J Stat Phys (2008) 133: 379–400
DOI 10.1007/s10955-008-9593-0

Large Deviations in the Superstable Weakly Imperfect Bose-Gas

J.-B. Bru · V.A. Zagrebnov

Received: 24 September 2007 / Accepted: 25 June 2008 / Published online: 6 August 2008

Abstract The *Superstable Weakly Imperfect Bose-Gas* (Sup-WIBG) was originally proposed to solve some inconsistencies of the Bogoliubov theory based on the WIBG. The grand-canonical thermodynamics of the Sup-WIBG has been recently studied in details but only out of the point of the (first order) phase transition. The present paper closes this gap. The key technical tools are the Large Deviations (LD) formalism and in particular the analysis of the Kac distribution function. It turns out that the condensate fraction discontinuity as a function of the chemical potential (that occurs at the phase transition point) disappears if one considers it as a function of the total particle density. We prove that at this point the equilibrium state of the Sup-WIBG is a mixture of two (low- and high-density) pure phases related to two critical particle densities. Non-zero Bose-Einstein condensate starts at the smaller critical density and continuously grows (for a constant chemical potential) until the second critical density. For higher particle densities, the Bose condensate fraction as well as the chemical potential both increase monotonously.

Keywords Superstable Weakly Imperfect Bose-Gas · Bose-Einstein condensation · Kac distribution · Large deviations · Equivalence of ensembles

1 Introduction

The proof of the *Large Deviation Principle* (LDP) for the *total* particle density distribution (the *Kac distribution*) in the *Perfect*- and in the *Mean-Field* boson gases goes back to [1]. In recent papers [2, 3], the authors addressed to the proof of the LDP for the particle density in *sub-domains* both for the perfect and interacting rarified quantum gases (Fermi or Bose).

J.-B. Bru (✉)
Fakultät für Physik, Universität Wien, Boltzmanngasse 5, 1090 Vienna, Austria
e-mail: jean-bernard.bru@univie.ac.at

V.A. Zagrebnov
Université Aix-Marseille II, Centre de Physique Théorique–UMR 6207, Luminy-Case 907, 13288 Marseille, Cedex 09, France
e-mail: Valentin.Zagrebnov@cpt.univ-mrs.fr

In the present paper we extend the proof of the LDP for the Kac distribution to the *Superstable Weakly Imperfect Bose-Gas* (Sup-WIBG) [4], known also as the Superstable Bogoliubov model [5, 6]. The study of this model out of the phase transition regime started in [4, 7] was recently completed in [8–11].

This model results from a weaker (comparing to the Bogoliubov WIBG) truncation of the full interacting Hamiltonian and allows to solve some inconsistencies between the grand-canonical WIBG description and the Bogoliubov theory of superfluidity, see [6] for discussion. For example the Sup-WIBG exists for *any* values of the chemical potential $\mu \in \mathbb{R}$, whereas the WIBG exists only for its *non-positive* values $\mu \leq 0$. On the thermodynamic level the Sup-WIBG was rigorously solved in the grand-canonical ensemble by [9, 11]. It turns out that the Sup-WIBG (similar to the WIBG) manifests a phase transition with a *nonconventional* (or *dynamical*) zero-mode Bose condensation, which is entirely due to the particle *interaction* [5, 6]. In WIBG this transition occurs at low temperatures β^{-1} and for a sufficiently *strong* (non-diagonal) interaction at a negative critical chemical potential $\mu_c(\beta)$, whereas in Sup-WIBG it takes place for any value of this interaction as soon as the chemical potential is large enough [9, 11].

This and other differences as well as similarities are discussed below in Sect. 2.

Here we only notice that this interaction leads also to the phenomenon of the condensate *depletion*: even at zero temperature, i.e. for an inverse temperature $\beta \to \infty$, only a fraction of the total particle density stays in the zero-mode condensate. This phenomenon is known since the pioneer Bogoliubov's paper [12] and it makes a difference with perfect or mean-field interacting boson gases. Another unusual property of Sup-WIBG is that (similar to WIBG) the phase transition mentioned above occurs in the grand-canonical ensemble for increasing chemical potential μ with a *discontinuity* of the total particle density $\rho(\beta, \mu)$ from $\rho_- := \rho(\beta, \mu_c(\beta) - 0)$ to $\rho_+ := \rho(\beta, \mu_c(\beta) + 0) > \rho(\beta, \mu_c(\beta) - 0)$ for $\beta < \infty$. Moreover, this is related to a strictly positive jump of the condensate density as a function of the chemical potential at the critical value $\mu_c := \mu_c(\beta)$.

The aim of this paper is to study the coexistence of the low- and high-density phases in the Sup-WIBG. (In fact, it was not carefully done even for the WIBG in [5, 6].) In particular, we solve the problem of the value of the Bose condensate density when $\rho \in [\rho_-, \rho_+]$. Several scenarios are possible *à priori*. For example, since this phase transition is characterized by the appearance of the *nonconventional* Bose condensation, which is due to the particle interaction, it might be that there is no condensate at all in the whole domain $\rho \in (\rho_-, \rho_+)$, i.e. the condensate density jumps from zero to a strictly positive value for $\rho > \rho_+$. Here we show that this discontinuity is of a more standard nature. In fact it disappears if the condensate density is considered as a function of the total particle density ρ (canonical ensemble). In particular, at the point of the phase coexistence, the quantum Gibbs state of the Sup-WIBG (or WIBG) model is a linear convex combination of *two* of phases corresponding to ρ_-- and ρ_+-grand-canonical equilibrium states. Moreover, the last one is an integral over pure states enumerated by the condensate gauge parameter. A similar observation was made for a particular example of a "non-convex" *Mean-Field* (MF) interaction in [1], using the large deviations technique description of the total particle density by the Kac distribution [1].

In the present paper we follow this strategy for the Sup-WIBG to verify the LDP for the Bose condensate density distribution as well as for the Kac distribution for all densities including the point of the phase transition. We show that the discontinuity of the zero-mode Bose condensate and its depletion, visible as a function of the chemical potential μ, appears differently, if it is considered as a function of the total particle density. For example, the Bose condensate density is a continuously increasing function of $\rho \geq 0$. When the particle density ρ exceeds the first critical value ρ_-, the Bose condensate density continuously grows but the corresponding chemical potential $\overline{\mu}(\beta,\rho)$ stays constant: $\overline{\mu}(\beta,\rho)=\mu_c(\beta)$ for $\rho\in[\rho_-,\rho_+]$. For higher particle densities: $\rho>\rho_+$, the Bose condensate as well as the chemical potential $\overline{\mu}(\beta,\rho)>\mu_c$ both increase monotonously. Here $\overline{\mu}(\beta,\rho)$ is the solution of the total particle density equation in the grand-canonical state fixed by (β,μ), see Sect. 2.2.

In Sect. 2 we briefly recall the results on the grand-canonical thermodynamics of the Sup-WIBG for a particle density ρ, i.e. for the chemical potential $\overline{\mu}(\beta,\rho)$. Our main results are formulated in Sect. 3 and the proofs are collected in Sect. 4. For the reader convenience, we quote in Appendix some main definitions and technical results related to LDP.

Recall that throughout this paper $\beta>0$ denotes the inverse temperature, whereas μ and $\rho>0$ are respectively the chemical potential and the total particle density. Also, we reserve the notation $\langle -\rangle_{H_\Lambda}(\beta,\mu)$ for the (*finite-volume*) *grand-canonical* Gibbs state corresponding to the Hamiltonian H_Λ.

Notice that our analysis essentially concerns the case with a fixed value of $\beta>0$. Hence, for a short-hand we omit this parameter as argument in notations and definitions, if it is obviously clear.

2 Superstable Weakly Imperfect Bose Gas

2.1 The Hamiltonian

Let a homogeneous gas of n spinless bosons with mass m be enclosed in a cubic box $\Lambda\subset\mathbb{R}^3$ of volume $V:=|\Lambda|$ with periodic boundary conditions for one-particle Schrödinger operator. Then the one-particle energy spectrum is $\varepsilon_k:=\hbar^2k^2/2m$ with $\Lambda^*:=2\pi\mathbb{Z}^3/V^{1/3}$ as the set of wave vectors k. We consider a system with interaction defined by a two-body potential $\varphi(x)\equiv\varphi(\|x\|)$ such that:

(A) $\varphi(x)\in L^1(\mathbb{R}^3)$ (absolute integrability).
(B) Its Fourier transformation $\widehat{\varphi}(\|k\|)=:\lambda_k$ satisfies: $\lambda_{k=0}\geq 0$ and $0\leq\lambda_k\leq\lambda_0$ for $k\in\mathbb{R}^3$.

The Sup-WIBG Hamiltonian (also known as the AVZ Hamiltonian [9] or the Superstable Bogoliubov Hamiltonian [8]), was proposed for the first time in [4]:

$$H^{SB}_{\Lambda,\lambda_0}:=H^B_{\Lambda,0}+U^{MF}_{\Lambda,\lambda_0}. \tag{2.1}$$

Here $H^B_{\Lambda,0}:=H^B_{\Lambda,\lambda_0=0}$ is the Hamiltonian of the WIBG without the *zero-mode* interaction term

$$U^{BMF}_{\Lambda}:=\frac{\lambda_0}{2V}a_0^{*2}a_0^2+\frac{\lambda_0}{V}a_0^*a_0\sum_{k\in\Lambda^*\setminus\{0\}}a_k^*a_k, \tag{2.2}$$

see e.g. [6]. More precisely, the Hamiltonian

$$H^B_{\Lambda,0}:=T_\Lambda+U^D_{\Lambda,0}+U^{ND}_{\Lambda}, \tag{2.3}$$

with the kinetic-energy term $T_\Lambda:=\sum_{k\in\Lambda^*}\varepsilon_k a_k^*a_k$ (note that $\varepsilon_0=0$) and with (*truncated*: $\lambda_0=0$) diagonal $U^D_{\Lambda,0}$ and non-diagonal U^{ND}_Λ Bogoliubov interactions [6]:

$$U^D_{\Lambda,0}:=\sum_{k\in\Lambda^*\setminus\{0\}}\frac{\lambda_k}{2}\frac{a_0^*a_0}{V}(a_k^*a_k+a_{-k}^*a_{-k}),$$

$$U_{\Lambda}^{ND} := \sum_{k\in\Lambda^*\setminus\{0\}} \frac{\lambda_k}{2}\left(a_k^* a_{-k}^* \frac{a_0^2}{V} + \frac{a_0^{*2}}{V} a_k a_{-k}\right).$$

The pressure and the free-energy density of Sup-WIBG are calculated in the thermodynamic limit in [10, 11]. The repulsive interaction U_{Λ}^{MF}, which involves *all modes*, corresponds to the "forward scattering" interaction:

$$U_{\Lambda,\lambda_0}^{MF} := \frac{\lambda_0}{2V} \sum_{k_1,k_2\in\Lambda^*} a_{k_1}^* a_{k_2}^* a_{k_2} a_{k_1} = \frac{\lambda_0}{2V}\left(N_{\Lambda}^2 - N_{\Lambda}\right), \tag{2.4}$$

with the particle-number operator:

$$N_{\Lambda} := \sum_{k\in\Lambda^*} a_k^* a_k.$$

Here $a_k^* := (a(\psi_k))^*$ and $a_k := a(\psi_k)$ are the usual boson creation/annihilation operators in the one-particle eigenfunctions for periodic boundary conditions:

$$\left\{\psi_k(x) := e^{ikx}/\sqrt{V}\right\}_{k\in\Lambda^*} \subset L^2\left(\Lambda^{n=1}\right).$$

These operators act in the boson Fock space

$$\mathcal{F}_{\Lambda}^{B} := \bigoplus_{n=0}^{\infty} \mathcal{H}_B^{(n)}, \quad \text{with } \mathcal{H}_B^{(n)} := \left(L^2\left(\Lambda^n\right)\right)_{\text{symm}}, \, \mathcal{H}_B^{(0)} := \mathbb{C}, \tag{2.5}$$

where $\{\mathcal{H}_B^{(n)}\}_{n=1}^{\infty}$ are symmetrized n-particle Hilbert spaces. By assumptions (A)–(B) the interaction (2.4) ensures the *superstability* of $H_{\Lambda,\lambda_0>0}^{SB}$, see [4, 14].

Notice that for general values of $\lambda > 0$ the interaction $U_{\Lambda,\lambda}^{MF}$ (2.4) is also known as the Mean-Field (MF) boson interaction, see e.g. [1].

Below we consider a *generalized version* $H_{\Lambda,\lambda}^{SB}$ (2.1) of the Sup-WIBG. One of the motivation for this is the (essential) independence of the Sup-WIBG thermodynamic properties of the parameter $\lambda > 0$, see [10, 11]. Recall that the WIBG Hamiltonian retains only a *part* $U_{\Lambda,\lambda_0}^{BMF}$ (2.2) of the total "forward scattering" interaction (2.4) for $\lambda = \lambda_0$. Then the corresponding Hamiltonian of the WIBG (cf. (2.3) and [6]) can be considered as a *truncation* of the Sup-WIBG (2.1):

$$H_{\Lambda,\lambda_0}^{WIBG} := H_{\Lambda,0}^{B} + U_{\Lambda,\lambda_0}^{BMF}. \tag{2.6}$$

Remark 2.1 Let $\mathcal{H}_{k=0,\Lambda} \subset L^2(\Lambda)$ be one-dimensional zero-mode subspace spanned by the vector $\psi_{k=0}(x) = 1/\sqrt{V}$. Then $\mathcal{F}_{\Lambda}^{B} \approx \mathcal{F}_{0\Lambda} \otimes \mathcal{F}_{\Lambda}'$ where $\mathcal{F}_{0\Lambda}$ and $\mathcal{F}_{\Lambda}'$ denote the boson Fock spaces constructed on the space $\mathcal{H}_{0,\Lambda}$ and on its orthogonal complement $\mathcal{H}_{0,\Lambda}^{\perp}$ respectively.

2.2 Grand-Canonical Thermodynamics for a Fixed Particle Density

The grand-canonical thermodynamics of the Sup-WIBG is based on two ingredients: the c-number Bogoliubov substitution $a_0/\sqrt{V} \to c \in \mathbb{C}$ proved in [15] (then justified in a great generality in [16]) and the proof [10, 11] of commutation of sup and inf based on particular convexity-concavity properties of the corresponding (y,α)-function defined in (4.9).

Before to formulate these results, we first define the Bogoliubov *approximation* (or c-number Bogoliubov substitution) of the Hamiltonian $H^B_{\Lambda,0} - \alpha(N_\Lambda - a_0^* a_0)$, which, combined with the gauge transformation $a_k \to e^{i2\arg c} a_k$, equals

$$H^B_{\Lambda,0}(\alpha, x) := \sum_{k\in\Lambda^*\setminus\{0\}} \left\{ (\varepsilon_k - \alpha)\, a_k^* a_k + \frac{x\lambda_k}{2} \left(a_k^* a_k + a_{-k}^* a_{-k} \right) + \frac{x\lambda_k}{2} \left(a_k^* a_{-k}^* + a_k a_{-k} \right) \right\}. \tag{2.7}$$

Here $x = |c|^2 \geq 0$ and $\alpha \leq 0$ are still free parameters. Actually, this operator is used as a trial Hamiltonian via its infinite-volume pressure

$$p_0^B(\beta, \alpha, x) := \lim_{\Lambda} \frac{1}{\beta V} \ln \mathrm{Tr}_{\mathcal{F}'_\Lambda} \left\{ e^{-\beta(H^B_{\Lambda,0}(\alpha,x) - \alpha x V)} \right\}. \tag{2.8}$$

In particular, by variational problem for trail parameters (α, x), it leads to the infinite-volume Sup-WIBG pressure:

Proposition 2.2 [10, 11] *The thermodynamic limit of the grand-canonical pressure associated with the Sup-WIBG model $H^{SB}_{\Lambda,\lambda}$ is equal to*

$$\begin{aligned} p^{SB}(\beta,\mu) &= \sup_{x\geq 0} \left\{ \inf_{\alpha\leq 0} \left\{ p_0^B(\beta,\alpha,x) + \frac{(\mu-\alpha)^2}{2\lambda} \right\} \right\} \\ &= \inf_{\alpha\leq 0} \left\{ p_0^B(\beta,\alpha,x_\mu(\beta)) + \frac{(\mu-\alpha)^2}{2\lambda} \right\}, \end{aligned} \tag{2.9}$$

for any chemical potential μ and any inverse temperature $\beta > 0$.

Notice that to obtain the last line and the *definition* of $x_\mu(\beta)$ in the variational problem (2.9) one uses the following argument. Let $\widehat{\alpha}(\beta,\mu,x)$ be a *minimizer* in the first line of (2.9):

$$p^{SB}(\beta,\mu) = \sup_{x\geq 0} \left\{ p_0^B(\beta, \widehat{\alpha}(\beta,\mu,x), x) + \frac{(\mu - \widehat{\alpha}(\beta,\mu,x))^2}{2\lambda} \right\}.$$

If now $x_\mu := x_\mu(\beta)$ is a *maximizer* of this last variational problem, then by definition of $\widehat{\alpha}$ one gets the identity:

$$\begin{aligned} p^{SB}(\beta,\mu) &= p_0^B(\beta, \widehat{\alpha}(\beta,\mu,x_\mu), x_\mu) + \frac{(\mu - \widehat{\alpha}(\beta,\mu,x_\mu))^2}{2\lambda} \\ &= \inf_{\alpha\leq 0} \left\{ p_0^B(\beta,\alpha,x_\mu(\beta)) + \frac{(\mu-\alpha)^2}{2\lambda} \right\}, \end{aligned}$$

which proves (2.9). Notice that maximizer x_μ might be a discontinuous function of μ, see Proposition 2.6. Below we put $\alpha_\mu(\beta) := \widehat{\alpha}(\beta,\mu,x_\mu)$ and use (2.9) to express the LDP for the condensate distribution.

By this proposition, one obtains the behaviour of the pressure $p^{SB}(\beta,\mu)$ as well as the grand-canonical total particle density $\rho(\beta,\mu)$ as a function of μ:

Proposition 2.3 [10, 11] *Let* $\lambda > 0$ *and* $\beta > 0$. *Then there is a critical value of the chemical potential* $\mu_c(\beta)$ *such that the pressure* (2.9) *has a cusp at* $\mu = \mu_c(\beta)$:

$$\rho_-(\beta) := \partial_\mu p^{SB}(\beta, \mu_c(\beta) - 0) \leq \partial_\mu p^{SB}(\beta, \mu_c(\beta) + 0) =: \rho_+(\beta). \tag{2.10}$$

Therefore, *the grand-canonical total particle density* $\rho(\beta, \mu) = \partial_\mu p^{SB}(\beta, \mu)$ *has a jump*

$$\Delta\rho(\beta, \mu_c(\beta)) := \rho_+(\beta) - \rho_-(\beta) \tag{2.11}$$

at the point $\mu = \mu_c(\beta)$.

Remark 2.4 Notice that the Sup-WIBG model has no sense for $\lambda < 0$, since the grand partition function diverges in this case. It is also difficult to compare Sup-WIBG with WIBG. For the latter model: $\lambda \equiv \lambda_0 \geq \lambda_k$ is compulsory (2.6), and this model exists only for $\mu \leq 0$. On the other hand, under certain conditions the WIBG also manifests a phase transition with a jump of the total particle density, which is related to the jump of the nonconventional condensation, as in Fig. 1. To make a contact between these two models let us introduce the parameter

$$M(\lambda) := \lambda - \frac{1}{2(2\pi)^3} \int d^3k \frac{\lambda_k^2}{\varepsilon_k}. \tag{2.12}$$

Here the second term corresponds to effective *attractive* interaction [5, 6] of bosons in the zero-mode due to non-diagonal interaction U_Λ^{ND} (2.3). The condition for a jump in the WIBG (condition (C)) is $M(\lambda_0) < 0$, whereas for $M(\lambda_0) \geq 0$ this model is equivalent to a Perfect Bose Gas (PBG). Notice that $M(\lambda_0)$ can change from positif to negative values for two-body potentials φ with non-zero radius (see conditions (A) and (B) in Sect. 2.1) by a simple scaling: $\varphi \mapsto \alpha\varphi$ with increasing $\alpha > 0$, see [5, 6]. In contrast to WIBG the Sup-WIBG model manifests a phase transition with a jump of the total particle density for any $\lambda > 0$. If $M(\lambda) \geq 0$, the value of the jump is *independent* of $\lambda > 0$ and converges to zero when $\beta \to \infty$, whereas for $M(\lambda) < 0$ it is *strictly decreasing* with $\lambda > 0$ [11].

Below we consider the Sup-WIBG in the grand-canonical ensemble (β, μ) defined by a given total particle density ρ, i.e. by the chemical potential $\overline{\mu}_\Lambda(\beta, \rho)$, which for any finite domain Λ is a solution of the equation

$$\rho = \left\langle \frac{N_\Lambda}{V} \right\rangle_{H_{\Lambda,\lambda}^{SB}} (\beta, \mu). \tag{2.13}$$

Since the right-hand side of (2.13) is a monotonously increasing function of μ [9], the solution $\overline{\mu}_\Lambda(\beta, \rho)$ is unique for any $\rho > 0$. In the thermodynamic limit, $\overline{\mu}_\Lambda(\beta, \rho)$ converges to

$$\mu_\rho(\beta) := \lim_\Lambda \overline{\mu}_\Lambda(\beta, \rho) \in \mathbb{R}, \tag{2.14}$$

with the following properties:

Proposition 2.5 [9–11] *The solution* $\mu_\rho(\beta)$ *is a strictly increasing function of* ρ *except for some interval* $[\rho_-(\beta), \rho_+(\beta)]$, *where it rests constant*:

$$\mu_c(\beta) := \mu_\rho(\beta), \quad \textit{for } \rho \in [\rho_-(\beta), \rho_+(\beta)]. \tag{2.15}$$

The interval in (2.15) *is non-zero as soon as* $\lambda > 0$, *but gets smaller as* $\beta \to \infty$, *see Fig.* 1.

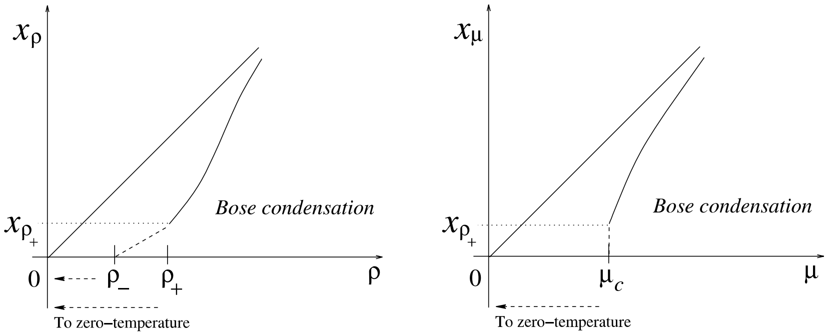

Fig. 1 Illustration of the Bose condensate density, x_ρ as a function of the total particle density $\rho > 0$, and x_μ as a function of the chemical potential $\mu \in \mathbb{R}$. The *dashed line* "closing" continuously the gap between $x_{\rho_-} = 0$ and x_{ρ_+} is an illustration of the condensation x_ρ in the mixture of the extreme phases corresponding the total particle density $\rho \in [\rho_-, \rho_+]$ that we study in the present paper. Here each of the *asymptotic straight lines* are: $x_\rho = \rho$, or $x_\mu = \mu/\lambda$. They correspond to the limits: $x_{\rho\to\infty}$, or $x_{\mu\to\infty}$, when the Bose condensation reachs the saturated value

The next statements make precise the relation between the first-order transition jump of the density and a jump of the nonconventional zero-mode condensation which in Sup-WIBG is due to the same mechanism of non-diagonal interaction U_Λ^{ND} (see (2.3)) as in the case of the WIBG.

Proposition 2.6 [9–11] *Let* $\lambda > 0$ *and* $\beta > 0$. *Then one obtains that*:
(a) *For* $\mu > \mu_c(\beta)$ *the Sup-WIBG manifests a nonconventional zero-mode Bose condensation*:

$$x_\mu = \lim_\Lambda \left\langle \frac{a_0^* a_0}{V} \right\rangle_{H_{\Lambda,\lambda}^{SB}} (\beta, \mu) = \begin{cases} = 0 & for\ \mu < \mu_c(\beta), \\ > 0 & for\ \mu > \mu_c(\beta), \end{cases} \tag{2.16}$$

which coincides with the corresponding solution of the variational problem (2.9). *By the same reason as in the case of the WIBG* (*effective attraction of the zero-mode bosons*, *see* [5, 6]) *the condensation* (2.16) *appears with a jump from zero to the non-zero value*:

$$x_{\mu_c(\beta)+0} - x_{\mu_c(\beta)-0} = x_{\mu_c(\beta)+0} > 0. \tag{2.17}$$

(b) *By virtue of Proposition* 2.5 *and by* (2.16) *one also finds the behaviour of the nonconventional condensation as a function of the total density*:

$$x_\rho := \lim_\Lambda \left\langle \frac{a_0^* a_0}{V} \right\rangle_{H_{\Lambda,\lambda}^{SB}} (\beta, \overline{\mu}_\Lambda(\beta, \rho)) = \begin{cases} = 0 & for\ \rho < \rho_-(\beta), \\ > 0 & for\ \rho > \rho_+(\beta), \end{cases} \tag{2.18}$$

i.e. by (2.15) *the value of* $x_{\rho_+} := x_{\rho_+(\beta)+0}$ *coincides with* $x_{\mu_c(\beta)+0}$ *in* (2.17).
(c) *From the variational problem* (2.9) *we obtain*:

$$p^{SB}(\beta, \mu) = p_0^B(\beta, \alpha_\mu, x_\mu)) + \frac{(\mu - \alpha_\mu)^2}{2\lambda}, \tag{2.19}$$

with maximizer $x_\mu = x_\mu(\beta)$ *and with minimizer* $\alpha_\mu := \alpha_\mu(\beta)$. *Combining* (2.14) *with* (b) *we get that the zero-mode condensate density* (2.18) *for* $\mu_\rho(\beta) \neq \mu_c(\beta)$ *is equal to*

$$x_\rho := x_{\mu_\rho(\beta)}(\beta) \equiv x_{\mu_\rho}(\beta). \tag{2.20}$$

At critical point, $\mu_\rho(\beta) = \mu_c(\beta)$, *the variational problem* (2.9) *has two solutions*: $(0, \alpha_{\mu_c(\beta)-0})$ *and* $(x_{\rho+} = x_{\mu_c(\beta)+0}, \alpha_{\mu_c(\beta)+0})$.
(d) *By* (2.8), (2.9) *and* (2.13), (2.19) *one obtains* [9–11] *the relation*:

$$\rho(\beta,\mu) = \lim_\Lambda \left\langle \frac{N_\Lambda}{V} \right\rangle_{H^{SB}_{\Lambda,\lambda}} (\beta,\mu) = \frac{\mu - \alpha_\mu}{\lambda}. \tag{2.21}$$

Since for any density ρ *we have the identity* $\rho = \rho(\beta, \mu_\rho(\beta))$, *the pressure as function of particle density* $p^{SB}(\beta,\rho)$ *is the Legendre transformation of* $p^{SB}(\beta,\mu)$. *By virtue of* (2.19) *and* (2.21) *we get that*

$$p^{SB}(\beta,\rho) := p^{SB}(\beta,\mu_\rho(\beta)) = p_0^B(\beta,\alpha_\rho,x_\rho) + \frac{\lambda}{2}\rho^2 \tag{2.22}$$

is a convex function of ρ, *where we put* $\alpha_\rho := \alpha_{\mu_\rho(\beta)}(\beta)$.

Remark 2.7 These propositions indicate that the Sup-WIBG manifests a first-order phase transition due to the jump of the zero-mode Bose condensate density. Illustrations of the behaviour of the Bose condensate density x_ρ as a function of ρ, and condensate density x_μ as a function of μ, are presented in Fig. 1. Notice that it is similar to the phase transition in WIBG, but with two essential differences:
(a) Since $\lambda > 0$, the range of the μ for the Sup-WIBG is $\mathbb{R}$, whereas the WIBG exists only for $\mu \leq 0$. The latter implies *coexistence* of the saturated nonconventional and conventional Bose condensations at the extremal point $\mu = 0$. Since for the Sup-WIBG the value of μ is unbounded this phenomenon does not appear for the Sup-WIBG.
(b) Since $\lambda > 0$, the canonical and grand canonical ensembles for the Sup-WIBG are (strongly) equivalent. By virtue of (2.1) and (2.4) with $\lambda_0 = \lambda$, the canonical Gibbs state for the Sup-WIBG are defined only by the Hamiltonian $H^B_{\Lambda,0}$, i.e. by the WIBG without the *zero-mode* interaction term U^{BMF}_Λ, i.e. for $\lambda_0 = 0$, see (2.3). The WIBG free-energy density $f^{WIBG}_{\lambda_0}(\beta,\rho)$ as a function of ρ is convex for $M(\lambda_0) \geq 0$ and non-convex for $M(\lambda_0) < 0$. In the last case one gets the first order transition at some critical chemical potential $\mu^{WIBG}_c(\beta)$ with a jump of the particle density corresponding to the nonconventional Bose condensation jump at this point [5, 6]. Since for $H^B_{\Lambda,0}$ we always have $M(\lambda_0 = 0) < 0$, the Sup-WIBG free-energy density $f^{SB}_{\lambda=0}(\beta,\rho)$ is non-convex, as a function of ρ. Moreover, by [9–11] the "stabilized" free-energy density: $f^{SB}_\lambda(\beta,\rho) = f^{SB}_{\lambda=0}(\beta,\rho) + \lambda\rho^2/2$ rests non-convex for any $\lambda > 0$. Hence, in contrast to WIBG the Sup-WIBG always manifests the first-order phase transition at the chemical potential $\mu_c(\beta)$, see Proposition 2.3.

3 LDP for the Zero-Mode Bose Condensate Density

To define the (finite volume) distribution function $\mathbb{D}_{\Lambda,\rho}$ for the zero-mode Bose condensate density, we first recall the definition of the *Bogoliubov approximation* due to Ginibre [15], see also a more recent paper [16].

For any complex $c \in \mathbb{C}$, a coherent vector $|c\rangle$ in the zero-mode boson Fock space $\mathcal{F}_{0\Lambda}$ (see Remark 2.1) satisfies $a_0|c\rangle = c\sqrt{V}|c\rangle$. In fact, if Ω_0 is the vacuum of $\mathcal{F}_\Lambda^B$, then $|c\rangle := \exp\{-V|c|^2/2 + c\sqrt{V}a_0^*\}\Omega_0$ for any $c \in \mathbb{C}$. Then the Bogoliubov approximation of the self-adjoint operator A with domain in $\mathcal{F}_\Lambda^B \approx \mathcal{F}_{0\Lambda} \otimes \mathcal{F}'_\Lambda$ is the operator $\mathrm{A}(c)$ defined in the boson Fock space $\mathcal{F}'_\Lambda$ of non-zero modes by its sesquilinear form:

$$a_c[\psi'_1, \psi'_2] := \left\langle \psi'_1 \right| \mathrm{A}(c) \left| \psi'_2 \right\rangle := \left\langle c \otimes \psi'_1 \right| \mathrm{A} \left| c \otimes \psi'_2 \right\rangle, \tag{3.1}$$

for $|c \otimes \psi'_{1,2}\rangle$ in the form-domain of A.

For any chemical potential $\mu \in \mathbb{R}$ the (finite volume) grand-canonical pressure associated with $H_{\Lambda,\lambda}^{SB}$ is equal to

$$p_\Lambda^{SB}(\beta, \mu) := \frac{1}{\beta V} \ln \mathrm{Tr}_{\mathcal{F}_\Lambda^B} \left\{ e^{-\beta(H_{\Lambda,\lambda}^{SB} - \mu N_\Lambda)} \right\}. \tag{3.2}$$

Here we put $W_{\Lambda,\mu} := e^{-\beta(H_{\Lambda,\lambda}^{SB} - \mu N_\Lambda)}$ for the grand-canonical *statistical operator* (density matrix) generated by $H_{\Lambda,\lambda}^{SB}$.

Using completeness of the family of coherent vectors $\{|c\rangle\}_{c\in\mathbb{C}}$, one can rewrite the trace Tr in (3.2) as

$$\begin{aligned} p_\Lambda^{SB}(\beta, \mu) &= \frac{1}{\beta V} \ln \int_{\mathbb{C}} \mathrm{d}^2 c \ \mathrm{Tr}_{\mathcal{F}'_\Lambda} \left\{ W_{\Lambda,\mu}(c) \right\} \\ &= \frac{1}{\beta V} \ln \int_{\mathbb{C}} \mathrm{d}^2 c \, e^{\beta V p_\Lambda^{SB}(\beta,\mu,c)}, \end{aligned} \tag{3.3}$$

where $\mathrm{d}^2 c := V\pi^{-1} \mathrm{d}c_1 \mathrm{d}c_2$ with $c := c_1 + ic_2$, and $W_{\Lambda,\mu}(c)$ results from the Bogoliubov approximation (3.1) of the statistical operator $W_{\Lambda,\mu}$. Let

$$p_\Lambda^{SB}(\beta, \mu, c) := \frac{1}{\beta V} \ln \mathrm{Tr}_{\mathcal{F}'_\Lambda} \left\{ W_{\Lambda,\mu}(c) \right\} \tag{3.4}$$

be the pressure defined by the partial trace over subspace $\mathcal{F}'_\Lambda$. Then for any μ, the grand-canonical *condensate-density* distribution function $\mathbb{D}_{\Lambda,\mu}$ is defined by

$$\mathbb{D}_{\Lambda,\mu}[\mathcal{A}] := e^{-\beta V p_\Lambda^{SB}(\beta,\mu)} \int_{\mathcal{A}} \mathrm{d}^2 c \, e^{\beta V p_\Lambda^{SB}(\beta,\mu,c)}, \tag{3.5}$$

on the Borel subsets $\mathcal{A} \subset \mathbb{C}$.

In Sect. 4 we give a proof of the Large Deviation Principle (LDP) for the *canonical* condensate distribution $\mathbb{D}_{\Lambda,\rho} := \mathbb{D}_{\Lambda,\overline{\mu}_\Lambda(\beta,\rho)}$, i.e. when the total particle density $\rho > 0$ is fixed.

Theorem 3.1 (LDP for *canonical* condensate distribution) *For any $\rho > 0$ the sequence of probability measures $\{\mathbb{D}_{\Lambda,\rho}\}_\Lambda$ satisfies the LDP (for the increasing sequence $\beta V \to \infty$) with the rate function (cf. with variational problem (2.9)):*

$$\begin{aligned} \mathrm{I}_\rho(x) : = \sup_{x\geq 0} \left\{ \inf_{\alpha\leq 0} \left\{ p_0^B(\beta, \alpha, x) + \frac{(\mu_\rho - \alpha)^2}{2\lambda} \right\} \right\} \\ - \inf_{\alpha\leq 0} \left\{ p_0^B(\beta, \alpha, x) + \frac{(\mu_\rho - \alpha)^2}{2\lambda} \right\}, \end{aligned} \tag{3.6}$$

where $x = |c|^2 \geq 0$, *the pressure* p_0^B *is defined by* (2.8) *and the chemical potential for a given density* μ_ρ *is equal to* (2.14).

This theorem shows in particular that the probability to observe the zero-mode condensate density $n_0/V \in \mathcal{A}$ of bosons enclosed in Λ for a fixed particle density $\rho > 0$ decreases *exponentially* with the volume $V = |\Lambda|$, if

$$\inf_{n_0/V \in \mathcal{A}} |x_\rho - n_0/V| > 0.$$

Behaviour of the function x_ρ is described by (3.9).

Our next step is to evaluate the limiting probability measure, in particular at the point of the phase transition defined for a particle density $\rho \in [\rho_-, \rho_+]$. Recall that by Proposition 2.6 the Bose condensate density x_ρ converges to 0, when $\rho \to \rho_- - 0$ and to a strictly positive value x_{ρ_+}, when $\rho \to \rho_+ + 0$.

Theorem 3.2 (Limit of distributions $\mathbb{D}_{\Lambda,\rho\notin[\rho_-,\rho_+]}$) *For* $\rho \notin [\rho_-, \rho_+]$ *and* $\Lambda \uparrow \mathbb{R}^3$ *the sequence* $\{\mathbb{D}_{\Lambda,\rho}\}_\Lambda$ *converges weakly on the set of probability measures* $\mathcal{M}_1(\mathbb{C})$ *to the uniform singular measure with density*:

$$\begin{aligned}\mathbb{D}_\rho[\mathrm{d}c_1\,\mathrm{d}c_2] &:= \lim_\Lambda \mathbb{D}_{\Lambda,\rho}[\mathrm{d}c_1\,\mathrm{d}c_2]\\ &= \int_0^{2\pi}\frac{\mathrm{d}\theta}{2\pi}\,\delta(c_1-\sqrt{x_\rho}\cos\theta)\delta(c_2-\sqrt{x_\rho}\sin\theta)\,\mathrm{d}c_1\,\mathrm{d}c_2,\end{aligned}\qquad(3.7)$$

with support on the circle $\{c \in \mathbb{C} : |c| = x_\rho^{1/2}\}$, *where* x_ρ *is the Bose condensate density determined by Proposition* 2.6(b).

Notice that for $\beta \to +\infty$ both $\rho_-(\beta)$ and $\rho_+(\beta)$ *could* converge to zero, depending on the interaction potential and $M(\lambda)$, see Remark 2.4. In contrast, at finite temperature, one always has $\rho_+ > \rho_-$ and the limit of $\{\mathbb{D}_{\Lambda,\rho}\}_\Lambda$ for $\rho \in [\rho_-, \rho_+]$ is one of the main result of the present paper.

Theorem 3.3 (Limit of distributions $\mathbb{D}_{\Lambda,\rho\in[\rho_-,\rho_+]}$) *Let* $\beta > 0$, *i.e.* $\rho_+(\beta) > \rho_-(\beta)$. *For* $\Lambda \uparrow \mathbb{R}^3$, *the distribution* $\mathbb{D}_{\Lambda,\rho}$ *of the condensate converges weakly in* $\mathcal{M}_1(\mathbb{C})$ *towards a convex linear combination of singular measures with densities*:

$$\begin{aligned}\mathbb{D}_\rho[\mathrm{d}c_1\,\mathrm{d}c_2] &:= \lim_\Lambda \mathbb{D}_{\Lambda,\rho}[\mathrm{d}c_1\,\mathrm{d}c_2]\\ &= \left(1-\kappa_\rho\right)\delta(c_1)\delta(c_2)\,\mathrm{d}c_1\,\mathrm{d}c_2\\ &\quad+\kappa_\rho\int_0^{2\pi}\frac{\mathrm{d}\theta}{2\pi}\delta(c_1-\sqrt{x_{\rho_+}}\cos\theta)\delta(c_2-\sqrt{x_{\rho_+}}\sin\theta)\,\mathrm{d}c_1\,\mathrm{d}c_2,\end{aligned}\qquad(3.8)$$

where $\kappa_\rho := (\rho-\rho_-)/(\rho_+-\rho_-)$ *for any* $\rho \in [\rho_-, \rho_+]$.

Note that $\kappa_\rho : [\rho_-, \rho_+] \mapsto [0, 1]$ is a strictly increasing and continuous function. This result gives an evidence that at the point of the phase transition the corresponding Gibbs state is not a *pure* phase anymore, but a convex combination of *two* phases [13], see also example in Sect. 4 of [1]. One of them corresponds to the limiting Gibbs state $\langle-\rangle(\beta, \rho_-(\beta))$ with $x_{\rho_-}(\beta) = 0$, whereas in the state $\langle-\rangle(\beta, \rho_+(\beta))$ the condensate density $x_{\rho_+}(\beta) > 0$, see

Proposition 2.6(b). Notice that the state with condensate is not pure: it is a linear combination (integral) of pure phases fixed by the gauge parameter θ of condensed states, see (3.8).

Finally, integrating the probability density $\mathbb{D}_\rho[c]$ with function $\varphi(c) = |c|^2$, we obtain the Bose condensate density (2.18) for all values of ρ, including in the domain of coexistence of two phases when $\rho \in [\rho_-, \rho_+]$.

Corollary 3.4 (Zero-mode condensate density) *The zero-mode Bose condensate density x_ρ as a function of the total particle density ρ has the form*:

$$x_\rho = \lim_\Lambda \left\langle \frac{a_0^* a_0}{V} \right\rangle_{H^{SB}_{\Lambda,\lambda}} = \begin{cases} 0 & \text{for } \rho \le \rho_-, \\ \dfrac{\rho - \rho_-}{\rho_+ - \rho_-} x_{\rho_+} & \text{for } \rho \in [\rho_-, \rho_+], \\ x_\rho > 0 & \text{for } \rho \ge \rho_+. \end{cases} \tag{3.9}$$

Notice that it is continuous as a function of $\rho > 0$ and is linearly increasing in domain: $\rho \in [\rho_-, \rho_+]$, see Fig. 1.

As a function of the density $\rho > 0$ in the grand-canonical ensemble, the phase transition is of order two if $\rho_+ > \rho_-$ whereas it is of order one as a function of the chemical potential. In particular, take $\rho < \rho_-$, then the system behaves as the so-called Mean-Field Bose Gas, i.e. the model defined by the Hamiltonian

$$H^{MF}_\Lambda := \sum_{k\in\Lambda^*} \varepsilon_k a_k^* a_k + \frac{\lambda}{2V}\left(N_\Lambda^2 - N_\Lambda\right),$$

with no Bose condensation. Increase now the particle density. The chemical potential $\mu_\rho \le \mu_c(\beta)$ normally grows until we reach $\rho = \rho_-$. By further increasing of the density, the Bose condensation sets in and the condensate density reaches continuously the value x_{ρ_+} for $\rho = \rho_+$. Meanwhile, the corresponding chemical potential μ_ρ stays constant at the phase transition: $\mu_\rho = \mu_c$ for $\rho \in [\rho_-, \rho_+]$. Finally, at higher particle densities, i.e. for $\rho > \rho_+$, the Bose condensate as well as the chemical potential $\mu_\rho > \mu_c(\beta)$ both increase.

4 Proofs: LDP for a Generalized Kac Distribution

In this section we prove the LDP for condensate- and "out of condensate" particles distributions of the Sup-WIBG in the grand-canonical ensemble for any fixed total particle density $\rho > 0$, i.e. for chemical potentials $\{\overline{\mu}_\Lambda(\beta, \rho)\}_\Lambda$, see (2.13) and (2.14). The corresponding finite-volume distribution $\mathbb{K}_{\Lambda,\mu}[\cdot, \cdot]$ is a *generalized* Kac distribution [1]: it is a *joint distribution* of particles outside the condensate and the condensed particles, cf. (3.5). The corresponding statement is expressed by Theorem 4.2, which is therefore a generalization of Theorem 3.1. To take into account the phase transition at $\mu_c(\beta)$ and the mixture of two extreme phases, we use a *generalized quasi-average procedure* [1] by taking a "perturbed" critical chemical potential:

$$\tilde{\mu}_c(\Lambda) := \mu_c(\beta) + \frac{\gamma}{\beta V} + o\left(\frac{1}{\beta V}\right) \quad \text{for } \gamma \in \mathbb{R}. \tag{4.1}$$

We analyze the thermodynamic limit of the generalized Kac distribution at the sequence of these chemical potentials, see Theorem 4.4.

As a consequence, the generalized quasi-average procedure (4.1) gives the finite volume asymptotics of the chemical potential $\overline{\mu}_\Lambda(\beta,\rho)$, which is a solution of (2.13) at the phase transition point, i.e. for $\rho \in [\rho_-, \rho_+]$ when $\rho_+ > \rho_-$. Indeed, by applying the distribution $\mathbb{K}_{\Lambda,\mu}$ to an appropriate function, we obtain the mean particle density at a chemical potential $\tilde{\mu}_c(\Lambda)$ for any $\gamma \in \mathbb{R}$. This procedure will then imply that for $\rho \in [\rho_-, \rho_+]$ there is a unique and explicit γ_ρ such that $\overline{\mu}_\Lambda(\beta,\rho) = \tilde{\mu}_c(\Lambda)$ with $|\gamma_\rho| = o(V)$, see Sect. 4.2.

Meanwhile, the LDP for $\mathbb{K}_{\Lambda,\mu}$ given by Theorem 4.2 directly implies Theorem 3.1 for any $\rho > 0$. Applying the result of Theorem 4.4 to the chemical potential $\overline{\mu}_\Lambda(\beta,\rho) = \tilde{\mu}_c(\Lambda)$ for $\gamma = \gamma_\rho$, we also get Theorem 3.3 for $\rho \in [\rho_-, \rho_+]$. If $\rho \notin [\rho_-, \rho_+]$, the generalized quasi-average procedure is not necessary and Theorem 3.2 is a simple consequence of Theorem 3.1. We give now the promised proofs.

4.1 Large Deviations for Generalized Kac Distribution

In the grand-canonical ensemble the particle number density is a random variable defined by the probability measure, known as the Kac distribution [1]. We introduce here a *generalized* Kac distribution associated with the condensate- and out of the condensate (depletion) particle densities.

Definition 4.1 The generalized Kac distribution is defined on the Borel subsets $\mathcal{A} \times \mathcal{B}$, where $\mathcal{A} \subset \mathbb{C}$ and $\mathcal{B} \subset \mathbb{R}_+$, by integration over the zero-mode coherent states and over the particle counting measure ν_Λ:

$$\begin{aligned} &\mathbb{K}_{\Lambda,\mu}\left[\mathcal{A} \times \mathcal{B}\right] \\ &\quad := e^{-\beta V p_\Lambda^{SB}(\beta,\mu)} \int_{\mathcal{A}} \mathrm{d}^2 c \int_{\mathcal{B}} \nu_\Lambda\left(\mathrm{d}y\right) e^{\beta V[\mu(y+|c|^2) - f_\Lambda^{SB}(\beta,y,c)]}. \end{aligned} \tag{4.2}$$

Here the counting measure

$$\nu_\Lambda\left(\mathrm{d}y\right) := \sum_{n=1}^{\infty} \delta\left(\left[|yV|\right] - n\right) \mathrm{d}y, \tag{4.3}$$

where $[|a|]$ stands for integer part of $a \geq 0$, and the (partial) canonical free-energy

$$f_\Lambda^{SB}(\beta,y,c) := -\frac{1}{\beta V} \ln \mathrm{Tr}_{\mathcal{H}_{B,k\neq 0}^{[yV]}} \left\{\left[W_{\Lambda,0}(c)\right]_{k\neq 0}^{[|yV|]}\right\} \tag{4.4}$$

corresponds to the Bogoliubov approximation $W_{\Lambda,\mu=0}(c)$ (3.1) of the statistical operator $W_{\Lambda,\mu}$, cf. (3.4), restricted to the *non-zero* mode of the $[|yV|]$-particle boson Fock subspace $\mathcal{H}_{B,k\neq 0}^{[|yV|]}$.

Our first result concerns the large deviations for the generalized Kac distributions $\mathbb{K}_{\Lambda,\mu}[\,\cdot\,]$ in the grand-canonical ensemble.

Theorem 4.2 (LDP for generalized Kac distributions) *In the grand-canonical ensemble* (β,μ) *the family of Kac distributions* $\{\mathbb{K}_{\Lambda,\mu}\}_\Lambda$ *satisfies the LDP for the increasing sequence* βV *with the rate function*:

$$\mathrm{K}_\mu\left(x,y\right) := p^{SB}\left(\beta,\mu\right) + f_0^B\left(\beta,y,x\right) + \frac{\lambda}{2}\left(y+x\right)^2 - \mu\left(y+x\right), \tag{4.5}$$

see Appendix. Here $x := |c|^2 \geq 0$, $y \geq 0$ and

$$f_0^B(\beta, y, x) := \sup_{\alpha \leq 0} \left\{ \alpha(y+x) - p_0^B(\beta, \alpha, x) \right\} \tag{4.6}$$

is the Legendre-Fenchel transformation of the trial pressure $p_0^B(\beta, \alpha, x)$ defined in (2.8).

Proof Notice that the pressure $p_0^B(\beta, \alpha, x)$ is defined by bilinear Hamiltonian (2.7) and thus it can be calculated explicitly for any $\alpha \leq 0$:

$$\begin{aligned} p_0^B(\beta, \alpha, x) = \alpha x &- \frac{1}{\beta(2\pi)^3} \int_{\mathbb{R}^3} \mathrm{d}^3 k \ln\left(1 - e^{-\beta E_k(\alpha, x)}\right) \\ &+ \frac{1}{2(2\pi)^3} \int_{\mathbb{R}^3} \mathrm{d}^3 k (\varepsilon_k - \alpha + x\lambda_k - E_k(\alpha, x)). \end{aligned} \tag{4.7}$$

Here

$$E_k(\alpha, x) := \sqrt{(\varepsilon_k - \alpha)(\varepsilon_k - \alpha + 2x\lambda_k)}.$$

Since $p_0^B(\beta, \alpha, x)$ is a convex function of $\alpha \leq 0$, it can be expressed as the (inverse) Legendre-Fenchel transform of the convex function (4.6):

$$p_0^B(\beta, \alpha, x) = \sup_{y \geq 0} \left\{ \alpha(y+x) - f_0^B(\beta, y, x) \right\}.$$

Combination of the last identity with the result of Proposition 2.2 implies that

$$\begin{aligned} &p^{SB}(\beta, \mu) \\ &= \sup_{x \geq 0} \left\{ \inf_{\alpha \leq 0} \left\{ \sup_{y \geq 0} \left\{ \alpha(y+x) - f_0^B(\beta, y, x) + \frac{(\mu - \alpha)^2}{2\lambda} \right\} \right\} \right\}. \end{aligned} \tag{4.8}$$

In general, a *supremum* and an *infimum* do not commute, i.e. we can not exchange infimum over $\alpha \leq 0$ and supremum over $y \geq 0$. But in this particular case, this is however possible. Indeed, for any fixed $x \geq 0$ the function

$$\Psi(y, \alpha) := \alpha(y+x) - f_0^B(\beta, y, x) + \frac{(\mu - \alpha)^2}{2\lambda} \tag{4.9}$$

is a strictly concave for $y \geq 0$ and strictly convex as the function of $\alpha \leq 0$. Therefore, the stationary (*saddle*) point $(\tilde{y}, \tilde{\alpha})$ of the function (4.9) is unique and it is solution of equations:

$$\partial_y \Psi(y, \alpha) = 0 \quad \text{and} \quad \partial_\alpha \Psi(y, \alpha) = y + x + \frac{\alpha - \mu}{\lambda} = 0.$$

In particular, this allows to commute the infimum over $\alpha \leq 0$ and the supremum over $y \geq 0$ in (4.8) to obtain

$$p^{SB}(\beta, \mu) = \sup_{(x,y) \in \mathbb{R}_+^2} \left\{ \mu(y+x) - f_0^B(\beta, y, x) - \frac{\lambda}{2}(y+x)^2 \right\}, \tag{4.10}$$

which implies the rate function $\mathrm{K}_\mu(x, y) \geq 0$, cf. (4.5). Moreover, due to (4.6) and to the explicit expression (4.7), one finds that for any $\lambda > 0$ there are strictly positive constants

$M, B > 0$ such that solutions (x_μ, y_μ) of the variational problem (4.10) are localized in a finite domain: $\mathcal{D}_M := \{|c_\mu|^2 := x_\mu < M, y_\mu < M\}$, whereas for any $(|c|^2 = x, y) \in \mathcal{D}_M^c := \{\mathbb{C} \times \mathbb{R}_+\} \setminus \mathcal{D}_M$ we have the estimate:

$$\mu (y + x) - f_0^B (\beta, y, x) - \frac{\lambda}{2} (y + x)^2 \leq -B (y + x) . \tag{4.11}$$

The latter implies that for these values of arguments the rate function can be estimated from below by

$$\mathrm{K}_\mu (x, y) > p^{SB} (\beta, \mu) + B (y + x) . \tag{4.12}$$

After these preliminaries we are in position to check the LDP for the sequence of distributions $\{\mathbb{K}_{\Lambda,\mu}\}_\Lambda$, see Appendix for basic notations and definitions.

By virtue of (4.6), (4.7) and (4.10) it gets evident that the rate function $\mathrm{K}_\mu(x, y)$ is not identical to ∞ and that it has compact level sets, i.e. for each $m < \infty$, the subset $\{(x, y) : \mathrm{K}_\mu(x, y) \leq m\}$ is compact (LD1).

Consider now $\mathbb{K}_{\Lambda,\mu}$ on any closed set $\mathcal{C} := \mathcal{C}_0 \times \mathcal{C}_1$ of $\mathbb{C} \times \mathbb{R}_+$. By (4.2), (4.10) and (4.12) we obtain the estimate:

$$\begin{aligned} \mathbb{K}_{\Lambda,\mu} [\mathcal{C}_0 \times \mathcal{C}_1] \leq e^{\beta V} & \Big\{ \sup_{\{\mathcal{C}_0 \times \mathcal{C}_1\} \cap \mathcal{D}_M} \left\{ \mu (y + |c|^2) - f_\Lambda^{SB}(\beta, y, c) \right\} - p_\Lambda^{SB} (\beta, \mu) \Big\} \\ & \times \int_{\{\mathcal{C}_0 \times \mathcal{C}_1\} \cap \mathcal{D}_M} \mathrm{d}^2 c \, \nu_\Lambda (\mathrm{d}y) \\ & + \int_{\{\mathcal{C}_0 \times \mathcal{C}_1\} \cap \mathcal{D}_M^c} \mathrm{d}^2 c \, \nu_\Lambda (\mathrm{d}y) \, e^{-\beta V \{B(x+y) + p_\Lambda^{SB}(\beta,\mu)\}}. \end{aligned} \tag{4.13}$$

Now definitions (4.2) and (4.10) combined with Lemma 5.2 imply:

$$\limsup_\Lambda \frac{1}{\beta V} \ln \mathbb{K}_{\Lambda,\mu} [\mathcal{C}_0 \times \mathcal{C}_1] \leq - \inf_{\mathcal{C}_0 \times \mathcal{C}_1} \mathrm{K}_\mu \left(|c|^2, y \right),$$

which is equivalent to the large deviations *upper bound* (5.11) for distributions $\mathbb{K}_{\Lambda,\mu}$ for the sequence βV with the rate function K_μ (LD2).

It remains to establish the corresponding large deviation lower bound (5.12). Let $\mathcal{G} := \mathcal{G}_0 \times \mathcal{G}_1$ be an arbitrary open subset of $\mathbb{C} \times \mathbb{R}_+$ and take a point $(\hat{c}, \hat{y}) \in \mathcal{G}_0 \times \mathcal{G}_1$. Denote by $\mathcal{G}_\delta(\hat{c}, \hat{y})$ a δ-vicinity of the point $(\hat{c}, \hat{y})$ such that $\mathcal{G}_\delta(\hat{c}, \hat{y}) = \mathcal{G}_{0,\delta}(\hat{c}) \times \mathcal{G}_{1,\delta}(\hat{y}) \subset \mathcal{G}$. Then one obviously has:

$$\begin{aligned} & \mathbb{K}_{\Lambda,\mu}[\mathcal{G}] \geq \mathbb{K}_{\Lambda,\mu}[\mathcal{G}_\delta(\hat{c}, \hat{y})] \\ & \qquad \geq e^{-\beta V p_\Lambda^{SB}(\beta,\mu)} e^{\beta V [\inf_{\mathcal{G}_\delta(\hat{c},\hat{y})} \{\mu(y+|c|^2) - f_\Lambda^{SB}(\beta,y,c)\}]} \int_{\mathcal{G}_{0,\delta}(\hat{c})} \mathrm{d}^2 c \int_{\mathcal{G}_{1,\delta}(\hat{y})} \nu_\Lambda (\mathrm{d}y) . \end{aligned} \tag{4.14}$$

Since inequality (4.14) holds for each point $(\hat{c}, \hat{y})$ of $\mathcal{G}$, by virtue of Lemma 5.2 and by continuity of functions $\{\mu(y + |c|^2) - f_\Lambda^{SB}(\beta, y, c)\}$ in variables c, y for any large βV, this implies:

$$\liminf_\Lambda \frac{1}{\beta V} \ln \mathbb{K}_{\Lambda,\mu} [\mathcal{G}] \geq - \inf_{\mathcal{G}_0 \times \mathcal{G}_1} \mathrm{K}_\mu \left(|c|^2, y \right),$$

i.e. the corresponding large deviation *lower bound* (5.12) for $\mathbb{K}_{\Lambda,\mu}$ holds for the sequence βV with the rate function K_μ (LD3). □

By Theorem 4.2 we can then deduce the convergence of the distribution $\mathbb{K}_{\Lambda,\mu}$ as $\Lambda \uparrow \mathbb{R}^3$ for $\mu \neq \mu_c$:

Corollary 4.3 (Limit of Distributions $\mathbb{K}_{\Lambda,\mu\neq\mu_c}$) *The sequence of generalized Kac distributions $\{\mathbb{K}_{\Lambda,\mu}\}_\Lambda$ verifies the LDP and converges weakly on the set of probability measures $\mathcal{M}_1(\mathbb{C}\times\mathbb{R}_+)$ to the product of atomic and of degenerate singular measure on the circle*

$$\begin{aligned}\mathbb{K}_\mu & \left[\mathrm{d}c_1\mathrm{d}c_2 \times \mathrm{d}y\right] \\ &= \lim_\Lambda \mathbb{K}_{\Lambda,\mu}\left[\mathrm{d}c_1\mathrm{d}c_2 \times \mathrm{d}y\right] \\ &= \int_0^{2\pi}\frac{\mathrm{d}\theta}{2\pi}\delta(c_1-\sqrt{x_\mu}\cos\theta)\delta(c_2-\sqrt{x_\mu}\sin\theta)\,\mathrm{d}c_1\mathrm{d}c_2\delta(y-y_\mu)\,\mathrm{d}y, \end{aligned} \tag{4.15}$$

for $\mu > \mu_c$ whereas for $\mu < \mu_c$, i.e. $x_{\mu<\mu_c} = 0$,

$$\mathbb{K}_{\mu<\mu_c}\left[\mathrm{d}c_1\mathrm{d}c_2 \times \mathrm{d}y\right] = \delta(c_1)\delta(c_2)\,\mathrm{d}c_1\mathrm{d}c_2\delta(y-y_\mu)\,\mathrm{d}y. \tag{4.16}$$

Proof By virtue of the LDP (Theorem 4.2), if $\lim_\Lambda \mathbb{K}_{\Lambda,\mu}[\cdot] = \mathbb{K}_\mu[\cdot]$ exists, the support of the limit Kac measure $\operatorname{supp}\mathbb{K}_\mu$ is contained in the set $\{(x,y) : \mathrm{K}_\mu(x,y) = 0\}$. However, if this support consists of more than one point the *Helly selection principle* guarantees that $\{\mathbb{K}_{\Lambda,\mu}\}_\Lambda$ contains subsequences converging to *atomic* measures with supports in these points. By [9] the variational problem (4.10) has for any $\mu \neq \mu_c$ a *unique* solution $(x_\mu = |c_\mu|^2, y_\mu) \in \operatorname{supp}\mathbb{K}_\mu$. Notice that in contrast to atomic measure with support at $y = y_\mu$ the condition $x_\mu = |c_\mu|^2$ defines in the complex plane $\mathbb{C}$ a two-dimensional *degenerate* probability measure on the circle $\{c \in \mathbb{C} : |c| = |c_\mu| = \sqrt{x_\mu}\}$. Hence, we obtain (4.15). Since there is no zero-mode condensation for $\mu < \mu_c$, i.e. $x_{\mu<\mu_c} = 0$, the measure (4.15) reduces in this case to the product of atomic measures (4.16). □

If $\rho_+ > \rho_-$, then at the critical point $\mu = \mu_c$ the variational problem (4.10) has two solutions: $(0, y_{\mu_c-0} = \rho_-)$ and $(x_{\mu_c+0}, y_{\mu_c+0})$, where $y_{\mu_c+0} = \rho_+ - x_{\mu_c+0}$, see [9] and [11]. We analyze this special case in our next theorem.

Theorem 4.4 (Generalized Kac distribution at the critical point) *Let $\beta > 0$, i.e. $\rho_+ > \rho_-$. Then for $\tilde{\mu}_c(\Lambda)$ defined by (4.1) the Kac distributions $\{\mathbb{K}_{\Lambda,\tilde{\mu}_c(\Lambda)}\}_\Lambda$ converge weakly in $\mathcal{M}_1(\mathbb{C}\times\mathbb{R}_+)$ to the family of linear convex combinations of two limit Kac distributions*:

$$\begin{aligned}\mathbb{K}_{\mu_c,\gamma}\left[\mathrm{d}c_1\mathrm{d}c_2 \times \mathrm{d}y\right] &= \lim_\Lambda \mathbb{K}_{\Lambda,\tilde{\mu}_c(\Lambda)}\left[\mathrm{d}c_1\mathrm{d}c_2 \times \mathrm{d}y\right] \\ &= \xi_\gamma \mathbb{K}_{\mu_c-0}\left[\mathrm{d}c_1\mathrm{d}c_2 \times \mathrm{d}y\right] + (1-\xi_\gamma)\mathbb{K}_{\mu_c+0}\left[\mathrm{d}c_1\mathrm{d}c_2 \times \mathrm{d}y\right], \end{aligned} \tag{4.17}$$

with coefficients $\xi_\gamma := (1 + e^{\gamma(\rho_+-\rho_-)})^{-1} \in (0,1)$, for $\gamma \in \mathbb{R}$. Here

$$\mathbb{K}_{\mu_c-0}\left[\mathrm{d}c_1\mathrm{d}c_2 \times \mathrm{d}y\right] := \delta(c_1)\delta(c_2)\,\mathrm{d}c_1\mathrm{d}c_2\,\delta(y-y_{\mu_c-0})\,\mathrm{d}y \tag{4.18}$$

and

$$\begin{aligned}\mathbb{K}_{\mu_c+0}&\left[\mathrm{d}c_1\mathrm{d}c_2 \times \mathrm{d}y\right] \\ &:= \int_0^{2\pi}\frac{\mathrm{d}\theta}{2\pi}\delta(c_1-\sqrt{x_{\mu_c+0}}\cos\theta)\delta(c_2-\sqrt{x_{\mu_c+0}}\sin\theta)\,\mathrm{d}c_1\mathrm{d}c_2\,\delta(y-y_{\mu_c+0})\,\mathrm{d}y \end{aligned} \tag{4.19}$$

correspond to extreme points ρ_- and ρ_+. Varying γ from $-\infty$ to $+\infty$, one scans over mixture of coexisting extreme Gibbs states $\langle - \rangle_{\rho_\mp}(\beta, \mu_c)$:

$$\langle - \rangle_{\rho(\gamma)}(\beta, \mu_c) = \xi_\gamma \langle - \rangle_{\rho_-}(\beta, \mu_c) + (1-\xi_\gamma)\langle - \rangle_{\rho_+}(\beta, \mu_c) \tag{4.20}$$

with the total particle density $\rho(\gamma) = \xi_\gamma \rho_- + (1-\xi_\gamma)\rho_+ \in [\rho_-, \rho_+]$.

Proof Since for $\rho_+ > \rho_-$ the rate function $\mathrm{K}_{\mu_c}(x,y)$ has two degenerate distinct minima at the points $(0,\rho_-)$ and $(x_{\rho_+} := x_{\mu_c+0}, y_{\rho_+} := y_{\mu_c+0})$, we take $\varepsilon \in (0, x_{\rho_+}) \cap (0, y_{\rho_+} - \rho_-)$ and define in $\mathbb{R}_+^2$ two subsets:

$$\mathcal{A}_- := \{c \in \mathbb{C} : |c|^2 \in (0, x_{\rho_+} - \varepsilon]\} \times (\rho_-, y_{\rho_+} - \varepsilon]$$

and

$$\mathcal{A}_+ := \{c \in \mathbb{C} : |c|^2 \in (x_{\rho_+} - \varepsilon, +\infty)\} \times (y_{\rho_+} - \varepsilon, +\infty).$$

By $\mathrm{K}_{\mu_c^-}$ and $\mathrm{K}_{\mu_c^+}$ we define the restrictions of K_{μ_c} onto $\mathcal{A}_-$ and $\mathcal{A}_+$. Now we see that $\mathrm{K}_{\mu_c^-}$ and $\mathrm{K}_{\mu_c^+}$ have both unique minimizers, respectively at $(0,\rho_-)$ and at (x_{ρ_+}, y_{ρ_+}). Let us define on $\mathbb{R}_+^2$ two probability measures:

$$\mathbb{L}_\Lambda^-[\mathcal{A}] := \frac{\mathbb{K}_{\Lambda,\mu_c}[\mathcal{A} \cap \mathcal{A}_-]}{\mathbb{K}_{\Lambda,\mu_c}[\mathcal{A}_-]} \quad \text{and} \quad \mathbb{L}_\Lambda^+[\mathcal{A}] := \frac{\mathbb{K}_{\Lambda,\mu_c}[\mathcal{A} \cap \mathcal{A}_+]}{\mathbb{K}_{\Lambda,\mu_c}[\mathcal{A}_+]},$$

which satisfy the LDP respectively with rate functions $\mathrm{K}_{\mu_c^-}$ and $\mathrm{K}_{\mu_c^+}$. Take a positive continuous function $\varphi(c,y) : \mathbb{C} \times \mathbb{R}_+ \mapsto \mathbb{R}_+$ and remark that

$$\begin{aligned}
&\int_{\mathbb{R}_+^2} \varphi(c,y)\, \mathbb{K}_{\Lambda,\tilde{\mu}_c(\Lambda)}\left[\mathrm{d}c_1 \mathrm{d}c_2 \times \mathrm{d}y\right] \\
&\quad = \frac{\int_{\mathbb{C}} \mathrm{d}^2 c \int_{\mathbb{R}_+} \nu_\Lambda(\mathrm{d}y) \varphi(c,y) e^{\beta V(\tilde{\mu}_c(y+|c|^2) - f_\Lambda^{SB}(\beta,y,c))}}{\int_{\mathbb{C}} \mathrm{d}^2 c \int_{\mathbb{R}_+} \nu_\Lambda(\mathrm{d}y) e^{\beta V(\tilde{\mu}_c(\Lambda)(y+|c|^2) - f_\Lambda^{SB}(\beta,y,c))}} = \Phi_\Lambda^- + \Phi_\Lambda^+,
\end{aligned}$$

where

$$\Phi_\Lambda^- := \frac{\int_{\mathcal{A}_-} \varphi(c,y) e^{\{\gamma+o(1)\}(y+|c|^2)} \mathbb{L}_\Lambda^-[\mathrm{d}c_1 \mathrm{d}c_2 \times \mathrm{d}y]}{\int_{\mathcal{A}_-} e^{\{\gamma+o(1)\}(y+|c|^2)} \mathbb{L}_\Lambda^-[\mathrm{d}c_1 \mathrm{d}c_2 \times \mathrm{d}y] + \Theta_\Lambda \int_{\mathcal{A}_+} e^{\{\gamma+o(1)\}(y+|c|^2)} \mathbb{L}_\Lambda^+[\mathrm{d}c_1 \mathrm{d}c_2 \times \mathrm{d}y]},$$

$$\Phi_\Lambda^+ := \frac{\int_{\mathcal{A}_+} \varphi(c,y) e^{\{\gamma+o(1)\}(y+|c|^2)} \mathbb{L}_\Lambda^+[\mathrm{d}c_1 \mathrm{d}c_2 \times \mathrm{d}y]}{\Theta_\Lambda^{-1} \int_{\mathcal{A}_-} e^{\{\gamma+o(1)\}(y+|c|^2)} \mathbb{L}_\Lambda^-[\mathrm{d}c_1 \mathrm{d}c_2 \times \mathrm{d}y] + \int_{\mathcal{A}_+} e^{\{\gamma+o(1)\}(y+|c|^2)} \mathbb{L}_\Lambda^+[\mathrm{d}c_1 \mathrm{d}c_2 \times \mathrm{d}y]},$$

and

$$\Theta_\Lambda := \frac{\int_{\mathcal{A}_+} \mathrm{d}^2 c\, \nu_\Lambda(\mathrm{d}y) e^{\beta V\{\mu_c(y+|c|^2) - f_\Lambda^{SB}(\beta,y,c)\}}}{\int_{\mathcal{A}_-} \mathrm{d}^2 c\, \nu_\Lambda(\mathrm{d}y) e^{\beta V\{\mu_c(y+|c|^2) - f_\Lambda^{SB}(\beta,y,c)\}}}. \tag{4.21}$$

By Lemma 5.2 the sequence $\{\mu_c(y+|c|^2) - f_\Lambda^{SB}(\beta,y,c)\}_\Lambda$ converges in the thermodynamic limit to the function

$$\mu_c(y+|c|^2) - f_0^B\left(\beta, y, |c|^2\right) - \frac{\lambda}{2}\left(y+|c|^2\right)^2,$$

which has degenerate suprema at $(0, \rho_-)$ and $(e^{i\theta}x_{\rho_+}, y_{\rho_+})$ for any $\theta \in [0, 2\pi]$. Consequently, in the thermodynamic limit we obtain for coefficient (4.21): $\lim_\Lambda \Theta_\Lambda = 1$. Since $\rho_+ = y_{\rho_+} + x_{\rho_+}$, then by the LDP for the measures $\mathbb{L}_\Lambda^\mp$ one gets that

$$\lim_\Lambda \Phi_\Lambda^- = \xi_\gamma \varphi(0, \rho_-) \quad \text{and} \quad \lim_\Lambda \Phi_\Lambda^+ = (1-\xi_\gamma) \int_0^{2\pi} \frac{d\theta}{2\pi} \varphi(\sqrt{x_{\rho_+}} e^{i\theta}, y_{\rho_+}).$$

Applying these results to the function $\varphi(c, y) = e^{-t(c+y)}$ with $t > 0$, by bijectivity of the probability measures and its Laplace transformation, one concludes that Kac distributions $\{\mathbb{K}_{\Lambda,\tilde{\mu}_c(\Lambda)}\}_\Lambda$ converge weakly on the set of measures $\mathcal{M}_1(\mathbb{C} \times \mathbb{R}_+)$ to (4.17).

Notice that the function $\xi_\gamma : \mathbb{R} \to (0, 1)$ is strictly decreasing. Therefore, by integrating $\varphi(c, y) = |c|^2 + y$ with the measures $\mathbb{K}_{\Lambda,\tilde{\mu}_c(\Lambda)}$ we obtain that the particle density in the Gibbs state (4.20) can converge to any fixed density in the open set (ρ_-, ρ_+):

$$\lim_\Lambda \left\langle \frac{N_\Lambda}{V} \right\rangle_{H^{SB}_{\Lambda,\lambda}} (\beta, \tilde{\mu}_c(\Lambda)) = \xi_\gamma \rho_- + \left(1 - \xi_\gamma\right) \rho_+, \tag{4.22}$$

and

$$\rho_\mp = \lim_{\gamma \to \mp\infty} \left\{\xi_\gamma \rho_- + (1-\xi_\gamma)\rho_+\right\}. \tag{4.23}$$

In particular, one obtains these results if in (4.1) we put the coefficient $\gamma = \gamma_\Lambda = \mp o(V)$. □

4.2 Generalized Kac Distribution and Particle Density Parameter

Here we give some additional comments about the concept of the total particle density as a parameter that defines the grand-canonical ensemble. Theorem 3.1 and Theorem 3.2 are direct consequences respectively of Theorem 4.2 and Corollary 4.3 for the chemical potential μ_ρ defined as the thermodynamic limit of $\overline{\mu}_\Lambda(\beta, \rho)$ (2.13). The only remaining question is to study the case of fixed particle densities at the point of phase transition, i.e. in domain: $\rho \in (\rho_-, \rho_+)$ for $\rho_+ > \rho_-$. From (4.22), we obtain that

$$\lim_\Lambda \left\langle \frac{N_\Lambda}{V} \right\rangle_{H^{SB}_{\Lambda,\lambda}} (\beta, \tilde{\mu}_c(\Lambda)) = \rho \in (\rho_-, \rho_+)\,,$$

for chemical potentials:

$$\tilde{\mu}_c(\Lambda) = \mu_c(\beta) + \frac{\gamma_\rho}{\beta V} + o\left(\frac{1}{\beta V}\right) \quad \text{with } \gamma_\rho := \frac{1}{\rho_+ - \rho_-} \ln\left(\frac{\rho - \rho_-}{\rho_+ - \rho}\right), \tag{4.24}$$

cf. (4.1). Therefore,

$$\overline{\mu}_\Lambda(\beta, \rho) = \mu_c(\beta) + \frac{\gamma_\rho}{\beta V} + o\left(\frac{1}{\beta V}\right).$$

In particular, from Theorem 4.4 with $\gamma = \gamma_\rho$ we get Theorem 3.3 for $\rho \in (\rho_-, \rho_+)$. Recall also (4.23). In other words, if $\rho = \rho_-$ then $\gamma_\rho < 0$ ($|\gamma_\rho| = o(V)$) would diverge to $-\infty$, whereas if $\rho = \rho_+$ then $\gamma_\rho = o(V) \to +\infty$. It follows that Theorem 3.3 is proven for any $\rho \in [\rho_-, \rho_+]$.

Acknowledgements We are most grateful to Joel Lebowitz for interest to this project, for his help and inspiring discussions. We also wish to thank him for hospitality extended to us in the Rutgers University (NJ) that allowed to discuss different aspects of the paper. The present version of the manuscript was finalized during the J.-B. Bru visit of the Centre de Physique Théorique–Luminy UMR-6207. He is thankful to Pierre Duclos for this invitation to CPT.

Appendix

In this appendix, we first establish some auxiliary results that we need for the proof of Theorems 4.2 and 4.4. Next, for the reader convenience, we shortly recall some basic notions of Large Deviation Principle (LDP).

Some Technical Statements and Proofs

The thermodynamic limit of $p_\Lambda^{SB}(\beta,\mu,c)$ (3.4) is first analyzed in order to obtain next the one of the free-energy density $f_\Lambda^{SB}(\beta,y,c)$ (4.4), which is given in Lemma 5.2.

Lemma 5.1 (Thermodynamic limit of the pressure $p_\Lambda^{SB}(\beta,\mu,c)$) *For any $c\in\mathbb{C}$, $\mu\in\mathbb{R}$ and $\beta>0$, the pressure $p_\Lambda^{SB}(\beta,\mu,c)$ converges towards*

$$p^{SB}(\beta,\mu,c):=\lim_{\Lambda} p_\Lambda^{SB}(\beta,\mu,c)=\inf_{\alpha\le 0}\left\{p_0^B(\beta,\alpha,x)+\frac{(\mu-\alpha)^2}{2\lambda}\right\}.$$

Here $x=|c|^2\ge 0$ and recall that $p_0^B(\beta,\alpha,x)$ is defined in (2.8), cf. also (4.7).

Proof The proof is obtained by a comparison between suitable lower and upper bounds for $p_\Lambda^{SB}(\beta,\mu,c)$. We start by the lower bound. By taking any orthonormal basis $\{\langle\psi_n'|\}_{n=1}^\infty$ of $\mathcal{F}_\Lambda'$,

$$\mathrm{Tr}_{\mathcal{F}_\Lambda'}\left\{W_{\Lambda,\mu}(c)\right\}=\sum_{n=1}^{\infty}\left\langle c\otimes\psi_n'\right|e^{-\beta(H_{\Lambda,\lambda}^{SB}-\mu N_\Lambda)}\left|c\otimes\psi_n'\right\rangle,$$

and so, by the Peierls-Bogoliubov inequality we get

$$\begin{aligned}\mathrm{Tr}_{\mathcal{F}_\Lambda'}\left\{W_{\Lambda,\mu}(c)\right\}&\ge\sup_{\{\psi_n'\}_{n=1}^\infty}\left\{\sum_{n=1}^{\infty}e^{-\beta\langle c\otimes\psi_n'|H_{\Lambda,\lambda}^{SB}-\mu N_\Lambda|c\otimes\psi_n'\rangle}\right\}\\&=\mathrm{Tr}_{\mathcal{F}_\Lambda'}\left\{e^{-\beta H_{\Lambda,\lambda}^{SB}(c,\mu)}\right\},\end{aligned}\tag{5.1}$$

see e.g. [17, 18], where $H_{\Lambda,\lambda}^{SB}(c,\mu)$ results from the Bogoliubov approximation (3.1) of $\{H_{\Lambda,\lambda}^{SB}-\mu N_\Lambda\}$. From [9] we already know that

$$\lim_{\Lambda}\frac{1}{\beta V}\ln\mathrm{Tr}_{\mathcal{F}_\Lambda'}\left\{e^{-\beta H_{\Lambda,\lambda}^{SB}(c,\mu)}\right\}=\inf_{\alpha\le 0}\left\{p_0^B(\beta,\alpha,|c|^2)+\frac{(\mu-\alpha)^2}{2\lambda}\right\}.\tag{5.2}$$

Consequently, the inequality (5.1) implies in the thermodynamic limit the lower bound

$$p^{SB}(\beta,\mu,c)\ge\inf_{\alpha\le 0}\left\{p_0^B(\beta,\alpha,|c|^2)+\frac{(\mu-\alpha)^2}{2\lambda}\right\},\tag{5.3}$$

for any $c \in \mathbb{C}$, $\mu \in \mathbb{R}$ and $\beta > 0$.

To obtain an upper bound on $p^{SB}(\beta, \mu, c)$, we follow the idea of [16], and use the coherent state representation of $\{H^{SB}_{\Lambda,\lambda} - \mu N_\Lambda\}$ given by

$$H^{SB}_{\Lambda,\lambda} - \mu N_\Lambda = \int_{\mathbb{C}} \mathrm{d}^2 c \left\{ \hat{H}^{SB}_{\Lambda,\lambda}(c, \mu) \left| c \right\rangle \left\langle c \right| \right\},$$

where the Hamiltonian $\hat{H}^{SB}_{\Lambda,\lambda}(c, \mu)$ is defined on $\mathcal{F}'_\Lambda$ by

$$\hat{H}^{SB}_{\Lambda,\lambda}(c, \mu) := H^{SB}_{\Lambda,\lambda}(c, \mu) + \Delta,$$

with

$$\Delta := \mu - 2\lambda |c|^2 + \frac{\lambda}{V} - \frac{1}{V} \sum_{k \in \Lambda^* \setminus \{0\}} (\lambda + \lambda_k)\, a_k^* a_k. \tag{5.4}$$

Actually, $\hat{H}^{SB}_{\Lambda,\lambda}(c, \mu)$ is derived by replacing the operators $a_0^* a_0$, $a_0 a_0$, $a_0^* a_0^*$, and $a_0^* a_0^* a_0 a_0$ in $\{H^{SB}_{\Lambda,\lambda} - \mu N_\Lambda\}$ respectively by $|Vc|^2 - 1$, Vc^2, $V\bar{c}^2$ and $V^2|c|^4 - 4V|c|^2 + 2$. Let $\{\langle \psi'_n(c)|\}_{n=1}^\infty$ be an orthonormal basis of eigenvectors of $\hat{H}^{SB}_{\Lambda,\lambda}(c, \mu)$. Since for any $z, c \in \mathbb{C}$

$$\langle z | c \rangle = e^{-\frac{1}{2}\{(\bar{z}-\bar{c})(z-c)+\bar{c}z-\bar{z}c\}},$$

it follows that

$$\begin{aligned}
\mathrm{Tr}_{\mathcal{F}'_\Lambda}\left\{W_{\Lambda,\mu}(c)\right\} &= \sum_{n=1}^{\infty} \langle c \otimes \psi'_n(c) | e^{-\beta \int_{\mathbb{C}} \mathrm{d}^2 z \hat{H}^{SB}_{\Lambda,\lambda}(z,\mu)|z\rangle\langle z|} | c \otimes \psi'_n(c) \rangle \\
&= \sum_{n=1}^{\infty} \left\{ 1 + \sum_{m=1}^{\infty} \frac{(-\beta)^m}{m!} \int_{\mathbb{C}^m} \mathrm{d}^2 z_1 \cdots \mathrm{d}^2 z_m \right. \\
&\quad \times e^{-\frac{V}{2}\{\mathrm{R}_m(z_1,\ldots,z_m) + i \mathrm{I}_m(z_1,\ldots,z_m)\}} \\
&\quad \left. \times \prod_{j=1}^{m} \langle \psi'_n(c) | \hat{H}^{SB}_{\Lambda,\lambda}(z_j, \mu) | \psi'_n(c) \rangle \right\},
\end{aligned} \tag{5.5}$$

with the two real-valued functions R_m and I_m of $(z_1, \ldots, z_m) \in \mathbb{C}^m$ defined by

$$\mathrm{R}_m(z_1, \ldots, z_m) := |z_1 - c|^2 + \sum_{j=1}^{m} \left| z_{j-1} - z_j \right|^2 + |z_m - c|^2,$$

$$\mathrm{I}_m(z_1, \ldots, z_m) := i\,(\bar{z}_1 c - \bar{c} z_1) + i \sum_{j=1}^{m} \left(\bar{z}_j z_{j-1} - \bar{z}_{j-1} z_j \right) + i\,(\bar{c} z_m - \bar{z}_m c).$$

Since $\mathrm{I}_m(c, \ldots, c) = 0$ and

$$\inf_{(z_1,\ldots,z_m)\in\mathbb{C}^m} \mathrm{R}_m(z_1, \ldots, z_m) = \mathrm{R}_m(c, \ldots, c) = 0,$$

by virtue of (5.5) combined with large deviations arguments, one can obtain in the thermodynamic limit that

$$p^{SB}(\beta, \mu, c) = \lim_{\Lambda} \frac{1}{\beta V} \ln \mathrm{Tr}_{\mathcal{F}'_\Lambda} \left\{ e^{-\beta \hat{H}^{SB}_{\Lambda,\lambda}(c,\mu)} \right\}. \tag{5.6}$$

Justification of the LD technique in sums (5.5) is based on the *Lebesgue domination* theorem and it follows the line of reasoning developed in [16]. Meanwhile, by using the Bogoliubov convexity inequality [6] it follows that

$$\mathrm{Tr}_{\mathcal{F}'_\Lambda}\left\{e^{-\beta \hat{H}^{SB}_{\Lambda,\lambda}(c,\mu)}\right\} \leq \frac{1}{\beta V}\ln \mathrm{Tr}_{\mathcal{F}'_\Lambda}\left\{e^{-\beta H^{SB}_{\Lambda,\lambda}(c,\mu)}\right\} - \frac{1}{V}\left\langle \Delta\right\rangle_{\hat{H}^{SB}_{\Lambda,\lambda}(c,\mu)}, \tag{5.7}$$

where

$$\langle - \rangle_{\hat{H}^{SB}_{\Lambda,\lambda}(c,\mu)} := \frac{\mathrm{Tr}_{\mathcal{F}'_\Lambda}\{-e^{-\beta \hat{H}^{SB}_{\Lambda,\lambda}(c,\mu)}\}}{\mathrm{Tr}_{\mathcal{F}'_\Lambda}\{e^{-\beta \hat{H}^{SB}_{\Lambda,\lambda}(c,\mu)}\}}.$$

In particular, since by our assumption (B) on the interaction potential one has: $0 \leq \lambda_k \leq \lambda_0$ for $k \in \mathbb{R}^3$, the inequality (5.7) together with (5.4) yields

$$\begin{aligned}\frac{1}{\beta V}\ln \mathrm{Tr}_{\mathcal{F}'_\Lambda}\left\{e^{-\beta \hat{H}^{SB}_{\Lambda,\lambda}(c,\mu)}\right\} &\leq \frac{1}{\beta V}\ln \mathrm{Tr}_{\mathcal{F}'_\Lambda}\left\{e^{-\beta H^{SB}_{\Lambda,\lambda}(c,\mu)}\right\} \\ &\quad + \frac{2|c|^2\lambda - \mu}{V} - \frac{\lambda}{V^2} + \frac{\lambda+\lambda_0}{V^2}\sum_{k\in\Lambda^*\backslash\{0\}}\left\langle a_k^* a_k\right\rangle_{\hat{H}^{SB}_{\Lambda,\lambda}(c,\mu)}. \end{aligned} \tag{5.8}$$

The last term can be explicitly computed. We omit the details. In fact, for any $\mu \in \mathbb{R}$ one can check that

$$\frac{1}{V}\sum_{k\in\Lambda^*\backslash\{0\}}\left\langle a_k^* a_k\right\rangle_{\hat{H}^{SB}_{\Lambda,\lambda}(c,\mu)} = O(1) \quad \text{as } \Lambda \uparrow \mathbb{R}^3.$$

Therefore, from (5.8) together with (5.2) and (5.6) one deduces that

$$p^{SB}(\beta,\mu,c) \leq \inf_{\alpha\leq 0}\left\{p_0^B(\beta,\alpha,|c|^2) + \frac{(\mu-\alpha)^2}{2\lambda}\right\}.$$

Together with the lower bound (5.3), this inequality proves the lemma. □

Lemma 5.2 (Thermodynamic limit of $f_\Lambda^{SB}(\beta,y,c)$) *For any $c \in \mathbb{C}$, $y \geq 0$ and $\beta > 0$, the thermodynamic limit $f^{SB}(\beta,y,c)$ of the free-energy density $f_\Lambda^{SB}(\beta,y,c)$ (4.4) equals*

$$f^{SB}(\beta,y,c) := \lim_{\Lambda} f_\Lambda^{SB}(\beta,y,c) = f_0^B(\beta,y,x) + \frac{\lambda}{2}(y+x)^2, \tag{5.9}$$

with $x = |c|^2 \geq 0$, and $f_0^B(\beta,y,x)$ defined as the Legendre-Fenchel transform of $p_0^B(\beta,\alpha,x)$ (2.8), cf. Theorem 4.2.

Proof The pressure $p_\Lambda^{SB}(\beta,\mu,c)$ (3.4) can be rewritten as

$$p_\Lambda^{SB}(\beta,\mu,c) = \frac{1}{\beta V}\ln\int_{\mathbb{R}_+} e^{\beta V(\mu y - f_\Lambda^{SB}(\beta,y,c))}\nu_\Lambda(\mathrm{d}y) + \mu|c|^2,$$

with $\nu_\Lambda(\mathrm{d}y)$ defined in (4.3). It is then straightforward to check that the thermodynamic limit $p^{SB}(\beta,\mu,c)$ of $p_\Lambda^{SB}(\beta,\mu,c)$ (3.4) equals

$$p^{SB}(\beta,\mu,c) = \sup_{y\geq 0}\left\{\mu y - f^{SB}(\beta,y,c)\right\} + \mu|c|^2,$$

with $f^{SB}(\beta, y, c) < \infty$ for $y \geq 0$. The derivative of the pressure $p^{SB}(\beta, \mu, c)$ is continuous as a function of μ, cf. Lemma 5.1 and (4.7). Thus, by using the *Tauberien theorem* proven in [19], the existence of $p^{SB}(\beta, \mu, c)$ already implies the convexity of $f^{SB}(\beta, y, c)$ as a function of $y \geq 0$. In particular, it yields that

$$f^{SB}(\beta, y, c) = \sup_{\mu \in \mathbb{R}} \left\{ \mu(y + |c|^2) - p^{SB}(\beta, \mu, c) \right\} \quad \text{for } y \geq 0. \tag{5.10}$$

By using the explicit form of $p^{SB}(\beta, \mu, c)$, given by Lemma 5.1, a straightforward computation then gives:

$$f^{SB}(\beta, y, c) = \sup_{\alpha \leq 0} \left\{ \alpha(y + |c|^2) - p_0^B(\beta, \alpha, |c|^2) \right\} + \frac{\lambda}{2}(y + x)^2,$$

which proves the assertion (5.9). □

Large Deviation Principle (LDP)

Let $\mathcal{X}$ denote a complete separable metric vector space. A lower semi-continuous function $\mathrm{I} : \mathcal{X} \to [0, \infty]$ is called a *rate* function, if I is not identical ∞ and has compact level sets, i.e. if $\mathrm{I}^{-1}([0, m]) = \{x \in \mathcal{X} : \mathrm{I}(x) \leq m\}$ is compact for any $m \geq 0$ (LD1). A sequence $\{X_l\}_{l=1}^{\infty}$ of $\mathcal{X}$-valued random variables X_l or the corresponding sequence $\{\mathbb{P}_l\}_{l=1}^{\infty}$ of probability measures on the Borel subsets of $\mathcal{X}$ satisfy the large deviations *upper* bound (LD2) for the sequence a_l and rate function I if, for any closed subset $\mathcal{C}$ of $\mathcal{X}$,

$$\limsup_{l \to \infty} \frac{1}{a_l} \ln \mathbb{P}_l (X_l \in \mathcal{C}) = \limsup_{l \to \infty} \frac{1}{a_l} \ln \mathbb{P}_l (\mathcal{C}) \leq - \inf_{\mathcal{C}} \mathrm{I}(x), \tag{5.11}$$

and they satisfy the large deviations *lower* bound (LD3) if, for any open subset $\mathcal{G}$ of $\mathcal{X}$,

$$\liminf_{l \to \infty} \frac{1}{a_l} \ln \mathbb{P}_l (X_l \in \mathcal{G}) = \liminf_{l \to \infty} \frac{1}{a_l} \ln \mathbb{P}_l (\mathcal{G}) \geq - \inf_{\mathcal{G}} \mathrm{I}(x). \tag{5.12}$$

If both, upper and lower bound, are satisfied, one says that $\{X_l\}_{l=1}^{\infty}$ or $\{\mathbb{P}_l\}_{l=1}^{\infty}$ satisfy a *Large Deviation Principle* (LDP). The LDP is called *weak*, if the upper bound in (5.11) holds only for compact sets $\mathcal{C}$. This notion easily extends to the situation where the distribution of X_l is not normalized, but a sub-probability distribution only. Observe also that one of the most important conclusions from a LDP is the *Varadhan* lemma, which says that, for any bounded and continuous function $\varphi : \mathcal{X} \to \mathbb{R}$,

$$\lim_{l \to \infty} \frac{1}{a_l} \ln \int \exp(a_l \varphi(X_l)) \mathrm{d}\mathbb{P} = - \inf_{x \in \mathcal{X}} \{\mathrm{I}(x) - \varphi(x)\}.$$

For the main results and a comprehensive treatment of the theory of large deviations, see e.g. [20].

References

1. Lewis, J.T., Pulé, J.V., Zagrebnov, V.A.: The large deviation principle for the Kac distribution. Helv. Phys. Acta **61**, 1063–1078 (1988)

2. Lebowitz, J.L., Lenci, M., Spohn, H.: Large deviations for ideal quantum systems. J. Math. Phys. **41**, 1224–1243 (2000)
3. Gallavotti, G., Lebowitz, J.L., Mastropietro, V.: Large deviations in rarefied quantum gases. J. Stat. Phys. **108**(5–6), 831–861 (2002)
4. Angelescu, N., Verbeure, A., Zagrebnov, V.A.: On Bogoliubov's model of superfluidity. J. Phys. A Math. Gen. **25**, 3473–3491 (1992)
5. Bru, J.-B., Zagrebnov, V.A.: On condensations in the Bogoliubov Weakly Imperfect Bose-Gas. J. Stat. Phys. **99**, 1297 (2000)
6. Zagrebnov, V.A., Bru, J.-B.: The Bogoliubov model of Weakly Imperfect Bose Gas. Phys. Rep. **350**, 291–434 (2001)
7. Angelescu, N., Verbeure, A., Zagrebnov, V.A.: Superfluidity III. J. Phys. A Math. Gen. **30**, 4895–4913 (1997)
8. Adams, S., Bru, J.-B.: Critical analysis of the Bogoliubov theory of superfluidity. Physica A **332**, 60–78 (2004)
9. Adams, S., Bru, J.-B.: Exact solution of the AVZ-Hamiltonian in the grand canonical ensemble. Ann. Henri Poincaré **5**, 405–434 (2004)
10. Adams, S., Bru, J.-B.: A new microscopic theory of superfluidity at all temperatures. Ann. Henri Poincaré **5**, 435–476 (2004)
11. Bru, J.-B.: Beyond the dilute Bose gas. Physica A **359**, 306–344 (2006)
12. Bogoliubov, N.N.: On the theory of superfluidity. J. Phys. (Mosc.) **11**, 23–32 (1947)
13. Brattelli, O., Robinson, D.W.: Operator Algebras and Quantum Statistical Mechanics, vol. II, 2nd edn. Springer, New York (1996)
14. Ruelle, D.: Statistical Mechanics: Rigorous Results. Benjamin, New York (1969)
15. Ginibre, J.: On the asymptotic exactness of the Bogoliubov approximation for many Bosons systems. Commun. Math. Phys. **8**, 26–51 (1968)
16. Lieb, E.H., Seiringer, R., Yngvason, J.: Justification of c-number substitutions in Bosonic Hamiltonians. Phys. Rev. Lett. **94**, 080401 (2005)
17. Reed, M., Simon, B.: Methods of Modern Mathematical Physics. Functional Analysis, vol. I. Academic Press, New York (1972)
18. Simon, B.: The Statistical Mechanics of Lattice Gases, vol. I. Princeton Univ. Press, Princeton (1993)
19. Minlos, R.A., Povzner, A.Ja.: Thermodynamic limit for entropy. Trans. Mosc. Math. Soc. **17**, 269 (1967)
20. Dembo, A., Zeitouni, O.: Large Deviations Techniques and Applications, 2nd edn. Springer, New York (1998)