle for the pressure [17] or by a self-consistency relation. There exists a rigorous result about this approximation [17–19], which is valid only for the full superstable interaction (1.1). In the Bogoliubov theory, the meaning of this result for temperature states created long debates [20–23]. The rigorous result [16] turns out to hold here only in the region $\mu \leqslant -\frac{1}{2}\phi(0)$. Anyway in this approximation [16, 20–23] $H_V^B - \mu N_V$ becomes

$$\mathcal{H}_V^B(c,\mu) = \sum_{k\neq 0}(\varepsilon_k - \mu + |c|^2(v(0)+v(k)))a_k^* a_k + \tfrac{1}{2}\sum_{k\neq 0} v(k)(c^2 a_k^* a_{-k}^* + \bar{c}^2 a_{-k}a_k) \\ -\mu|c|^2 V + \tfrac{1}{2}v(0)|c|^4 V. \tag{1.2a}$$

It is easy to verify (see the remark after proposition 2.2) that without further assumptions the spectrum of $\mathcal{H}_V^B(c,\mu)$ is in general parabolic and has a gap for $\mu < |c|^2 v(0)$, hence not so relevant for superfluidity. Therefore a supplementary conceptually *ad hoc* condition is usually added, namely $\mu = |c|^2 v(0)$, for which model (1.2*a*) is still stable. This choice of the parameter $|c|^2$, which is at the border line of the stability domain of system (1.2*a*), closes the gap in the spectrum, but it obviously creates an inconsistency with the variational principle for pressure or ground state of (1.2*a*) (see [20–23]). Indeed, the relation $\mu = |c|^2 v(0)$ results from the minimization of only the last two terms of (1.2*a*), called the Landau part of the thermodynamic potential.

Hence, despite the stabilization of the Bogoliubov Hamiltonian (1.2) by the Bogoliubov approximation which suppresses condensate fluctuations, one still faces an oppressive alternative: either to follow a thermodynamic variational principle for the pressure and obtain a gap in the spectrum, or to insist on the relation fixing $\mu v(0) = |c|^2$ and working out arguments in favour of it, which are out of the frame of the theory of Bogoliubov. For instance, one can refer to some kind of 'renormalized' Bogoliubov theory [20–22]. In view of the above difficulties, our aim is to first try a construction of a model of the same type as the Bogoliubov one, but which is free from basic obscurities, as discussed above.

First we stabilized the Bogoliubov Hamiltonian (1.2) by adding the 'forward scattering' repulsive interactions between particles above zero mode ($k \neq 0$) and propose the Hamiltonian:

$$\tilde{H}_V = H_V^B + \frac{1}{2V}v(0)\sum_{k,k'\neq 0} a_k^* a_{k'}^* a_{k'} a_k \tag{1.2b}$$

where H_V^B is defined in (1.2), such that $\tilde{H}_V - \mu N_V$ is stable for $\mu \in \mathbb{R}$. In fact, Bogoliubov [2] himself proposed this model. The additional term $\frac{1}{2}v(0)N_V(N_V-1)$ however, which he declared to be a 'constant' despite the fact that the Hamiltonian $\mathcal{H}_V^B(c,\mu)$ is not gauge invariant. System (1.2*b*) is nevertheless exactly soluble in the grand canonical ensemble [13]. In this paper we discuss its solutions, which show properties not shared by superfluid liquids (see further).

In [13, 16], we introduced a modification of (1.2*b*), i.e. retaining the 'forward scattering' repulsive interactions, in fact we started from the imperfect Bose gas Hamiltonian [24–26], added the Bogoliubov terms

$$\sum_{k\neq 0}|c|^2((v(0)+v(k))a_k^* a_k + \tfrac{1}{2}\sum_{k\neq 0} v(k)(b^2 a_k^* a_{-k}^* + \mathrm{hc})$$

and proposed the following model:

$$\tilde{H}_V(b) = \sum_{k\neq 0}(\varepsilon_k + |b|^2 v(k))a_k^* a_k + \tfrac{1}{2}\sum_{k\neq 0} v(k)(a_k^* a_{-k}^* b^2 + \bar{b}^2 a_{-k}a_k) + \tfrac{1}{2}v(0)N_V(N_V-1). \tag{1.3}$$

Remark that in the N_V^2/V-term of the imperfect Bose gas contribution we do not consider the approximation $a_0 \approx \sqrt{V}b$, but we keep the full operator a_0. The Hamiltonian contains a constant b, which is to be determined as a function solely of the condensate.

The idea is that, within some range of temperature and density, the perturbational diagrammatic approach yields an effective Hamiltonian involving 'dressed' Bosons, see e.g. [23]. This Hamiltonian has the imperfect Bose gas as a main part which is soluble. The perturbational part of it contains residual interactions between quasiparticles, which are in fact not the original ones, but renormalized ones, in due case non-local and long ranged. That b is a constant solely dependent on the condensate, i.e. on the expectation values c of $\frac{a_0}{\sqrt{V}}$, means in particular, that the ground-state fluctuations are driven to zero in these interaction terms. The problem which we explore is, how such a Hamiltonian might yield the equilibrium states with the desired properties of a superfluid phase? This is the very spirit of Bogoliubov's approach. We start from his original idea that condensation takes place in the $k = 0$ mode, and the main interactions are between $(k, -k)$-pairs via the non-fluctuating zero mode. Our programme started in [16], where we showed, using standard means of quantum statistical mechanics, that models (1.3) are thermodynamically stable and yield the correct (i.e. linear for small k) spectral properties to ensure its relevance for the theory of superfluidity. In [13], we gave a variational solution of one of the models (1.3) namely for $b = c$.

The aim of this paper is to refine the previous model to ensure a decent thermodynamic behaviour. We consider in particular two versions of (1.3), namely the model

$$\tilde{H}_V(b = c) \tag{1.3a}$$

and the model

$$\tilde{H}_V(b = c\sqrt{r(|c|^2)}) \tag{1.3b}$$

where r is a suitably chosen function: the parameter c 'renormalized' by fluctuations of the condensate. We show that model (1.3*a*) does not have satisfactory thermodynamics, while (1.3*b*) ensures it for a proper choice of $r(|c|^2)$.

The structure of the paper is as follows. In section 2, we rigorously formulate our variational problem and the main statements about the equilibrium states and the spectral properties for models (1.2) and (1.3). The thermodynamic properties of these models are discussed in section 3. Section 4 contains a discussion of the results.

2. Symmetry considerations and spectra

The approach we shall follow throughout the paper to derive the solutions of the various interacting-Boson models under consideration is based on the variational principle for the free energy or pressure. For convenience, we shall first sketch the procedure in general terms and afterwards specialize it to particular models.

A general (infinite-volume) state ω of a Bose system is determined if all its correlation functions: $\omega(a^*(f_1)\dots a^*(f_n)a(g_1)\dots a(g_m))$, for all $n, m \geqslant 0$ and all test functions f_i, g_i, are known.

A particular class of states, called quasifree states [27], is defined by the property that all its correlation functions can be expressed as sums of products of one- and two-point correlations:

$$\text{if } Q_{1\dots n} = \prod_{i=1}^{n}(a^{\#}(f_i) - \omega(a^{\#}(f_i))) \tag{2.1}$$

then

$$\omega(Q_{1\ldots n}) = \sum_{P\in\mathcal{P}} \omega(Q_{P_1})\ldots\omega(Q_{P_r}) \tag{2.2}$$

where the sum runs over the set $\mathcal{P}$ of all partitions $P = \{P_1, \ldots, P_r\}$ of $\{1, \ldots, n\}$ into two-point sets P_i, and the operators within each P_i are in the same order as in $Q_{1\ldots n}$.

Let us now consider a model defined by the finite-volume Hamiltonians H_V. For each translation-invariant (general) state ω, one defines particle-, energy- and entropy-densities by:

$$n(\omega) = \lim_{V\to\infty} V^{-1}\omega_V(N_V) \tag{2.3}$$

$$e(\omega) = \lim_{V\to\infty} V^{-1}\omega_V(H_V) \tag{2.4}$$

$$s(\omega) = \lim_{V\to\infty} V^{-1}S(\omega_V) \tag{2.5}$$

respectively, where $N_V = \sum_k a_k^* a_k$ is the particle-number operator in V, ω_V denotes the restriction of the state ω to local observables in the volume V and $S(\omega_V)$ is its entropy.

The variational principle of statistical mechanics is as follows. The equilibrium states of the model H_V at inverse temperature $\beta = (kT)^{-1}$ and particle density ρ are the minimizers of the free energy: $f(\omega) = e(\omega) - \beta^{-1}s(\omega)$, over all translation-invariant states ω, such that $n(\omega) = \rho$.

It is convenient to take into account the constraint by the Lagrange multiplier method. One defines:

$$p_\mu(\omega) = f(\omega) - \mu(n(\omega) - \rho) \tag{2.6}$$

and solves the unconstrained minimum problem for p_μ. Let $\omega_{\beta,\mu}$ denote the minimizer of p_μ, $\mu \in \mathbb{R}$; one determines $\mu(\rho)$ from the subsidiary condition:

$$n(\omega_{\beta,\mu}) = \rho. \tag{2.7}$$

Then $\omega_{\beta,\mu(\rho)}$ is an equilibrium state and $p_{\mu(\rho)}(\omega_{\beta,\mu(\rho)})$ is the equilibrium pressure functional corresponding to β and ρ. Note that the physical pressure equals $-p_\mu(\omega)$.

A model H_V is exactly solvable if the associated energy density (2.4) is expressed solely in terms of the one- and two-point functions of ω, i.e. $\omega(a^\#(x))$ and $\omega(a^\#(x)a^\#(y))$. In such cases, the variational principle can be simplified considerably, in that the minimum of p_μ (2.6), can be taken only within the class of quasifree states. Indeed, every state ω determines a quasifree state ω_{qf}: it has the same one- and two-point correlations as ω, and, of course, all its higher correlations are put equal to zero. Then, $n(\omega_{qf}) = n(\omega)$ and, by assumption, $e(\omega_{qf}) = e(\omega)$. Moreover, it is always true (cf for example [28]) that $s(\omega_{qf}) \geqslant s(\omega)$. Therefore, $p_\mu(\omega_{qf}) \leqslant p_\mu(\omega)$ for all states ω, the assertion follows.

As already pointed out, models (1.2)–(1.2*b*) and (1.3) presented in the introduction are exactly solvable. In order to apply the variational principle, we need a convenient parametrization of the set of quasifree states.

First, we consider the one-point function:

$$\omega(a(x)) =: c \tag{2.8}$$

as a parameter characterizing the $k = 0$ mode, for example we have for finite V, $\omega(a_0) = V^{1/2}c$ and $\omega(a_0^* a_0) = V|c|^2$.

The two-point correlations are more conveniently described in Fourier representation, i.e. we take the functions $\omega(a_k^* a_k)$ and $\omega(a_k^* a_{-k}^*) = \overline{\omega(a_{-k}a_k)}$ for $k \in \mathbb{R}^3\backslash\{0\}$ as non-trivial parameters.

Remark that we consider quasifree states which are not necessarily gauge invariant, which enables us to take into account spontaneous symmetry breaking. Indeed, models (1.2)–(1.2*b*) have global gauge symmetry (expressing the conservation of their particle number); model (1.3) is not invariant under global gauge transformations, but is instead invariant for gauge transformations in the $k = 0$ mode (expressing conservation of the number of particles with $k = 0$). The thermodynamic limit of finite-volume Gibbs states shares the symmetries of the Hamiltonian, but, like any equilibrium state, it has a decomposition into ergodic states, and the latter are not necessarily preserving the symmetry of the Hamiltonian. The quasifree minimizers we are looking for are the ergodic equilibrium states [27]. In both cases (1.2*b*) and (1.3), it can be checked that, in a minimizing state ω, the phases of the complex numbers $\omega(a_k^* a_{-k}^*)$ are independent of k: for model (1.2*b*) they equal the phase of $\bar{c}^2$, while for (1.3) they equal the phase of $\bar{b}^2$, which—by the self-consistency equations—should be put equal to that of $\bar{c}^2$. Thereby, the energy density $e(\omega)$ is independent of this phase. Therefore, if $c \neq 0$ in a minimizing state ω, then all states obtained from ω by simultaneously changing the phases of $\omega(a_k^* a_{-k}^*)$ and of $\bar{c}^2$ will also be minimizers.

So, for simplicity of the presentation, we shall assume henceforth, without any loss, that c and $\omega(a_k^* a_{-k}^*)$ are reals (and, of course, $b \in \mathbb{R}$ in (1.3)). Also, because $\varepsilon_k = \varepsilon_{-k}$ and $v_k = v_{-k}$, one can assume $\omega(a_k^* a_k) = \omega(a_{-k}^* a_{-k})$.

In order to compute (and express in a simple form) the entropy functional $s(\omega)$, it is convenient to use another parametrization of the set of quasifree states. The new parameters will be a triple (c, m_k, α_k) ($k \in \mathbb{R}^3 \backslash \{0\}$), where $c \in \mathbb{R}$ is again the one-point function, and m_k, α_k are real-valued, even functions, subject to the constraint:

$$m_k \geqslant 1 \qquad \forall k \in \mathbb{R}^3 \backslash \{0\}. \tag{2.9}$$

The old parameters are expressed in terms of (m_k, α_k) by:

$$\omega(a_k^* a_k) = \tfrac{1}{2}(m_k \cosh 2\alpha_k - 1) \qquad \omega(a_k^* a_{-k}^*) = -\tfrac{1}{2} m_k \sinh 2\alpha_k. \tag{2.10}$$

It is clear that constraint (2.9) expresses the positivity of ω.

The new parameters appear naturally by going, via a Bogoliubov transformation, to a gauge-invariant formulation of ω, i.e. in terms of new Boson operators $b_k^{\#}$:

$$a_k = b_k \cosh \alpha_k + b_{-k}^* \sinh \alpha_k \qquad a_{-k} = b_{-k} \cosh \alpha_k + b_k^* \sinh \alpha_k \tag{2.11}$$

such that $\omega(b_k^* b_{-k}^*) = 0$. The latter equation defines $\alpha_k = \alpha_{-k}$, and $m_k = m_{-k}$ is taken as

$$m_k = 2\omega(b_k^* b_k) + 1. \tag{2.12}$$

In the gauge-invariant formulation, and using equation (2.12), the entropy density functional is calculated without difficulty and it has the following expression [29]:

$$s(\omega) = \frac{1}{(2\pi)^3} \int \mathrm{d}k \left(\frac{m_k + 1}{2} \log \frac{m_k + 1}{2} - \frac{m_k - 1}{2} \log \frac{m_k - 1}{2} \right). \tag{2.13}$$

Taking into account (2.10), it is now an easy matter to compute the functional $p_\mu(\omega)$ entering the variational principle. We consider separately models (1.2*b*) and (1.3).

2.1. Model (1.2b)

One has to minimize with respect to (c, m_k, α_k):

$$p_\mu^I(\omega) = \frac{1}{2(2\pi)^3} \int \mathrm{d}k \, [(\varepsilon_k + c^2 v_k)(m_k \cosh 2\alpha_k - 1) - c^2 v_k m_k \sinh 2\alpha_k]$$

$$+\tfrac{1}{2}v(0)n(\omega)^2 - \mu(n(\omega)-\rho)$$
$$-\frac{1}{\beta(2\pi)^3}\int \mathrm{d}k\,\left(\frac{m_k+1}{2}\log\frac{m_k+1}{2} - \frac{m_k-1}{2}\log\frac{m_k-1}{2}\right) \tag{2.14}$$

where:

$$n(\omega) = c^2 + \frac{1}{2(2\pi)^3}\int \mathrm{d}k\,(m_k\cosh 2\alpha_k - 1). \tag{2.15}$$

The stationarity conditions (Euler equations) for $p^I_\mu(\omega)$ read as:

$$cJ(x(\omega), c^2) = 0 \qquad \text{('condensate equation')} \tag{2.16}$$

$$\tanh 2\alpha_k = \frac{c^2 v(k)}{\varepsilon_k + x(\omega) + c^2 v(k)} \qquad k \neq 0 \tag{2.17}$$

$$\frac{1}{\beta}\log\frac{m_k+1}{m_k-1} = (\varepsilon_k + x(\omega) + c^2 v(k))\cosh 2\alpha_k - c^2 v(k)\sinh 2\alpha_k \qquad k \neq 0 \tag{2.18}$$

where the following notation has been used:

$$J(x,y) := x + \frac{1}{2(2\pi)^3}\int \mathrm{d}k\, v_k\left[\frac{\varepsilon_k + x}{E_k(x,y)}\coth\frac{\beta E_k(x,y)}{2} - 1\right] \tag{2.19}$$

with

$$E_k(x,y) = [(\varepsilon_k + x + yv(k))^2 - (yv(k))^2]^{1/2} \tag{2.20}$$

where $x(\omega)$ denotes the functional:

$$x(\omega) = v(0)n(\omega) - \mu. \tag{2.21}$$

System (2.16)-(2.18) can be reduced to a system of two equations for two unknowns $(x, y) \in \mathbb{R}^2_+$ as follows. If (c, m_k, α_k) is a solution to (2.16)–(2.18), denote x the value of $x(\omega)$ in this solution (cf equations (2.21) and (2.15)) and $y = c^2$. Due to equations (2.17) and (2.18) being fulfilled, one can express m_k, α_k in terms of x and y alone. Plugging these expressions into the r.h.s. of (2.21) and simply using the definitions of x, y in equation (2.16), one obtains:

$$x + \mu = v(0)I(x,y) \tag{2.22}$$

$$yJ(x,y) = 0 \tag{2.23}$$

where we defined:

$$I(x,y) = y + \frac{1}{2(2\pi)^3}\int \mathrm{d}k\,\left(\frac{\varepsilon_k + x + yv(k)}{E_k(x,y)}\coth\frac{\beta E_k(x,y)}{2} - 1\right). \tag{2.24}$$

Let us remark that, because of equation (2.17), one necessarily has $x = x(\omega) \geqslant 0$.

Conversely, if $(x, y) \in \mathbb{R}^2_+$ is a solution of system (2.22)–(2.23), one can recover a solution of (2.16)–(2.18), which we denote $\omega(x, y)$, by putting:

$$c = \sqrt{y} \qquad \alpha_k = \frac{1}{2}\tanh^{-1}\left(\frac{yv(k)}{\varepsilon_k + x + yv(k)}\right) \qquad m_k = \coth\frac{\beta E_k(x,y)}{2}. \tag{2.25}$$

The result concerning the equilibrium states for model (1.2*b*) is as follows.

Proposition 2.1. In an equilibrium state $\omega_{\beta,\mu}$, either: (i) $y = 0$ and x is the unique positive solution of the equation

$$x + \mu = v(0)I(x,0) = \frac{v(0)}{2(2\pi)^3}\int \mathrm{d}k\,\left(\coth\frac{\beta(\varepsilon_k + x)}{2} - 1\right) \tag{2.26}$$

or (ii) $y \neq 0$, and (x, y) is a solution of (2.22)–(2.23) with $x > 0$.

In fact, a value μ_1 exists, such that the alternative (i) is obtained for $\mu \in (-\infty, \mu_1)$ and the alternative (ii) for $\mu \in (\mu_1, \infty)$, where μ_1 is to be calculated by equating p_{μ_1} in the stationary points corresponding to the two alternatives.

Proof. The proof relies mainly on the properties of the set of solutions (x, y) of equation (2.23), which is independent of μ. This set is made of two disconnected parts: the half-axis $\{y = 0, x \geqslant 0\}$ and the solutions of $J(x, y) = 0$. To show that the two parts are disconnected, we take advantage of the fact that $J(x, y)$ (see equation (2.19)) is manifestly a strictly decreasing function of y for every fixed $x \geqslant 0$, and moreover:

$$J(x, 0) > x \tag{2.27}$$

$$\lim_{y\to\infty} J(x, y) = x - \frac{1}{2(2\pi)^3}\int \mathrm{d}k\, v(k) =: x - x_{\max}. \tag{2.28}$$

These properties allow us to solve equation (2.23) with respect to y for every $x \in [0, x_{\max})$; in this way, the set of solutions of $J(x, y) = 0$ is the graph of a function $\eta : [0, x_{\max}) \to \mathbb{R}_+$. Clearly, $\eta(x) > 0$ for all x, and $\lim_{x\nearrow x_{\max}} \eta(x) = +\infty$, so $\min \eta > 0$. The solutions of the system (2.22)–(2.23) are the intersection points of the above disconnected set, with the set $S(\mu)$ of solutions of equation (2.22), which depends in a monotonous way on μ. (A more detailed description of $S(\mu)$ will be given in lemma 3.1.) It follows that the only possible solution with $x = 0, y \neq 0$, namely $(0, \eta(0))$ may occur for at most one value of μ. We postpone the proof that $(0, \eta(0))$ never corresponds to a minimum to the next section. □

In order to give a clearer physical interpretation of the behaviour of model (1.2*b*), we construct the effective Hamiltonian $H^{\mathrm{eff}}(\omega_{\beta,\mu})$ in the quasifree equilibrium state $\omega_{\beta,\mu}$ minimizing $p_\mu(\omega)$.

A formal way of finding the effective Hamiltonian for a given local Hamiltonian H_V in such an equilibrium state $\omega_{\beta,\mu}$ in general, amounts to finding a Hamiltonian H^{eff}, bilinear in the creation and annihilation operators, such that, for any observables A, B, C:

$$\lim_{V\to\infty} \omega_{\beta,\mu}(B[H_V - \mu N_V, A]C) = \lim_{V\to\infty} \omega_{\beta,\mu}(B[H_V^{\mathrm{eff}}, A]C). \tag{2.29}$$

In order to solve our problem here, it is sufficient to choose $B = C = 1$ and to take alternatively $A = a_k^*$ for all k (including $k = 0$). One obtains, with $\omega_{\beta,\mu} = \omega(x, y)$ (cf equation (2.25)):

$$H_V^{\mathrm{eff}}(\omega_{\beta,\mu}) = J(x, y)(a_0^* - \sqrt{y})(a_0 - \sqrt{y}) + \sum_{k\neq 0} E_k(x, y) b_k^* b_k + c_V(x, y) \tag{2.30}$$

where $b_k^\#$ and the original $a_k^\#$ are related by the Bogoliubov transformation (2.11), in which α_k is solution (2.25), $c_V(x, y)$ is an explicit function of parameters x, y.

Using this picture (2.30), one has the following.

Proposition 2.2 (spectral properties of model (1.2b)). Model (1.2*b*) behaves like a system of free quasiboson particles and collective excitations with the spectrum $\{J(x, y) \cup (\cup_{k\neq 0} E_k(x, y) | x, y \text{ solutions of equation (2.23)})\}$

Remark that inequality (2.27) implies that, in the normal phase, the quasiparticle eigenvalue $J(x, y)$ is embedded in the continuous spectrum of collective excitations. On the other hand, if $y \neq 0$, the eigenvalue $J(x, y) = 0$ (see the condensate equation (2.23)), while

$$\lim_{k\to 0} E_k(x, y) = E_0(x, y) = \sqrt{x(x + 2yv(0))} > 0. \tag{2.31}$$

Therefore, there is a gap in the spectrum in the condensed phase. Moreover, the behaviour of the dispersion law $E_k(x, y)$ at low momenta is parabolic:

$$E_k(x, y) \approx E_0(x, y) + \frac{2x + yv(0)}{2E_0(x, y)}\varepsilon_k + \cdots \qquad (k \to 0). \tag{2.32}$$

Clearly, the spectral properties of model (1.2*b*) differ drastically from the usual Landau picture of the superfluid phase.

Remark. The original Bogoliubov model (1.2*a*) can be considered within the same variational approach. One obtains for it exactly the same equations (2.16)–(2.18), but with $x(\omega)$ defined as

$$x(\omega) = v(0)y - \mu. \tag{2.33}$$

The corresponding system of two equations for $x, y \in \mathbb{R}^2_+$ becomes $x = v(0)y - \mu$ and, again, the condensate equation (2.23). As the set of solutions of the latter is not connected (cf the proof above), it follows that a solution with $y \neq 0$ cannot be obtained continuously from the non-condensed ones, and, moreover, that the corresponding x does not vanish (spectral gap). In fact, as we proved in [16], no states corresponding to solutions (x, y) associated with $\mu > 0$ can be obtained as limit (grand-canonical) Gibbs states for (1.2*a*).

2.2. Models (1.3)

One has to minimize with respect to (c, m_k, α_k), the pressure

$$\begin{aligned} p^{II}_\mu(\omega, b) = {} & \frac{1}{2(2\pi)^3}\int \mathrm{d}k\,[(\varepsilon_k + b^2 v(k))(m_k \cosh 2\alpha_k - 1) - b^2 v(k) m_k \sinh 2\alpha_k] \\ & + \frac{1}{2} v(0) n(\omega)^2 - \mu(n(\omega) - \rho) \\ & - \frac{1}{\beta(2\pi)^3}\int \mathrm{d}k \left(\frac{m_k + 1}{2}\log\frac{m_k + 1}{2}\log\frac{m_k - 1}{2}\right) \end{aligned} \tag{2.34}$$

where, as before, $n(\omega)$ is given by equation (2.15). Among the minimizing states at a given μ, which are of course, labelled by b, one has to select those for which b is related to the one-point function c according to the self-consistency equations of the models (1.3) or (1.3*a*), (1.3*b*).

The Euler equations for $p^{II}_\mu(\omega, b)$ are:

$$cx(\omega) = 0 \tag{2.35}$$

$$\tanh 2\alpha_k = \frac{c^2 v_k}{\varepsilon_k + x(\omega) + b^2 v(k)} \tag{2.36}$$

$$\frac{1}{\beta}\log\frac{m_k + 1}{m_k - 1} = (\varepsilon_k + x(\omega) + b^2 v(k))\cosh 2\alpha_k - b^2 v_k \sinh 2\alpha_k \tag{2.37}$$

where $x(\omega)$ is defined as before by equation (2.21). The self-consistency equation should be added to (2.35)–(2.37) as a separate equation.

In the same way as for model (1.2), any solutions of (2.35)–(2.37) can be expressed in terms of a solution $(x, y) \in \mathbb{R}^2_+$ of the system of two equations:

$$xy = 0 \tag{2.38}$$

$$\frac{1}{v(0)}(x + \mu) = y + \frac{1}{2(2\pi)^3}\int \mathrm{d}k \left(\frac{\varepsilon_k + x + b^2 v(k)}{E_k(x, c^2)}\coth\frac{\beta E_k(x, b^2)}{2} - 1\right) \tag{2.39}$$

by the following formulae

$$c = \sqrt{y} \qquad \alpha_k = \frac{1}{2}\tanh^{-1}\frac{b^2 v(k)}{\varepsilon_k + x + b^2 v(k)} \qquad m_k = \coth\frac{\beta E_k(x, b^2)}{2}. \tag{2.40}$$

Therefore, by simply looking at equations (2.38)–(2.39), one can express the following alternative for the equilibrium states of the models defined by the Hamiltonian (1.3), irrespective of whether we consider b as a fixed parameter of the model, or select it in terms of c according to the self-consistency equations (1.3*a*) or (1.3*b*).

Proposition 2.3. In an equilibrium state of models (1.3), either: (i) $x = 0$ and equation (2.39) provides a solution $y = y(b^2, \mu) \geqslant 0$, or (ii) $y = 0$ and equation (2.39) provides a solution $x = x(b^2, \mu) \geqslant 0$.

In order to be more precise, we shall consider separately two cases.

(1) b is a fixed real parameter. Remark that such a model has the unpleasant aspect of containing a parameter without any physical significance or origin. Therefore, at this point, the model should be considered as an *artefact*, invented in order to analyse the role played by the individual different terms in the Hamiltonian (1.3).

In this case, the alternative (i) (i.e. $x = 0$) holds for $\mu \geqslant \mu_{cr}(b)$ and the alternative (ii) for $\mu \leqslant \mu_{cr}(b)$, where

$$\mu_{cr}(b) = \frac{v(0)}{2(2\pi)^3} \int \mathrm{d}k \left(\frac{\varepsilon_k + b^2 v(k)}{E_k(0, b^2)} \coth \frac{\beta E_k(0, b^2)}{2} - 1 \right). \tag{2.41}$$

Indeed, if $x = 0$, equation (2.39) becomes $y = v(0)^{-1}(\mu - \mu_{cr}(b))$, which is positive for $\mu \geqslant \mu_{cr}(b)$; if $y = 0$, then, because the r.h.s. of equation (2.39) is strictly decreasing in x, a positive solution to it will exist if, and only if, the value of the l.h.s. at $x = 0$, i.e. $v(0)^{-1}\mu$ is less than the r.h.s. at $x = 0$, i.e. than $v(0)^{-1}\mu_{cr}(b)$.

(2) $b^2 = y(b^2, \mu) = c^2$ (the self-consistency equation (1.3*a*)). Upon using $b^2 = y = c^2$, equation (2.39) becomes exactly equation (2.22).

If $y = 0$, it reads:

$$\frac{1}{v(0)}(x + \mu) = \frac{1}{2(2\pi)^3} \int \mathrm{d}k \left(\coth \frac{\beta(\varepsilon_k + x)}{2} - 1 \right) = I(x, 0) \tag{2.42}$$

which has a unique positive solution if, and only if,

$$\mu \leqslant \overline{\mu}_{cr} := v(0) I(0, 0). \tag{2.43}$$

If $x = 0$, equation (2.22) becomes

$$\frac{1}{v(0)}\mu = I(0, y). \tag{2.44}$$

As $\lim_{y\to\infty} I(0, y) = +\infty$, equation (2.44) will have solutions for all

$$\mu \geqslant \underline{\mu}_{cr} = \min_{y\geqslant 0} I(0, y). \tag{2.45}$$

As $\underline{\mu}_{cr} \leqslant \overline{\mu}_{cr}$, there exist solutions for all μ, either of type (i), or of type (ii).

Constructing in the same way as above (cf equation (2.29)), the effective Hamiltonian for this model ((1.3*a*), (1.3*b*)) in an equilibrium state, we obtain:

$$H_V^{\mathrm{eff}} = x a_0^* a_0 + \sum_{k\neq 0} E_k(x, y) b_k^* b_k + c_V(x, y). \tag{2.46}$$

If the state ω is normal ($y = 0$), then $E_k(x, 0) = \varepsilon_k + x$, therefore $x = \lim_{k\to 0} E_k(x, 0)$ and there is no gap in the spectrum. If ω is a condensed state, then $x = 0$ in view of the condensate equation (2.38) and hence also $\lim_{k\to 0} E_k(0, y) = 0$, therefore the spectrum is again gapless.

Moreover, the dispersion law behaves linearly at $k \approx 0$:

$$E_k(0, y) = \sqrt{\varepsilon_k(\varepsilon_k + 2y v(k))} \sim \sqrt{\frac{y v(0)}{2m}}|k|. \tag{2.47}$$

This behaviour of the excitation spectrum is in accordance with Landau's criteria for superfluidity.

Finally, it is instructive to look upon our results on the spectra of models (1.2*b*) and (1.3) in an equilibrium state from the point of view of the Goldstone theorem. For equilibrium states the Goldstone theorem is normally formulated in terms of cluster properties. More precisely, it states that if the correlations decay fast enough, then there is no spontaneous symmetry breaking [30]. On the other hand, for ground states and short-range interactions, the Goldstone theorem states that, if there is spontaneous symmetry breaking, then the Hamiltonian spectrum has no gap [31]. As we are able to derive the spectral properties for our models, we take the advantage of discussing our spectral results in the context of the symmetry of breaking showing up in the models.

Model (1.2*b*) is gauge invariant, because the Hamiltonian commutes with the total number operator N_V. For densities ρ larger than critical, the gauge symmetry is spontaneously broken. We remark that we found nevertheless an energy gap.

Models (1.3) are gauge invariant only for the zero mode gauge transformations, i.e. the Hamiltonian commutes with the zero momentum occupation number operator $a_0^* a_0$. For large densities, in the condensed phase, again the symmetry is spontaneously broken, and our result yields no energy gap, now in accordance with the Goldstone theorem.

Remark that all models, (1.2*b*) as well as (1.3), can be looked upon as perturbations of the imperfect Bose gas, which itself is described by the Hamiltonian

$$H_V^{IM} = \sum_k \varepsilon_k a_k^* a_k + \frac{1}{2} v(0) \frac{N_V^2}{V}. \tag{2.48}$$

This is a mean-field model and, as such, with long-range interactions. The spectrum of this model in the condensed phase does not show a spectral gap, as for model (1.3) and unlike model (1.2), and in accordance with the Goldstone theorem. On the other hand, this model has a parabolic behaviour at low momenta, like model (1.2*b*), making it unsuitable for the description of superfluidity.

3. The thermodynamics of the models

In the previous section, we discussed the spectral properties of models (1.2*b*) and (1.3*a*), (1.3*b*) in the states fulfilling the necessary conditions for a minimum of the pressure. The analysis should be completed by comparing the values of $p_\mu(\omega)$ at its various stationary points, in order to pick up the absolute minimum. We shall consider first models (1.2) and (1.3*a*). Let us remind at this point that, upon using in $p_\mu^{II}(\omega, c)$ the self-consistency equation (1.3*a*), one obtains the same functional $p_\mu(\omega)$ for both models under consideration. Using part of the Euler equation, we reduced the problem of finding the stationary points of $p_\mu(\omega)$ to that of finding the solution of a system of two equations for two positive unknowns ((2.22), (2.23) for model (1.2*b*), and (2.22), (2.38) for (1.3*a*)).

For arbitrary positive values of the two variables x, y, equation (2.25) provides a quasifree state $\omega(x, y)$. Our task now is to pick up the lowest value of

$$\begin{aligned} p_\mu(\omega(x,y)) = {} & \frac{v(0)}{2} I(x,y)^2 - \mu(I(x,y) - \rho) \\ & + \frac{1}{2(2\pi)^3} \int \mathrm{d}k \left[\frac{2}{\beta} \log 2 \sinh \frac{\beta E_k(x,y)}{2} - (\varepsilon_k + x + y v(k)) \right] \\ & - x \frac{1}{2(2\pi)^3} \int \mathrm{d}k \left(\frac{\varepsilon_k + x + y v(k)}{E_k(x,y)} \coth \frac{\beta E_k(x,y)}{2} - 1 \right) \end{aligned} \tag{3.1}$$

among the solutions (x, y) of the above-mentioned system. As a first step, we shall use

equation (2.22): $v(0)^{-1}(x+\mu) = I(x, y)$, to transform equation (3.1) into:

$$\overline{p}_\mu(x, y) = -\frac{(x+\mu)^2}{2v(0)} + xy + \mu\rho + \frac{1}{2(2\pi)^3}\int \mathrm{d}k \left[\frac{2}{\beta}\log 2\sinh\frac{\beta E_k(x, y)}{2} - (\varepsilon_k + x + yv(k))\right]. \tag{3.2}$$

Clearly, $p_\mu(\omega(x, y)) = \overline{p}_\mu(x, y)$ on the set $S(\mu)$ of solutions (x, y) of equation (2.22), but they are certainly different outside $S(\mu)$. However,

$$\frac{\partial \overline{p}_\mu}{\partial x}(x, y) = -\frac{x+\mu}{v(0)} + I(x, y) \qquad \frac{\partial \overline{p}_\mu}{\partial y}(x, y) = J(x, y) \tag{3.3}$$

so the stationary points of $\overline{p}_\mu(x, y)$ are given by the system (2.22), (2.23), and therefore coincide with the stationary points of $p_\mu(\omega(x, y))$ in $\mathbb{R}^2_+$.

At this stage, a more detailed description of the sets $S(\mu)$ and their dependence on μ is necessary.

Taking into account that $I(x, y)$ is strictly decreasing in x at fixed $y \geqslant 0$, equation (2.22) has at most one solution $x = \xi(\mu, y)$ for given μ, y, and this solution exists if, and only if, $y \in \mathcal{D}(\mu)$, where

$$\mathcal{D}(\mu) = \left\{y \geqslant 0 : \frac{1}{v(0)}\mu \leqslant I(0, y)\right\}. \tag{3.4}$$

Otherwise stated, $S(\mu)$ is the graph of the function $\xi(\mu, \cdot) : \mathcal{D}(\mu) \to \mathbb{R}_+$, defined implicitly by:

$$\xi(\mu, y) + \mu = v(0)I(\xi(x, y), y). \tag{3.5}$$

We collect some information on $S(\mu)$ in the following lemma.

Lemma 3.1. (i) If $\mu_1 < \mu_2$, then $\mathcal{D}(\mu_1) \supset \mathcal{D}(\mu_2)$ and $\xi(\mu_1, y) > \xi(\mu_2, y)$, $\forall y \in \mathcal{D}(\mu_2)$.

(ii) Let

$$\underline{\mu}_{cr} := v(0)\min_{y\geqslant 0} I(0, y) \tag{3.6}$$

then, for $\mu \leqslant \underline{\mu}_{cr}$, $\mathcal{D}(\mu) = \mathbb{R}_+$, while for $\mu > \underline{\mu}_{cr}$, there exists a maximal interval $[\overline{y}(\mu), +\infty) \subset \mathcal{D}(\mu)$, where $\overline{y}(\mu) > 0$.

(iii) Let

$$\overline{\mu}_{cr} := v(0)I(0, 0) \tag{3.7}$$

then, for $\mu \leqslant \overline{\mu}_{cr}$, $0 \in \mathcal{D}(\mu)$, and therefore there exists a largest interval $[0, \underline{y}(\mu)] \subset \mathcal{D}(\mu)$ (with $\underline{y}(\mu) < \overline{y}(\mu)$ if $\mu > \underline{\mu}_{cr}$ and $\underline{y}(\mu) = +\infty$ otherwise).

(iv) The sign of $\frac{\partial \xi}{\partial y}(\mu, y)$ equals sign $\frac{\partial I}{\partial y}(\xi(\mu, y), y)$, therefore $\xi(\mu, \cdot)$ is an increasing function at all points of its graph which belong to the positivity domain of $\frac{\partial I}{\partial y}(x, y)$. Thereby, $\frac{\partial I}{\partial y}$ is positive outside a compact neighbourhood of the origin, and $\frac{\partial I}{\partial y}(x, 0)$ has exactly one change from negative to positive sign as x increases from 0 to $+\infty$.

Proof. All these properties are easy consequences of the definitions and of the properties of $I(x, y)$, equation (2.24).

For (i), the inclusion is obvious from definition (3.4), and the inequality follows by taking the μ-derivative in equation (3.5):

$$\frac{\partial \xi}{\partial \mu}(\mu, y) = -\left(1 - v(0)\frac{\partial I}{\partial x}(\xi(\mu, y), y)\right)^{-1} < 0 \tag{3.8}$$

(because $\frac{\partial I}{\partial x} < 0$, as already remarked). Properties (ii) and (iii) follow directly from definition (3.4) and the fact that:

$$\lim_{y\to\infty} I(0, y) = +\infty \qquad (= \mathrm{O}(y) \text{ at } y \to \infty). \tag{3.9}$$

Finally, (iv) follows by taking the y-derivative of equation (3.5):

$$\frac{\partial \xi}{\partial y}(\mu, y) = v(0)\frac{\partial I}{\partial y}(\xi(\mu, y), y)\left(1 - v(0)\frac{\partial I}{\partial x}(\xi(\mu, y), y)\right)^{-1} \tag{3.10}$$

and again using $\frac{\partial I}{\partial x} < 0$. To prove the statements about sign $\frac{\partial I}{\partial y}$, we compute

$$\frac{\partial I}{\partial y}(x, y) = 1 + \frac{y}{2(2\pi)^3}\int \mathrm{d}k\, v^2(k)\left(\frac{\varepsilon_k + x}{E_k(x, y)^3}\coth\frac{\beta E_k(x, y)}{2} + \frac{\beta}{2(\varepsilon_k + x + 2yv(k))\sinh^2\frac{\beta E_k(x,y)}{2}}\right) - \frac{1}{2(2\pi)^3}\int \mathrm{d}k\,\frac{\beta v(k)}{2\sinh^2\frac{\beta E_k(x,y)}{2}}. \tag{3.11}$$

Because $E_k(x, y) \geqslant \sqrt{\varepsilon_k}\sqrt{x + 2yv(k)} \to \infty$, when x and/or $y \to \infty$, for all $k \neq 0$ such that $v_k > 0$, the negative term converges to 0. For $y = 0$, (3.11) becomes simply:

$$\frac{\partial I}{\partial y}(x, 0) = 1 - \frac{1}{2(2\pi)^3}\int \mathrm{d}k\,\frac{\beta v(k)}{2\sinh^2\frac{\beta(\varepsilon_k + x)}{2}} \tag{3.12}$$

on which the statement is manifest (as $1/\varepsilon_k^2$ is not integrable at 0). □

A few typical sets $S(\mu)$ are sketched in figure 1 ((1) for small μ; (2) for $\mu \leqslant \mu_{cr}$; (3) for $\underline{\mu}_{cr} < \mu \leqslant \overline{\mu}_{cr}$; (4) for $\mu > \overline{\mu}_{cr}$). The solutions (discussed in section 2) of the condensate equation (2.23) (i.e. $\{y = 0\}$ and the graph of the function $\eta(x)$ defined by $J(x, \eta(x)) = 0$) are also represented by heavy curves. Outside the broken line $\frac{\partial I}{\partial y} > 0$. $\frac{\partial \overline{p}_\mu}{\partial y} = J$ is negative at the right of the heavy curve and positive otherwise.

We are now prepared to discuss the phase transitions taking place in the two models.

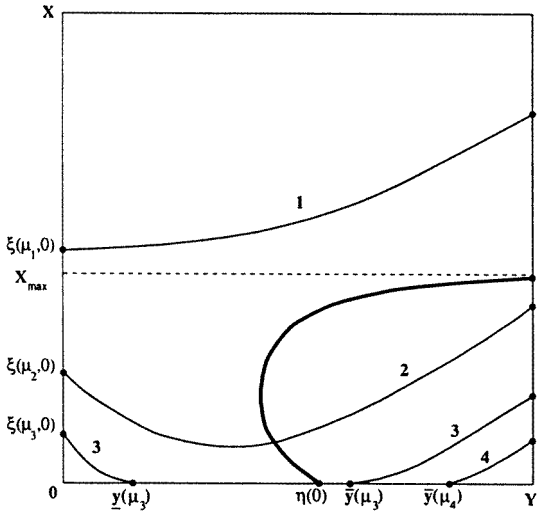

Figure 1.

3.1. Model (1.2b)

For low values of μ, $S(\mu)$ does not intersect the graph of $y(x)$, so the only stationary point is $(\xi(\mu, 0), 0)$, which is the absolute minimum. With increasing μ, $S(\mu)$, and hence also $\xi(\mu, 0)$, goes monotonously down, and the minimum value of p_μ, $\overline{p}_\mu(\xi(\mu, 0), 0)$ also decreases:

$$\frac{\mathrm{d}}{\mathrm{d}\mu}(\overline{p}_\mu(\xi(\mu, 0), 0)) = -I(\xi(\mu, 0), 0) < 0. \tag{3.13}$$

For the first value of μ at which $S(\mu)$ is tangent to the graph of $y(x)$, say in the point $(\xi(\mu, y_0), y_0)$, one has

$$\overline{p}_\mu(\xi(\mu, 0), 0) < \overline{p}_\mu(\xi(\mu, y_0), y_0) \tag{3.14}$$

because $\overline{p}_\mu(\xi(\mu, y), y)$ is increasing in y on $[0, y_0]$; indeed,

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}y}(\overline{p}_\mu(\xi(\mu, y), y)) &= \frac{\partial \overline{p}_\mu}{\partial x}(\xi(\mu, y), y)\frac{\partial \xi}{\partial y}(\mu, y) + \frac{\partial \overline{p}_\mu}{\partial y}(\xi(\mu, y), y) \\ &= \left[-\frac{\xi(\mu, y) + y}{v(0)} + I(\xi(\mu, y), y)\right]\frac{\partial \xi}{\partial y}(\mu, y) + J(\xi(\mu, y), y) \\ &= J(\xi(\mu, y), y) > 0 \end{aligned} \tag{3.15}$$

where (3.3), (3.5) and the positivity of J outside the graph of $\eta(x)$ have been used. Therefore, at this μ, $(\xi(\mu, 0), 0)$ is still the absolute minimum.

For $\mu > \overline{\mu}_{cr}$, $\mathcal{D}(\mu)$ no longer contains 0 and there is no solution on the axis $y = 0$. Therefore, all solutions, among which the absolute minimum, are the intersections of $S(\mu)$ with the graph of $\eta(x)$.

One concludes that the absolute minimum will jump at a certain intermediate value of μ from the axis $y = 0$ (normal phase) to a point on the graph of $\eta(x)$, therefore one has (at least one) first-order phase transition from a normal to a condensed phase.

Let us remark here that, by the same argument as for inequality (3.14) (cf equation (3.15)), when y increases, the entry points of $(\xi(\mu, y), y)$ into the region $\{J(x, y) \leqslant 0\}$ are local maxima and the exit points are local minima. If the point $(0, \eta(0))$ belongs to $S(\mu)$, then it is always an entry point, because $\frac{\partial \xi}{\partial y}(\mu, y) = 0$ whenever $\xi(\mu, y) = 0$, while $\eta'(0)$ is finite. Therefore $(0, \eta(0))$ is a local maximum. This completes the proof that $y > 0$ implies $x > 0$, i.e. condensation implies spectral gap.

The above discussion shows that model (1.2*b*) is not suited to being a superfluidity model both because it always has a spectral gap in the excitation spectrum in the condensed phase, and because it predicts a first-order transition.

3.2. Model (1.3a)

We have shown in section 2 that system (2.38), (2.22) has solutions for every $\mu \in \mathbb{R}$. These can be viewed as the intersections of $S(\mu)$ with the coordinate axis.

The solutions with $y = 0$ will be the same as for model (1.2), i.e. $(\xi(\mu, 0), 0)$, and the discussion done there applies.

The solutions with $x = 0$, $y > 0$ exist for $\mu \geqslant \mu_{cr}$, and they are the finite set of points $0 < y_1(\mu) < \cdots < y_n(\mu)$, such that $\xi(\mu, y_i) = 0$; typically, y_i are boundary points of $\mathcal{D}(\mu)$. According to the description in lemma 3.1, parts (i) and (ii), with increasing μ, these points appear and disappear in pairs, corresponding to the appearance of a gap in $\mathcal{D}(\mu)$ or to the disappearance of a connected component of $\mathcal{D}(\mu)$. (For example, if there is at

most one gap in $\mathcal{D}(\mu)$ (as we conjecture, but are unable to prove for a general v_k satisfying our assumptions), i.e. $\mathcal{D}(\mu) = [0, \underline{y}(\mu)] \cup [\overline{y}(\mu), \infty)$, then $\underline{y}(\mu)$ decreases with μ until it reaches 0 and disappears, while $\overline{y}(\mu)$ increases.) Therefore, none of these points will grow out from 0.

This shows that the transition from the normal to a condensed solution is achieved by a jump of y to a non-zero value at a certain chemical potential, i.e. it will be a first-order transition. In [13], when we considered in detail only the nature of the equilibrium states but not their thermodynamics of models (1.3) and (1.3*a*), it is stated in the introduction that the transition is second order. We take this occasion to correct that error. Hence, a most unpleasant feature of model (1.3*a*) is that the jump of y might entail a discontinuity of $p_\mu(\omega(x, y))$ (i.e. a discontinuity in the equilibrium free energy) at the transition.

It might be instructive at this stage to remark that the unphysical model with Hamiltonian (1.3), in which b^2 is viewed as a fixed parameter of the model (see section 2), without any relation to the one-point function, does not suffer from this disease. There, besides the fact that there is no gap in the spectrum, the thermodynamics is reasonable and predicts a second-order phase transition. In this case, if we solve equation (2.39) with respect to x, we obtain a family $\xi(\mu, y)$ of increasing functions in y, the graph of $\xi(\mu, \cdot)$ intersects exactly once either the x-, or y-axis and the solutions move, with increasing μ, downwards on the x-axis (until it reaches 0 at $\mu = \mu_{cr}(b)$) and then to the right on the y-axis.

It is clear, in the geometrical language above, that technically, the origin of the jump in the solution of model (1.3*a*) is the fact that $\xi(\mu, \cdot)$ is decreasing as a function of y for small y, if μ is near $\overline{\mu}_{cr}$.

As a conclusion, models (1.3) with b (a fixed constant), provide the expected equilibrium states and spectra of a superfluid phase and this is due to the suppressing of the interactions with the fluctuations of the $k = 0$ mode. However, a superimposed self-consistency equation such as (1.3*a*) may have unwanted consequences upon the thermodynamics. Now we show that replacing (1.3*a*) by an equation of type (1.3*b*) yields a good thermodynamics (i.e. second-order transition) without spoiling in any way the good properties of the excitation spectrum.

3.3. Model (1.3b)

For model (1.3) we take the modified self-consistency equation (1.3*b*), i.e.

$$b = c\sqrt{r(|c|^2)} \tag{3.16}$$

and we show that, with a suitable choice of the renormalization function r, model (1.3*b*) is able to give a correct qualitative picture of the superfluid transition, i.e. a second-order transition and a gapless, linear spectrum of excitations in the condensate phase. First, in view of the spectral properties, we repeat that the effective Hamiltonian is given by (see equation (2.46)):

$$H_V^{\text{eff}} = x a_0^* a_0 + \sum_{k \neq 0} E_k(x, y) b_k^* b_k + c_V(x, y)$$

where the pair (x, y) is a solution of equations (2.38) and (2.39), yielding the alternative, either no condensation: $y = c^2 = 0$ and $x \neq 0$, or condensation $y = c^2 \neq 0$ and $x = 0$. All the spectral properties remain qualitatively the same as for model (1.3*a*), analysed in [13, 16], independently of the choice of the function r, as far as $\lim_{y \to 0} yr(y) = 0$.

Finally, in order to provide a model which also shows good thermodynamic behaviour we consider model (1.3*b*) with a physically reasonable choice of the function r. We assume

that r satisfies:

$$\frac{\mathrm{d}}{\mathrm{d}y}(yr(y)) > 0 \qquad \lim_{y\to 0} yr(y) = 0 \qquad \lim_{y\to\infty} r(y) = 1 \tag{3.17}$$

meaning that:

(a) the renormalized coupling of the $(k, -k)$ pairs to the zero-mode is such that the latter increases monotonously with the number of the condensed particles;

(b) without macroscopic occupation of the $k = 0$ mode there is no contribution to the energy density coming from the interactions;

(c) there is no renormalization of the coupling in highly condensed states, i.e. for c large one has $b \simeq c$.

Of course, the approach used for models (1.3), (1.3*a*) applies here as well. One has to minimize the pressure functional (2.34) over the set of quasifree states and one obtains the Euler equations (2.35)–(2.37). Every solution is expressed by (2.40) to which equation (3.16) is added as a separate equation. One arrives now at solving the following systems of equations for (x, y):

$$xy = 0 \tag{3.18}$$

$$\frac{1}{v(0)}(x + \mu) = y(1 - r(y)) + I(x, yr(y)) =: I_r(x, y). \tag{3.19}$$

As the function $I_r(x, y)$, like $I(x, y)$, is a strictly decreasing function of x for fixed y, one can solve equation (3.19) for x, to obtain the set $S_r(\mu)$ of its solutions as the graph of a function;

$$\xi_r(\mu, \cdot) : \mathcal{D}_r(\mu) \to \mathbb{R}_+ \tag{3.20}$$

defined by (3.4), (3.5) with I_r replacing I.

We show now that, under assumptions on v_k, one can choose the function $r(y)$ such that conditions (3.17) are satisfied and, moreover:

$$\frac{\partial I_r(x, y)}{\partial y} > 0 \qquad \text{for all } (x, y) \in \mathbb{R}^2_+ \qquad \text{and} \qquad \text{all } \beta \geqslant \beta_0 > 0 \tag{3.21}$$

where β_0 is some finite, fixed inverse temperature. (We take advantage of the fact that superfluidity is a low-temperature phenomenon and are looking therefore at temperatures lower than the inverse of β_0.)

To this aim, compute

$$\frac{\partial I_r(x, y)}{\partial y} = 1 + \frac{\mathrm{d}\,(yr(y))}{\mathrm{d}y}\left(\frac{\partial I}{\partial y}(x, yr(y)) - 1\right) \tag{3.22}$$

and use (3.11) to identify the only negative term in (3.22) which we have to control. We see that it is sufficient to find a function r such that:

$$\frac{\mathrm{d}}{\mathrm{d}y}(yr(y))\frac{1}{2(2\pi)^3}\int \frac{\beta v_k}{2\sinh^2\frac{\beta E_k(x, yr(y))}{2}}\,\mathrm{d}k \leqslant 1 \qquad \forall (x, y) \in \mathbb{R}^2_+ \qquad \forall \beta \geqslant \beta_0. \tag{3.23}$$

We majorize the l.h.s. of (3.23), using the inequalities $\sinh\frac{\beta E}{2} \geqslant \frac{\beta E}{2}$, $\beta \geqslant \beta_0$, $E_k(x, yr(y)) \geqslant E_k(0, yr(y))$, $v_0 \geqslant v_k$, by:

$$\begin{aligned}
&\frac{\mathrm{d}}{\mathrm{d}y}(yr(y))\frac{1}{\beta_0(2\pi)^3}\int \frac{v_k}{\varepsilon_k(\varepsilon_k + 2yr(y)v(k))}\,\mathrm{d}k \\
&\qquad \leqslant \frac{\mathrm{d}}{\mathrm{d}y}(yr(y))\frac{1}{\beta_0(2\pi)^3}\int_{\text{supp of } v} \frac{v(0)}{\varepsilon_k(\varepsilon_k + 2yr(y)v(0))}\,\mathrm{d}k \\
&\qquad \leqslant \frac{\frac{\mathrm{d}}{\mathrm{d}y}(yr(y))}{\sqrt{yr(y)}}\frac{1}{\beta_0(2\pi)^3}\int_{\mathbb{R}^3} \frac{v(0)}{\varepsilon_k(\varepsilon_k + 2v(0))}\,\mathrm{d}k
\end{aligned} \tag{3.24}$$

where we also used a change of variables $k \to \frac{k}{\sqrt{yr(y)}}$ and an extension of the integral to $\mathbb{R}^3$.

The bound (3.24) shows that it is sufficient to choose the function r under the conditions (3.17) and such that

$$\max_{y \geqslant 0} \frac{\frac{\mathrm{d}}{\mathrm{d}y}(yr(y))'}{\sqrt{yr(y)}} \tag{3.25}$$

is sufficiently small. Here is a fancy example of renormalize coupling

$$r(y) = \frac{\lambda y}{1 + \lambda y}$$

with λ sufficiently small.

With such a choice of r, the analysis in lemma 3.1 shows that:

$$\mathcal{D}_r(\mu) = \begin{cases} \mathbb{R}_+ & \text{if } \mu \leqslant v(0) I_r(0,0) = v(0) I(0,0) = \overline{\mu}_{cr} \\ [\overline{y}_r(\mu), \infty) & \text{if } \mu \geqslant \overline{\mu}_{cr} \end{cases}$$

where $\overline{y}_r(\mu)$ is a continuous, increasing function of μ, with $\overline{y}(\overline{\mu}_{cr}) = 0$. Moreover, $\xi_r(\mu, 0) = \xi(\mu, 0)$ for $\mu \leqslant \overline{\mu}_{cr}$, so that the normal phase is not affected by the change of the self-consistency equation to (3.16). We proved this by the following proposition.

Proposition 3.1. The model

$$\tilde{H}_\Lambda(b) = \sum_{k \neq 0} (\varepsilon_k + |b|^2 v(k)) a_k^* a_k + \tfrac{1}{2} \sum_{k \neq 0} v(k) (a_k^* a_{-k}^* b^2 + \overline{b}^2 a_{-k} a_k) + \tfrac{1}{2} v(0) N_\Lambda (N_\Lambda - 1)$$

with self-consistency equation

$$b = c \sqrt{r(|c|^2)}$$

and the function r satisfying (3.17) and (3.25), is showing Bose condensation as a second-order phase transition and with a linear quasiparticle spectrum for small k. □

4. Conclusions

Our study of the original Bogoliubov model (1.2) shows that to give it any rigorous sense, one has to modify the Hamiltonian H_V^B.

As we discovered in [16], the system $H_V^B - \mu N_V$ either coincides with the perfect Bose gas ($\mu \leqslant 0$) or is unstable ($\mu > 0$).

To save H_V^B as the model of superfluidity, Bogoliubov proposed his famous substitution of the operators $a_0^\#/\sqrt{V}$ by c-numbers, which gives instead of $H_V^B - \mu N_V$, the operator $\mathcal{H}_V^B(c, \mu)$. The consequence of this procedure is twofold:

(1) the operator $\mathcal{H}_V^B(c, \mu)$ (1.2*a*) becomes stable for $\mu < v(0)|c|^2$;

(2) in the thermodynamic limit one can reach the boundary of stability $\mu = v(0)|c|^2$, which guarantees the absence of the gap in the Bogoliubov spectrum and finally a correct interpretation of the superfluidity.

It is clear that the substitution proposed by Bogoliubov is a way of excluding the fluctuations of the Bose condensate which serve as mediators for supplementary attraction between particles (stabilization). The next problem is the choice of the c-numbers in the Bogoliubov procedure: to close the energy gap, one has to put $\mu = v|c|^2$, but the variational principle gives another possibility, for a discussion, see [20–22].

That is why we proposed an alternative way to save Bogoliubov's prescription, namely: first stabilize the initial Bogoliubov Hamiltonian H_V^B by adding the 'forward scattering' interaction between particles above the condensate. The new Hamiltonian $\tilde{H}_V$ (1.2*b*) is superstable, i.e. $\tilde{H}_V - \mu N_V$ gives a finite pressure for all $\mu \in \mathbb{R}$.

The next point is that now one can pass to the substitution of the operators $a_0^{\#}/\sqrt{V}$ by c-numbers $b(\cdot)$ in the Bogoliubov part of the Hamiltonian $\tilde{H}_V$. But in order to take into account fluctuations of the condensate we propose that $b(\cdot)$ would be a function ('*form-factor*' of interaction with condensate) of the condensate density $|c|^2$, for example Bogoliubov prescription corresponds to the *specific choice* of this function namely, a *linear* function of the condensate with the coefficient 1: $b(c) = c$.

The advantage of the model $\tilde{H}_V$ is that the corresponding $\tilde{H}_V(b)$ (1.3) is stable for all $\mu \in \mathbb{R}$, so that we can apply a variational principle to our model (see sections 2 and 3), which gives a solution with a gapless spectrum. We would like to stress that the latter is *not* a result of the 'physical recipe' inspired by the will to close the gap (see the discussion above and [20, 21, 23]) and based essentially on the arguments outside the Bogoliubov theory (e.g. perturbation theory arguments), but a pure consequence of the *exact solution* of model (1.3) within the class of quasifree states.

Another important observation concerns the 'form-factor' $b(c)$. The precise form of this form-factor (which in fact should be, for example a result of perturbation-type calculations) can vary the thermodynamics of the model without changing its fundamental property to have a gapless spectrum of collective excitations. Our particular choice of this 'form-factor' in section 3 guarantees the proof of the convexity of the pressure.

The final point which we believe is important to mention is the problem of the spectrum of the system $\tilde{H}_V$ or $\tilde{H}_V(b)$. Besides the Bogoliubov spectrum of gapless collective excitations one obtains another branch in the spectrum of excitations (sections 2 and 3) related to zero-mode particles, i.e. to the spectrum of quasiparticles. Recent attempts to interpret the phonon-roton excitations in superfluid ^{4}He actually lead to a combination of the collective plus quasiparticle exciations [32, 33].

We will return to this important question in our next paper.

Acknowledgments

NA and VZ wish to thank the Instituut voor Theoretische Fysica, K U Leuven, for hospitality during the visit when the main ideas contained in the paper were formulated. AV acknowledges CPT-Luminy for hospitality during a later phase in the preparation of this paper.

References

[1] Bogoliubov N N 1947 *J. Phys. (USSR)* **11** 23
[2] Bogoliubov N N 1970 *Lectures on Quantum Statistics* vol 2 (London: Gordon and Breach)
[3] van den Berg M, Dorlas T C, Lewis J T and Pulé J V 1990 *Commun. Math. Phys.* **127** 41
[4] van den Berg M, Lewis J T and Pulé J V 1988 *Commun. Math. Phys.* **118** 61
[5] Dorlas T C, Lewis J T and Pulé J V 1991 *Helv. Phys. Acta* **64** 1200
[6] Dorlas T, Lewis J T and Pulé J V 1993 *Commun. Math. Phys.* **156** 37
[7] Zubarev D N and Tserkovnikov Yu A 1958 *Sov. Phys.-Dokl.* **3** 603
[8] Girardeau M 1959 *Phys. Rev.* **115** 1090
[9] Wentzel G 1960 *Phys. Rev.* **120** 1572
[10] Luban M 1962 *Phys. Rev.* **128** 956
[11] Pulé J V and Zagrebnov V A 1993 *Ann. Inst. Henri Poincaré* **59** 421

[12] Critchly R H and Solomon A I 1976 *J. Stat. Phys.* **14** 381
[13] Angelescu N and Verbeure A 1995 *Physica* **216A** 386
[14] Nozières P and Pines D 1990 *Theory of Quantum Liquids, vol II: Superfluid Bose Liquids* (Redwood City, CA: Addison-Wesley)
[15] Toyoda T 1983 *Ann. Phys., NY* **147** 244
[16] Angelescu N, Verbeure A and Zagrebnov V A 1992 *J. Phys. A: Math. Gen.* **25** 3473
[17] Ginibre J 1968 *Commun. Math. Phys.* **8** 26
[18] Fannes M, Pulé J V and Verbeure A 1982 *Helv. Phys. Acta* **55** 391
[19] Buffet E, de Smedt Ph and Pulé J V 1983 *J. Phys. A: Math. Gen.* **16** 4307
[20] Kobe D 1968 *Ann. Phys., NY* **47** 15
[21] Hohenberg P C and Martin P C 1965 *Ann. Phys., NY* **34** 291
[22] Weichman P B 1988 *Phys. Rev.* B **38** 8739
[23] Griffin A 1993 *Excitations in a Bose-Condensed Liquid* (Cambridge: Cambridge University Press)
[24] Davies E B 1972 *Commun. Math. Phys.* **28** 69
[25] van den Berg M, Lewis J T and de Smedt Ph 1984 *J. Stat. Phys.* **37** 697
[26] de Smedt Ph and Zagrebnov V A 1987 *Phys. Rev.* A **35** 4763
[27] Manuceau J and Verbeure A 1968 *Commun. Math. Phys.* **21** 293
[28] Fannes M, Sisson P N M, Verbeure A and Wolf J C 1976 *Ann. Phys.* **98** 38
[29] Fannes M 1978 *Ann. Inst. Henri Poincaré* **28** 187
[30] Martin Ph 1982 *Nuovo Cimento* B **68** 302
[31] Ezawa H and Swieca J A 1967 *Commun. Math. Phys.* **5** 330
[32] Glyde H R 1992 *Phys. Rev.* B **45** 7321
[33] Blagoveshchenskii N M *et al* 1994 *Phys. Rev.* B **50** 16 550