Large Deviations in the Superstable Weakly Imperfect Bose Gas

J.-B. Bru[a] and V.A. Zagrebnov[b]

[a] *Fakultät für Physik, Universität Wien, Boltzmanngasse 5, 1090 Vienna, Austria*
[b] *Université Aix-Marseille II and Centre de Physique Théorique - UMR 6207*
Luminy-Case 907, F-13288 Marseille, Cedex 09, France

Abstract

The superstable Weakly Imperfect Bose Gas (WIBG) was originally derived to solve the inconsistency of the Bogoliubov theory of superfluidity. Its grand-canonical thermodynamics was recently solved but not at point of the (first order) phase transition. This paper proposes to close this gap by using the large deviations formalism and in particular the analysis of the Kac distribution function. It turns out that, as a function of the chemical potential, the discontinuity of the Bose condensate density at the phase transition point disappears as a function of the particle density. Indeed, the Bose condensate continuously starts at the first critical particle density and progressively grows but the free-energy per particle stays constant until the second critical density is reached. At higher particle densities, the Bose condensate density as well as the free-energy per particle both increase monotonously.

Keywords : WIBG, Bose-Einstein condensation, Kac distribution, large deviations, equivalence of ensembles.

1. Introduction

The proof of large deviations for the distribution of the particle density (the Kac distribution) in the Perfect and in the Mean-Field Bose gases goes back to [1]. In recent papers [2, 3], the authors addressed to the large deviations in the particle density in a sub-domain both for the perfect and for rarified quantum gases (Fermi or Bose). In the present paper we extend the study of Large Deviations (LD) principle to the superstable Weakly Imperfect Bose Gas (WIBG) [4], known also as the Superstable Bogoliubov model [5]. The study of this model started in [4, 6] was recently completed in [7, 9, 10, 8].

Actually, this model originates from a *weaker truncation* than that of the Bogoliubov one in the grand-canonical ensemble. This new system served to solve some inconsistencies between the grand-canonical Bogoliubov theory of superfluidity and the WIBG description. This non-diagonal boson model was rigorously solved on the thermodynamic level for the grand-canonical ensemble in [8, 10]. It turns out that similar to the WIBG it manifests a phase transition with a *non-conventional* Bose condensation at high densities ρ or high inverse temperatures β. Meantime, even for $\beta \uparrow +\infty$, i.e. at a zero-temperature, only a fraction of the full density is in the condensate: i.e. there is a *coexistence* of particles inside and outside the boson condensate. This last phenomenon is known as *depletion* of the condensate. More interesting for our analysis is a discontinuity of the particle density from $\rho_- > 0$ to $\rho_+ > \rho_-$ related to a strictly positive jump of the condensate density at the phase transition defined by a fixed chemical potential μ_c. This *first-order* phase transition as a function of the chemical potential μ sounds unusual and seems to be not quite clear as far as it concerns its physical relevance.

In fact, the grand-canonical thermodynamics of the superstable WIBG is *unknown* at the point of coexistence of the low- and high-density phases. This paper proposes to close this gap using large deviations techniques description of the density distribution. For instance to answer the question, what is the value of the Bose condensate density when $\rho \in [\rho_-, \rho_+]$? In fact several scenarios are possible. Since this phase transition is characterized by the appearance of a non-conventional Bose condensation, which is due to particle interaction, a naive thought might be that there is no condensate at all in domain $\rho \in (\rho_-, \rho_+)$, i.e. the condensate density jumps from zero to a strictly positive value for $\rho > \rho_+$. In fact this scenario is *wrong*. Here we show that this discontinuity is a subtle function of the total particle density ρ. Formally, at the point of the phase coexistence, the corresponding quantum Gibbs state of the model is no more a pure state [11] but instead, a convex combination of some of them. A similar observation was made for example in Section 4 of [1].

Actually, we verify LD for the Bose condensate density for any given particle densities ρ in the grand-canonical ensemble, i.e. even at the point of the phase transition. A direct consequence of this study is a rigorous proof that the discontinuity of the Bose condensate and its depletion, visible as a function of the chemical potential μ, does not appear in the same grand-canonical ensemble if it is considered as a function of the total particle density $\rho > 0$. We show that the Bose condensate density continuously increases with $\rho > 0$. In others words, there is no jump and the phase transition in $\rho > 0$ is of the second order. When the particle density ρ (or the inverse temperature β) exceeds the first critical value ρ_-, the Bose condensate density continuously grows but the free-energy per particle, i.e., the corresponding chemical potential μ_ρ, stays constant: $\mu_\rho = \mu_c$ in domain: $\rho \in [\rho_-, \rho_+]$. At higher particle densities (or inverse temperatures β), the Bose condensate as well as the free-energy per particle $\mu_\rho > \mu_c$ both increase when $\rho > \rho_+$.

The structure of the paper is the following. In Section 2 we briefly review the grand-canonical thermodynamics of the superstable WIBG for a given particle density ρ. Our main results are formulated in Section 3. The proofs are collected in Section 4. For the reader convenience, we collect in Appendix (Section 5) some technical results as well as a short review on the LD principles.

To conclude, we 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 $\langle - \rangle_{H_\Lambda}$ for (*finite-volume*) grand-canonical Gibbs state corresponding to the Hamiltonian H_Λ.

2. The Superstable Weakly Imperfect Bose Gas

2.1 The Hamiltonian [4]

Let an homogeneous gas of n spinless bosons with mass m be enclosed in a cubic box $\Lambda \subset \mathbb{R}^3$ of volume $V := |\Lambda|$. The one-particle energy spectrum is then $\varepsilon_k := \hbar^2 k^2/2m$ and, using periodic boundary conditions, $\Lambda^* := (2\pi\mathbb{Z}/V^{1/3})^3 \subset \mathbb{R}^3$ is the set of wave vectors k. The considered system is with interactions defined via a (real) two-body soft potential $\varphi(x) = \varphi(||x||)$ such that:

(A) $\varphi(x) \in L^1(\mathbb{R}^3)$ (absolute integrability).

(B) Its (real) Fourier transformation $\lambda_k = \lambda_{||k||}$ satisfies: $\lambda_0 > 0$ and $0 \leq \lambda_k \leq \lambda_0$ for $k \in \mathbb{R}^3$.

The Superstable WIBG (also known as the AVZ Hamiltonian [8] or the Superstable Bogoliubov Hamiltonian [7]), was proposed for the first time in [4]. It is defined by

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

Here the weakly imperfect Bose gas

$$H^B_{\Lambda,0} := \sum_{k\in\Lambda^*\backslash\{0\}} \left\{ \varepsilon_k a_k^* a_k + \frac{\lambda_k}{2}\left(\frac{a_0^* a_0}{V}\left(a_k^* a_k + a_{-k}^* a_{-k}\right) + a_k^* a_{-k}^* \frac{a_0^2}{V} + \frac{a_0^{*2}}{V} a_k a_{-k} \right) \right\} \tag{2.2}$$

contains the kinetic-energy term* plus diagonal and non-diagonal interactions. It is solved in the canonical ensemble in [9, 10]. The repulsive interaction ensuring the superstability of $H^{SB}_{\Lambda,\lambda_0}$ by assumptions (A)-(B) is the "forward scattering" interaction

$$U^{MF}_\Lambda := \frac{\lambda_0}{2V} \sum_{k_1,k_2\in\Lambda^*} a_{k_1}^* a_{k_2}^* a_{k_2} a_{k_1} = \frac{\lambda_0}{2V}\left(N_\Lambda^2 - N_\Lambda\right), \text{ with } N_\Lambda := \sum_{k\in\Lambda^*} a_k^* a_k \tag{2.3}$$

defined as the particle-number operator within the grand-canonical framework. Indeed, a_k^* and a_k are the usual boson creation / annihilation operators in the one-particle state† $\chi_\Lambda(x) e^{ikx}/\sqrt{V}$, acting on the boson Fock space

$$\mathcal{F}^B_\Lambda := \bigoplus_{n=0}^{+\infty} \mathcal{H}_B^{(n)}, \text{ with } \mathcal{H}_B^{(n)} := \left(L^2(\Lambda^n)\right)_{\mathrm{symm}}, \ \mathcal{H}_B^{(0)} := \mathbb{C}, \tag{2.4}$$

*Recall that $\varepsilon_0 = 0$.

†Here $\chi_\Lambda(x)$ is the characteristic function of the box Λ.

defined as the symmetrized n-particle Hilbert spaces, see [11, 12].

Remark 2.1 *Let $\mathcal{H}_{0\Lambda} \subset L^2(\Lambda)$ be the one-dimensional subspace generated by $\psi_{k=0}(x) = 1/\sqrt{V}$. Then $\mathcal{F}_\Lambda^B \approx \mathcal{F}_{0\Lambda} \otimes \mathcal{F}'_\Lambda$ where $\mathcal{F}_{0\Lambda}$ and $\mathcal{F}'_\Lambda$ are the boson Fock spaces constructed out of $\mathcal{H}_{0\Lambda}$ and of its orthogonal complement $\mathcal{H}_{0\Lambda}^\perp$ respectively.*

2.2 Grand-canonical thermodynamics for a fixed particle density [8, 9, 10]

We consider here the grand-canonical ensemble (β, μ) defined by a given particle density ρ, or more precisely by the chemical potential $\mu_{\Lambda,\rho}$, which is a unique solution of the equation (2.5) below. In any finite volume, the corresponding particle density is strictly increasing by strict convexity of the pressure. Therefore, for any $\rho > 0$, there exists a unique $\mu_{\Lambda,\rho}$ such that

$$\left\langle \frac{N_\Lambda}{V} \right\rangle_{H_{\Lambda,\lambda_0}^{SB}} = \rho, \tag{2.5}$$

where $\langle - \rangle_{H_{\Lambda,\lambda_0}^{SB}}$ always represents the (finite volume) grand-canonical Gibbs states for $H_{\Lambda,\lambda_0}^{SB}$ taken at inverse temperature β and chemical potential $\mu_{\Lambda,\rho}$. In the thermodynamic limit, $\mu_{\Lambda,\rho}$ converges to $\mu_\rho \in \mathbb{R}$ for any $\rho > 0$. In fact, μ_ρ is strictly increasing except for $\rho \in [\rho_-, \rho_+]$ where it equals $\mu_c = \mu_c$. Here $\rho_+ > \rho_- > 0$ are two well-defined density only depending on the inverse temperature $\beta > 0$. Additionally, $\mu_\rho := \alpha_\rho + \lambda_0 \rho$ with $\alpha_\rho < 0$ and $\partial_{\lambda_0} \alpha_\rho = 0$ for $\rho \in [\rho_-, \rho_+]$.

Moreover, there is a non-conventional Bose condensation induced by the non-diagonal interaction U_Λ^{ND} for high particle densities:

$$x_\rho := \lim_\Lambda \left\langle \frac{a_0^* a_0}{V} \right\rangle_{H_{\Lambda,\lambda_0}^{SB}} = \begin{cases} = 0 \text{ for } \rho < \rho_-, \\ > 0 \text{ for } \rho > \rho_+, \end{cases} \tag{2.6}$$

with $\partial_{\lambda_0} x_\rho = 0$ for $\rho \notin [\rho_-, \rho_+]$. When $\rho \downarrow \rho_+$, note that the Bose condensate density x_ρ converges to $x_{\rho_+} > 0$. In particular, since $\mu_\rho = \mu_c$ for $\rho \in [\rho_-, \rho_+]$, the Bose condensate density x_μ as a function of the chemical potential μ jumps from 0 to x_{ρ_+} at $\mu = \mu_c$. An illustration of the behavior of x_ρ for a fixed density ρ (or x_μ at a fixed chemical potential μ) is performed in Figure 1.

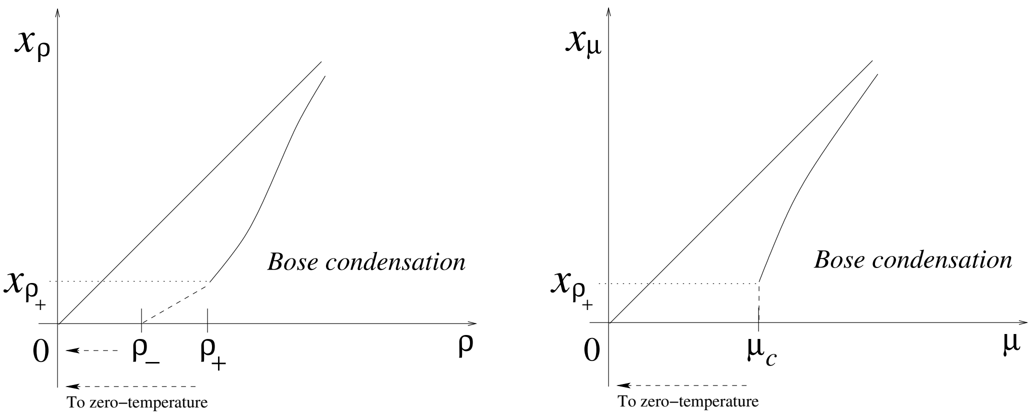

Figure 1: *Illustration of the Bose condensate density, x_ρ at fixed particle density $\rho > 0$ or x_μ at fixed chemical potential $\mu \in \mathbb{R}$. The dashed line closing continuously the gap between ρ_- and ρ_+ in the illustration of x_ρ is a consequence of results of the present paper. Here each of the asymptotic straight lines are : $x_\rho = \rho$, or $x_\mu = \mu/\lambda_0$. They correspond to the limits : $x_{\rho\to\infty}$, or $x_{\mu\to\infty}$, with 100% of the Bose condensate.*

We would like to stress that coexistence of different types of condensations is a subtle matter. For example a slight modification of interaction, see [8, 9, 10], excludes any coexistence of non-conventional and conventional Bose condensation, as it appears for high densities in the Bogoliubov WIBG [13, 14].

Below we consider coexistence a high and low density phases. For intermediate total density $\rho \notin [\rho_-, \rho_+]$ we find for the particle density outside the zero-mode

$$\lim_{\Lambda} \frac{1}{V} \sum_{k\in\Lambda^*\setminus\{0\}} \langle a_k^* a_k \rangle_{H^{SB}_{\Lambda,\lambda_0}} = \frac{1}{(2\pi)^3} \int_{\mathbb{R}^3} \left\{ \frac{f_k}{E_k \left[e^{\beta E_k} - 1\right]} + \frac{x_\rho^2 \lambda_k^2}{2E_k \left[f_k + E_k\right]} \right\} \mathrm{d}^3 k, \tag{2.7}$$

where $f_k := \varepsilon_k - \alpha_\rho + x_\rho \lambda_k$ and $E_k := (f_k^2 - x_\rho^2 \lambda_k^2)^{\frac{1}{2}}$.

Observe that the grand-canonical thermodynamic behavior of the superstable WIBG is unknown for $\rho \in [\rho_-, \rho_+]$ at fixed $\beta > 0$. When $\beta \rightarrow +\infty$, i.e. at zero temperature, the critical densities ρ_- and ρ_+ could both converge to zero depending on the interaction potential [8, 10], whereas the critical chemical potential μ_c converges to a negative value. Moreover, we have a non-zero particle density outside the zero-mode for any fixed $\rho > 0$ even at zero-temperature since

$$\lim_{\beta\rightarrow+\infty} \lim_{\Lambda} \frac{1}{V} \sum_{k\in\Lambda^*\setminus\{0\}} \langle a_k^* a_k \rangle_{H^{SB}_{\Lambda,\lambda_0}} > 0 \text{ and } \lim_{\beta\rightarrow+\infty} \lim_{\Lambda} \left\langle \frac{a_0^* a_0}{V} \right\rangle_{H^{SB}_{\Lambda,\lambda_0}} < \rho. \tag{2.8}$$

In other words, there is a depletion of the Bose condensate even at zero temperature.

To conclude, the grand-canonical pressure associated with $H^{SB}_{\Lambda,\lambda_0}$ in the thermodynamic limit equals

$$\begin{aligned} p^{SB}(\beta,\mu_\rho) &= \sup_{x\geq 0} \left\{ \inf_{\alpha\leq 0} \left\{ p_0^B(\beta,\alpha,x) + \frac{(\mu_\rho-\alpha)^2}{2\lambda_0} \right\} \right\} && (2.9)\\ &= \inf_{\alpha\leq 0} \left\{ p_0^B(\beta,\alpha,x_\rho) + \frac{(\mu_\rho-\alpha)^2}{2\lambda_0} \right\} && (2.10)\\ &= p_0^B(\beta,\alpha_\rho,x_\rho) + \frac{\lambda_0}{2}\rho^2, && (2.11) \end{aligned}$$

for any $\rho > 0$. In particular, x_ρ and α_ρ are solutions of the variational problems (2.9) and (2.10) respectively. For any $x \geq 0$ and $\alpha \leq 0$,

$$p_0^B(\beta,\alpha,x) := \lim_{\Lambda} \frac{1}{\beta V} \ln \mathrm{Tr}_{\mathcal{F}'_\Lambda} \left\{ e^{-\beta\left(H^B_{\Lambda,0}(x,\alpha) - \alpha x\right)} \right\} \tag{2.12}$$

is here the (infinite volume) pressure of the so-called Bogoliubov approximation[‡]

$$H^B_{\Lambda,0}(x,\alpha) := \sum_{k\in\Lambda^*\setminus\{0\}} \left\{ (\varepsilon_k - \alpha)\, a_k^* a_k + \frac{x\lambda_k}{2} \left(a_k^* a_k + a_{-k}^* a_{-k} + a_k^* a_{-k}^* + a_k a_{-k} \right) \right\} \tag{2.13}$$

of $\{H^B_{\Lambda,0} - \alpha(N_\Lambda - a_0^* a_0)\}$. Observe that $H^B_{\Lambda,0}(x,\alpha)$ is defined on the boson Fock space $\mathcal{F}'_\Lambda$ for non-zero momentum bosons, cf. Remark 2.1 and Section 3 for a rigorous definition of the so-called Bogoliubov approximation. Finally, note that the Hamiltonian $H^B_{\Lambda,0}(x,\alpha)$ represents, via a unitary transformation, a perfect Bose gas of quasi-particles with one-particle spectrum E_k for $k \in \Lambda^* \setminus \{0\}$, see for instance [8].

3. Large deviations for the Bose condensate at a fixed total particle density

To define the (finite volume) distribution $\mathbb{D}_{\Lambda,\rho}$ of the condensate, we first recall the rigorous definition of the Bogoliubov approximation due to Ginibre [15] and based on coherent vectors. For any complex $c \in \mathbb{C}$, a coherent vector $|c\rangle$ is an element of the boson Fock space $\mathcal{F}_{0\Lambda}$ for zero momentum bosons (cf. Remark 2.1), satisfying $a_0|c\rangle = c\sqrt{V}|c\rangle$. In fact, if Ω_0 is the vacuum of $\mathcal{F}^B_\Lambda$, then $|c\rangle := \exp\{-V|c|^2/2 + c\sqrt{V}a_0^*\}\Omega_0$ for any $c \in \mathbb{C}$. The Bogoliubov approximation of a self-adjoint operator A acting on $\mathcal{F}^B_\Lambda$ is the operator $\mathrm{A}(c)$ defined on the boson Fock space $\mathcal{F}'_\Lambda$ without the zero mode by its quadratic form

$$\langle \psi_1' |\, \mathrm{A}(c)\, | \psi_2' \rangle := \langle c \otimes \psi_1' |\, \mathrm{A}\, | c \otimes \psi_2' \rangle, \tag{3.1}$$

[‡]Combined with a gauge transformation $a_k \rightarrow e^{i\varphi} a_k$

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

Now, for any chemical potential $\mu \in \mathbb{R}$ the (finite volume) grand-canonical pressure associated with $H^{SB}_{\Lambda,\lambda_0}$ equals

$$p^{SB}_{\Lambda}(\beta,\mu) := \frac{1}{\beta V} \ln \mathrm{Tr}_{\mathcal{F}^B_\Lambda} \{W_\Lambda\}, \text{ with } W_\Lambda := e^{-\beta(H^{SB}_{\Lambda,\lambda_0} - \mu N_\Lambda)}. \tag{3.2}$$

By using the generating family of coherent vectors $|c\rangle$ for $c \in \mathbb{C}$, we can rewrite the trace Tr above to observe that

$$p^{SB}_{\Lambda}(\beta,\mu) = \frac{1}{\beta V} \ln \frac{1}{2\pi} \int_{\mathbb{C}} \mathrm{Tr}_{\mathcal{F}'_\Lambda} \{W_\Lambda(c)\} \, \mathrm{d}^2 c = \frac{1}{\beta V} \ln \frac{1}{2\pi} \int_{\mathbb{C}} e^{\beta V p^{SB}_\Lambda(\beta,\mu,c)} \mathrm{d}^2 c, \tag{3.3}$$

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

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

is the pressure defined by the partial trace. For any $\rho > 0$, the corresponding distribution $\mathbb{D}_{\Lambda,\mu}$ related to the Bose condensate number density, is now defined on the Borel subsets $\mathcal{A}$ of $\mathbb{C}$ by

$$\mathbb{D}_{\Lambda,\mu}[\mathcal{A}] := e^{-\beta V p^{SB}_\Lambda(\beta,\mu)} \frac{1}{2\pi} \int_{\mathcal{A}} e^{\beta V p^{SB}_\Lambda(\beta,\mu,c)} \mathrm{d}^2 c. \tag{3.5}$$

Then, at fixed particle density $\rho > 0$, we express a large deviations principle (Section 5.2) for the condensate distribution $\mathbb{D}_{\Lambda,\rho} := \mathbb{D}_{\Lambda,\mu_{\Lambda,\rho}}$.

Theorem 3.1 (LD principle for the condensate distribution at a fixed density ρ)
The sequence $\{\mathbb{D}_{\Lambda,\rho}\}$ satisfies a large deviation principle with speed βV and rate function

$$\mathrm{D}_\rho(x) := \inf_{\alpha \le 0} \left\{ p^B_0(\beta,\alpha,x_\rho) + \frac{(\mu_\rho - \alpha)^2}{2\lambda_0} \right\} - \inf_{\alpha \le 0} \left\{ p^B_0(\beta,\alpha,x) + \frac{(\mu_\rho - \alpha)^2}{2\lambda_0} \right\},$$

for $x = |c|^2 \ge 0$, cf. (2.9)-(2.10).

This theorem shows in particular that the probability to observe a density $n_0/V \in \mathcal{A}$ of condensed bosons enclosed in Λ for a fixed chemical potential $\mu \in \mathbb{R}$ decreases exponentially with the volume $V = |\Lambda|$ if the distance between the Bose condensate density x_ρ (2.6) and the set $\mathcal{A} \subset \mathbb{R}$ is strictly positive. Now, the next step is to evaluate the limiting probability measure, in particular at the phase transition defined for a chemical potential $\rho \in [\rho_-, \rho_+]$. Recall that the Bose condensate density x_ρ (2.6) converges to 0 when $\rho \uparrow \rho_-$ but to a strictly positive value $x_{\rho_+} > 0$ when $\rho \downarrow \rho_+$.

Theorem 3.2 (The condensate distribution outside the point of the phase transition)
The (finite volume) distribution $\mathbb{D}_{\Lambda,\rho}$ of the condensate converges weakly in the set of probability measures $\mathcal{M}_1(\mathbb{C})$ as $\Lambda \uparrow \mathbb{R}^3$ towards the singular measures

$$\mathbb{D}_\rho := \lim_\Lambda \mathbb{D}_{\Lambda,\rho} = \frac{1}{2\pi} \int_0^{2\pi} \delta\left(c - x_\rho^{1/2} e^{i\theta}\right) \mathrm{d}\theta,$$

for any $\rho \in (0,\rho_-) \cup (\rho_+, +\infty)$.

For $\beta \to +\infty$, i.e. at zero-temperature, observe that ρ_- and ρ_+ could both converge to zero, depending on the interaction potential. But, at finite temperature, i.e. at $\beta > 0$, one always has $\rho_+ > \rho_-$ and the convergence of $\mathbb{D}_{\Lambda,\rho}$ is not solved for $\rho \in [\rho_-, \rho_+]$. The corresponding result is therefore expressed in the next theorem.

Theorem 3.3 (The condensate distribution at the point of the phase transition)
Let $\rho_+ > \rho_-$. As $\Lambda \uparrow \mathbb{R}^3$, the (finite volume) distribution $\mathbb{D}_{\Lambda,\rho}$ of the condensate converges weakly in $\mathcal{M}_1(\mathbb{C})$ towards a convex combination of the singular measures

$$\mathbb{D}_\rho := \lim_\Lambda \mathbb{D}_{\Lambda,\rho} = (1-\kappa_\rho)\,\delta(c) + \frac{\kappa_\rho}{2\pi}\int_0^{2\pi} \delta\left(c - x_{\rho_+}^{1/2} e^{i\theta}\right) \mathrm{d}\theta,$$

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

Note that κ_ρ is a strictly increasing and continuous function from $[\rho_-, \rho_+]$ to $[0,1]$. This result gives a strong evidence that, at the phase transition, the corresponding Gibbs state is not a pure state anymore [11] but a convex combination of pure states, see for example Section 4 in [1].

Integrating $\mathbb{D}_{\Lambda,\rho}$ with the function $\varphi(c) = |c|^2$, we finally obtain the Bose condensate density (2.6) inside the phase transition, i.e. for $\rho \in [\rho_-, \rho_+]$.

Corollary 3.4 (Derivation of the Bose condensate density for any total density)
The Bose condensate density equals

$$\lim_\Lambda \left\langle \frac{a_0^* a_0}{V} \right\rangle_{H^{SB}_{\Lambda_j,\lambda_0}} = \begin{cases} 0 & \text{for } \rho \leq \rho_-. \\ \dfrac{\rho-\rho_-}{\rho_+-\rho_-} x_{\rho_+} & \text{for } \rho \in [\rho_-, \rho_+]. \\ x_\rho > 0 & \text{for } \rho \geq \rho_+. \end{cases}$$

In particular, it is continuous as a function of $\rho > 0$ and linearly increasing for $\rho \in [\rho_-, \rho_+]$, cf. figure 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

$$H_\Lambda^{MF} := \sum_{k\in\Lambda^*} \varepsilon_k a_k^* a_k + \frac{\lambda_0}{2V}\left(N_\Lambda^2 - N_\Lambda\right), \tag{3.6}$$

with no Bose condensations. Increase now the particle density. The free-energy per particle, i.e., the chemical potential $\mu_{\beta,\rho} \leq \mu_c$, normally grows until we reach $\rho = \rho_-$. By further increasing of the density, a Bose condensation continuously appears to reach 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 free-energy per particle $\mu_\rho > \mu_c$ both increase.

4. Proofs: Large Deviations for a generalized Kac distribution

We are going to study the grand-canonical ensemble at a fixed total particle density $\rho > 0$. But before doing this, we start our analysis at a fixed chemical potential μ. Then we prove the LD principle for the condensate plus "out of condensate" particle densities. The corresponding distribution $\mathbb{K}_{\Lambda,\mu}$ is a combination of the so-called *Kac distribution* [1] for particles outside the condensate with the condensate distribution $\mathbb{D}_{\Lambda,\mu}$. This is expressed by Theorem 4.1, which is therefore, a generalization of Theorem 3.1. To study the phase transition, we use the *generalized quasi-average procedure* [1] by taking a "perturbed" chemical potential

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

we analyze the thermodynamic limit of the generalized Kac distribution at this chemical potential, see Theorem 4.2.

As a consequence, the generalized quasi-average procedure (4.1) gives the finite volume behavior of the chemical potential $\mu_{\Lambda,\rho}$ solution of (2.5) at the phase transition, i.e. when $\rho \in [\rho_-, \rho_+]$ if $\rho_+ > \rho_-$. Indeed, by applying the distribution $\mathbb{K}_{\Lambda,\mu}$ to an appropriate function, we obtain the mean particle density at a chemical potential $\tilde{\mu}_c$ 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 $\mu_{\Lambda,\rho} = \tilde{\mu}_c$ with $|\gamma_\rho| = o(V)$, see Section 4.2.

Meanwhile, the large deviation principle for $\mathbb{K}_{\Lambda,\mu}$ given by Theorem 4.1 directly implies Theorem 3.1 for any $\rho > 0$. Applying the result of Theorem 4.2 to the chemical potential $\mu_{\Lambda,\rho} = \tilde{\mu}_c$ 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

The particle number density as a $\mathbb{R}$-valued random variable, is well-defined via a well-known probability measure, the so-called Kac distribution [1]. We give here a *generalized* version of the Kac distribution associated with the condensate and its depletion. This distribution is defined, on the Borel subsets $\mathcal{A} \subset \mathbb{C}$ and $\mathcal{B} \subset \mathbb{R}_+$ by integration over the zero-mode coherent state:

$$\mathbb{K}_{\Lambda,\mu}[\mathcal{A}] := e^{-\beta V p_\Lambda^{SB}(\beta,\mu)} \frac{1}{2\pi} \int\limits_{\mathcal{A}} \mathrm{d}^2 c \int\limits_{\mathcal{B}} \nu_\Lambda(\mathrm{d}y)\, e^{\beta V \left(\mu\left(y+|c|^2\right) - f_\Lambda^{SB}(\beta,y,c)\right)}, \tag{4.2}$$

with

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

Here $[.]$ is the integer part and

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

where $W_{\Lambda,0}(c)$ results from the Bogoliubov approximation (3.1) of the statistical operator $W_{\Lambda,0}$ (3.2) and $\mathrm{A}^{(n,k\neq 0)}$ is the restriction of any operator A acting on the boson Fock space $\mathcal{F}_B'$ to the space $\{\mathcal{H}_{0\Lambda}^{\perp}\}^{(n)}$ of n non-zero momentum bosons. Now we express our first result concerning large deviations for the generalized Kac distribution $\mathbb{K}_{\Lambda,\mu}$.

Theorem 4.1 (LD principle for the generalized Kac distribution)
The sequence $\{\mathbb{K}_{\Lambda,\mu}\}$ satisfies a large deviation principle with speed βV and rate function

$$\mathrm{K}_\mu(x,y) := p^{SB}(\beta,\mu) + f_0^B(\beta,y,x) + \frac{\lambda_0}{2}(y+x)^2 - \mu(y+x).$$

Here $x = |c|^2 \geq 0$, $y \geq 0$ and

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

is the Legendre-Fenchel transform of $p_0^B(\beta,\alpha,x)$ (2.12).

Proof. Let us start by some observations. The pressure $p_0^B(\beta,\alpha,x)$ defined in (2.12) and used in (2.9) can be explicitly computed. Indeed,

$$\begin{aligned} p_0^B(\beta,\alpha,x) &= \alpha x - \frac{1}{\beta(2\pi)^3} \int\limits_{\mathbb{R}^3} \ln\left(1 - e^{-\beta\sqrt{(\varepsilon_k-\alpha)(\varepsilon_k-\alpha+2x\lambda_k)}}\right) \mathrm{d}^3k + \\ &\quad + \frac{1}{2(2\pi)^3} \int\limits_{\mathbb{R}^3} \left\{\varepsilon_k - \alpha + x\lambda_k - \sqrt{(\varepsilon_k-\alpha)(\varepsilon_k-\alpha+2x\lambda_k)}\right\} \mathrm{d}^3k, \end{aligned} \tag{4.5}$$

for any $\alpha \leq 0$. Since $p_0^B(\beta,\alpha,x)$ is a convex function of $\alpha \leq 0$, it is also the Legendre-Fenchel transform of $f_0^B(\beta,y,x)$, i.e.

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

Combined with (2.9) this last inequality implies that

$$p^{SB}(\beta,\mu) = \sup_{x\geq 0}\left\{\inf_{\alpha\leq 0}\left\{\sup_{y\geq 0}\left\{\alpha(y+x) - f_0^B(\beta,y,x) + \frac{(\mu-\alpha)^2}{2\lambda_0}\right\}\right\}\right\}. \tag{4.7}$$

We would like to bring the infimum over $\alpha \leq 0$ inside the two other suprema. In general, a supremum and an infimum do not commute. In this peculiar case, this is however the case. Indeed, for any fixed $x \geq 0$ the function

$$\Psi(y,\alpha) := \alpha(y+x) - f_0^B(\beta,y,x) + \frac{(\mu-\alpha)^2}{2\lambda_0} \tag{4.8}$$

is a strictly concave function of $y \geq 0$ and a strictly convex function of $\alpha \leq 0$. Then, we obtain the uniqueness of the stationary point $(\tilde{y},\tilde{\alpha})$ solution of

$$\partial_y \Psi(y,\alpha) = 0 \text{ and } \partial_\alpha \Psi(y,\alpha) = y + x + \frac{\alpha-\mu}{\lambda_0} = 0. \tag{4.9}$$

In particular, we can commute the infimum over $\alpha \leq 0$ and the supremum over $y \geq 0$ in (4.7) to obtain

$$p^{SB}(\beta,\mu) = \sup_{(x,y)\in\mathbb{R}_+^2}\left\{\mu(y+x) - f_0^B(\beta,y,x) - \frac{\lambda_0}{2}(y+x)^2\right\}. \tag{4.10}$$

This result is coherent with the rate function $\mathrm{K}_\mu(x,y)$. By explicit computations, observe also that there are $M, B > 0$ such that any solution (x_μ, y_μ) of the variational problem (4.10) verifies $x_\mu < M$ and $y_\mu < M$ whereas for any $x \geq M$ and $y \geq M$ we have

$$\mu(y+x) - f_0^B(\beta,y,x) - \frac{\lambda_0}{2}(y+x)^2 \leq -B(y+x). \tag{4.11}$$

Now we are in position to analyze the LD principle for distribution $\mathbb{K}_{\Lambda,\mu}$ (Section 5.2).

From (4.5) the rate function $\mathrm{K}_\mu(x,y)$ is not identical ∞ and has compact level sets, i.e. for each $m < \infty$, the subset $\{(x,y) : \mathrm{K}_\mu(x,y) \leq m\}$ is compact.

Let a closed set $\mathcal{C} := \mathcal{C}_0 \times \mathcal{C}_1 \subset \mathbb{C} \times \mathbb{R}_+$. Remark that M can be taken arbitrary large (and B being the same). Then, without lost of generality, we can assume that any $c \in \mathcal{C}_0$ and $y \in \mathcal{C}_1$ satisfy $|c|^2 < M$ and $y < M$ respectively. By (4.11), we also obtain

$$\begin{aligned}\mathbb{K}_{\Lambda,\mu}[\mathcal{C}] \leq\ & \frac{1}{2\pi} e^{\beta V\left\{\sup_{\mathcal{C}}\left\{\mu(y+|c|^2) - f_\Lambda^{SB}(\beta,y,c)\right\} - p_\Lambda^{SB}(\beta,\mu)\right\}} \int_{\mathcal{C}_0} \mathrm{d}^2 c \int_{\mathcal{C}_1} \nu_\Lambda(\mathrm{d}y) + \\ & + \frac{1}{2\pi} e^{-\beta V\left\{p_\Lambda^{SB}(\beta,\mu) + 2BM\right\}} \int_{\mathbb{C}} \mathrm{d}^2 c \int_{\mathbb{R}_+} \nu_\Lambda(\mathrm{d}y)\, e^{-\beta V B\left(|c|^2 + y\right)}.\end{aligned} \tag{4.12}$$

For large enough M, one has

$$2BM + \sup_{\mathcal{C}}\left\{\mu(y+x) - f_0^B(\beta,y,x) - \frac{\lambda_0}{2}(y+x)^2\right\} > 0. \tag{4.13}$$

Consequently, the inequality (4.12) combined Lemma 5.2 implies that

$$\limsup_{\Lambda} \frac{1}{\beta V} \ln \mathbb{K}_{\Lambda,\mu}[\mathcal{C}] \leq -\inf_{\mathcal{C}} \mathrm{K}_\mu\left(|c|^2, y\right). \tag{4.14}$$

In other words, the large deviations upper bound (5.22) for $\mathbb{K}_{\Lambda,\mu}$ with speed βV and rate function K_μ is verified. It remains to analyze the corresponding large deviations lower bound (5.23).

Let $\mathcal{G}$ be an arbitrary open subset of $\mathbb{C} \times \mathbb{R}_+$. Note that

$$\mathbb{K}_{\Lambda,\mu}[\mathcal{G}] \geq \mathbb{K}_{\Lambda,\mu}[\{(c,y)\}] = e^{-\beta V p_\Lambda^{SB}(\beta,\mu)} e^{\beta V\left\{\mu([yV]+|c|^2) - f_\Lambda^{SB}(\beta,y,c)\right\}}, \tag{4.15}$$

with $(c, y) \in \mathcal{G}$. From Lemma 5.2, it yields that

$$\liminf_{\Lambda} \frac{1}{\beta V} \ln \mathbb{K}_{\Lambda,\mu}[\mathcal{G}] \geq -\mathrm{K}_{\mu}\left(|c|^2, y\right). \tag{4.16}$$

Since the last inequality holds for each point of $\mathcal{G}$, it means that

$$\liminf_{\Lambda} \frac{1}{\beta V} \ln \mathbb{K}_{\Lambda,\mu}[\mathcal{G}] \geq -\inf_{\mathcal{G}} \mathrm{K}_{\mu}\left(|c|^2, y\right), \tag{4.17}$$

i.e. the corresponding large deviation lower bound (5.23) for $\mathbb{K}_{\Lambda,\mu}$ holds with speed βV and rate function K_{μ}. □

For $\mu \neq \mu_c$ we already know [8] that the variational problem (4.10) has a unique solution (x_μ, y_μ). Therefore, as a direct consequence of the fact that the sequence $\{\mathbb{K}_{\Lambda,\mu}\}$ satisfies a large deviations principle with rate function K_μ having a unique minimum in $\mathbb{R}_+^2$ at (x_μ, y_μ) for any $\mu \neq \mu_c$, the distribution $\mathbb{K}_{\Lambda,\mu}$ converges weakly on the set of probability measures $\mathcal{M}_1(\mathbb{C}\times\mathbb{R}_+)$ as $\Lambda \uparrow \mathbb{R}^3$ towards the singular measure

$$\mathbb{K}_\mu := \lim_{\Lambda} \mathbb{K}_{\Lambda,\mu} = \frac{1}{2\pi}\int_0^{2\pi} \delta\left(c - x_\mu^{1/2} e^{i\theta}\right)\delta\left(y - y_\mu\right) \mathrm{d}\theta, \text{ for } \mu \neq \mu_c. \tag{4.18}$$

Now, the next step is to evaluate the limiting probability measure at the phase transition defined for a chemical potential $\mu = \mu_c$. Indeed, if $\rho_+ > \rho_-$, the solution (x_μ, y_μ) jumps when μ cross the critical chemical potential μ_c from $(0, \rho_-)$ to (x_{ρ_+}, y_{ρ_+}) with $x_{\rho_+} > 0$ and $y_{\rho_+} := \rho_+ - x_{\rho_+} > \rho_-$.

Theorem 4.2 (The generalized Kac distribution at the phase transition)
If $\rho_+ > \rho_-$, then the distribution $\mathbb{K}_{\Lambda,\tilde{\mu}_c}$ converges weakly in $\mathcal{M}_1(\mathbb{C}\times\mathbb{R}_+)$ as $\Lambda \uparrow \mathbb{R}^3$ towards

$$\lim_{\Lambda} \mathbb{K}_{\Lambda,\tilde{\mu}_c} = \xi_\gamma \delta(c)\,\delta(y-\rho_-) + \frac{(1-\xi_\gamma)}{2\pi}\int_0^{2\pi} \delta\left(c - x_{\rho_+}^{1/2} e^{i\theta}\right)\delta\left(y - y_{\rho_+}\right)\mathrm{d}\theta, \tag{4.19}$$

with $\xi_\gamma := (1 + e^{\gamma(\rho_+ - \rho_-)})^{-1} \in (0,1)$ and $\tilde{\mu}_c$ defined by (4.1) for any $\gamma \in \mathbb{R}$.

Proof. We have already mentioned that the rate function K_{μ_c} has two distinct minima in $\mathbb{R}_+^2$ at $(0, \rho_-)$ and (x_{ρ_+}, y_{ρ_+}). To get around this complication, take $\varepsilon \in (0, x_{\rho_+}) \cap (0, y_{\rho_+} - \rho_-)$ and define

$$\mathcal{A}_- := \left\{c \in \mathbb{C} : |c|^2 \in \left(0, x_{\rho_+} - \varepsilon\right]\right\} \times \left(\rho_-, y_{\rho_+} - \varepsilon\right] \tag{4.20}$$

and

$$\mathcal{A}_+ := \left\{c \in \mathbb{C} : |c|^2 \in \left(x_{\rho_+} - \varepsilon, +\infty\right)\right\} \times \left(y_{\rho_+} - \varepsilon, +\infty\right). \tag{4.21}$$

Now, let $\mathrm{K}_{\mu_c^-}$ and $\mathrm{K}_{\mu_c^+}$ be defined as the two restrictions of K_{μ_c} to $\mathcal{A}_-$ and $\mathcal{A}_+$ respectively and remark that $\mathrm{K}_{\mu_c^-}$ and $\mathrm{K}_{\mu_c^+}$ have both a unique minimizer in $\mathbb{R}_+^2$, respectively $(0, \rho_-)$ and (x_{ρ_+}, y_{ρ_+}). Define the corresponding probability measures

$$\mathbb{L}_\Lambda^-[\mathcal{A}] := \frac{\mathbb{K}_{\Lambda,\mu_c}[\mathcal{A}\cap\mathcal{A}_-]}{\mathbb{K}_{\Lambda,\mu_c}[\mathcal{A}_-]} \text{ and } \mathbb{L}_\Lambda^+[\mathcal{A}] := \frac{\mathbb{K}_{\Lambda,\mu_c}[\mathcal{A}\cap\mathcal{A}_+]}{\mathbb{K}_{\Lambda,\mu_c}[\mathcal{A}_+]}, \tag{4.22}$$

which satisfy a large deviations principle respectively with rate functions $\mathrm{K}_{\mu_c^-}$ and $\mathrm{K}_{\mu_c^+}$ (where $x = |c|^2$). Take any positive and continuous function $\varphi(c, y)$ of $(c, y) \in \mathbb{C}\times\mathbb{R}_+$ and observe that

$$\int_{\mathbb{R}_+^2} \varphi(c,y)\,\mathbb{K}_{\Lambda,\mu_{c,\Lambda}}\left(\mathrm{d}^2 c\right) = \frac{\int_{\mathbb{C}} \mathrm{d}^2 c \int_{\mathbb{R}_+} \nu_\Lambda(\mathrm{d}y)\,\varphi(c,y)\, e^{\beta V\left(\tilde{\mu}_c(y+|c|^2) - f_\Lambda^{SB}(\beta,y,c)\right)}}{\int_{\mathbb{C}} \mathrm{d}^2 c \int_{\mathbb{R}_+} \nu_\Lambda(\mathrm{d}y)\, e^{\beta V\left(\tilde{\mu}_c(y+|c|^2) - f_\Lambda^{SB}(\beta,y,c)\right)}} = \Phi_\Lambda^- + \Phi_\Lambda^+, \tag{4.23}$$

with

$$\Phi_\Lambda^- \quad : \quad = \frac{\int\limits_{\mathcal{A}_-} \varphi(c,y)\, e^{\{\gamma+o(1)\}(y+|c|^2)} \mathbb{L}_\Lambda^-\left(\mathrm{d}^2 c \mathrm{d} y\right)}{\int\limits_{\mathcal{A}_-} e^{\{\gamma+o(1)\}(y+|c|^2)} \mathbb{L}_\Lambda^-\left(\mathrm{d}^2 c \mathrm{d} y\right) + \Theta_\Lambda \int\limits_{\mathcal{A}_+} e^{\{\gamma+o(1)\}(y+|c|^2)} \mathbb{L}_\Lambda^+\left(\mathrm{d}^2 c \mathrm{d} y\right)}, \tag{4.24}$$

$$\Phi_\Lambda^+ \quad : \quad = \frac{\int\limits_{\mathcal{A}_+} \varphi(c,y)\, e^{\{\gamma+o(1)\}(y+|c|^2)} \mathbb{L}_\Lambda^+\left(\mathrm{d}^2 c \mathrm{d} y\right)}{\Theta_\Lambda^{-1} \int\limits_{\mathcal{A}_-} e^{\{\gamma+o(1)\}(y+|c|^2)} \mathbb{L}_\Lambda^-\left(\mathrm{d}^2 c \mathrm{d} y\right) + \int\limits_{\mathcal{A}_+} e^{\{\gamma+o(1)\}(y+|c|^2)} \mathbb{L}_\Lambda^+\left(\mathrm{d}^2 c \mathrm{d} y\right)}, \tag{4.25}$$

and

$$\Theta_\Lambda := \frac{\int\limits_{\mathcal{A}_+} e^{\beta V\left\{\mu_c(y+|c|^2) - f_\Lambda^{SB}(\beta,y,c)\right\}} \nu_\Lambda(\mathrm{d}y)\, \mathrm{d}^2 c}{\int\limits_{\mathcal{A}_-} e^{\beta V\left\{\mu_c(y+|c|^2) - f_\Lambda^{SB}(\beta,y,c)\right\}} \nu_\Lambda(\mathrm{d}y)\, \mathrm{d}^2 c}. \tag{4.26}$$

By Lemma 5.2 the function

$$\mu_c(y+|c|^2) - f_\Lambda^{SB}(\beta,y,c) \tag{4.27}$$

converges in the thermodynamic limit to

$$\mu_c(y+|c|^2) - f_0^B\left(\beta,y,|c|^2\right) - \frac{\lambda_0}{2}\left(y+|c|^2\right)^2, \tag{4.28}$$

which has suprema at $(0,\rho_-)$ and $(e^{i\theta}x_{\rho_+}, y_{\rho_+})$ for any $\theta \in [0,2\pi]$. Consequently, the coefficient Θ_Λ (4.26) converges to 1 in the thermodynamic limit. Since $\rho_+ = y_{\rho_+} + x_{\rho_+}$, it is then straightforward to see that

$$\lim_\Lambda \Phi_\Lambda^- = \xi_\gamma \varphi(0,\rho_-) \text{ and } \lim_\Lambda \Phi_\Lambda^+ = \frac{(1-\xi_\gamma)}{2\pi} \int\limits_0^{2\pi} \varphi(x_{\rho_+}^{1/2} e^{i\theta}, y_{\rho_+}) \mathrm{d}\theta. \tag{4.29}$$

Let us apply these limits to the function $\varphi(c,y) = e^{-t(c+y)}$ with $t>0$. Then, by bijectivity of the Laplace transform, it follows that $\mathbb{K}_{\Lambda,\tilde{\mu}_c}$ converges weakly on $\mathcal{M}_1(\mathbb{C}\times\mathbb{R}_+)$ as $\Lambda \uparrow \mathbb{R}^3$ to (4.19). □

Notice that the function $\xi_\gamma : \mathbb{R} \to (0,1)$ defined in Theorem 4.2 is strictly decreasing and in fact bijective. Therefore, by applying $\mathbb{K}_{\Lambda,\tilde{\mu}_c}$ to $\varphi(c,y) = |c|^2 + y$, we have shown that the particle density can converge to any fixed density in the open set (ρ_-,ρ_+) :

$$\lim_\Lambda \left\langle \frac{N_\Lambda}{V} \right\rangle_{H_{\Lambda,\lambda_0}^{SB}} = \xi_\gamma \rho_- + (1-\xi_\gamma)\rho_+. \tag{4.30}$$

Note that all these results are coherent since we have

$$\rho_- = \lim_{\gamma\to-\infty} \{\xi_\gamma\rho_- + (1-\xi_\gamma\rho_+)\} \text{ and } \rho_+ = \lim_{\gamma\to+\infty} \{\xi_\gamma\rho_- + (1-\xi_\gamma\rho_+)\}. \tag{4.31}$$

In particular, if $\gamma = \gamma_\Lambda = o(\pm V)$ in (4.1) diverges to $\pm\infty$, then we would obtain one of the previous limit, depending if $\gamma_\Lambda \downarrow -\infty$ or $\gamma_\Lambda \uparrow +\infty$.

4.2 Application of the generalized Kac distribution for a fixed particle density

Let us consider now the total particle density as a parameter that defines the grand-canonical ensemble. Theorems 3.1 and 3.3 are direct consequences respectively of Theorem 4.1 and (4.18) for the chemical potential μ_ρ defined as the thermodynamic limit of $\mu_{\Lambda,\rho}$ (2.5). The only remaining question is to study the case of fixed particle densities at the the point of phase transition, i.e. in domain: $\rho \in (\rho_-,\rho_+)$ for $\rho_+ > \rho_-$. From (4.30), we obtain that

$$\lim_\Lambda \left\langle \frac{N_\Lambda}{V} \right\rangle_{H_{\Lambda,\lambda_0}^{SB}} = \rho \in (\rho_-,\rho_+), \tag{4.32}$$

for a chemical potential

$$\mu = \mu_c + \frac{\gamma_\rho}{\beta V} + o\left(\frac{1}{\beta V}\right) \text{ with } \gamma_\rho := \frac{1}{\rho_+ - \rho_-} \ln\left(\frac{\rho - \rho_-}{\rho_+ - \rho}\right), \tag{4.33}$$

cf. (4.1). Therefore,

$$\mu_{\Lambda,\rho} = \mu_c + \frac{\gamma_\rho}{\beta V} + o\left(\frac{1}{\beta V}\right). \tag{4.34}$$

In particular, from (4.2) with $\gamma = \gamma_\rho$ we get Theorem 3.3 for $\rho \in (\rho_-, \rho_+)$. Recall also (4.31). In other words, if $\rho = \rho_-$ then $\gamma_\rho < 0$ ($|\gamma_\rho| = o(V)$) would diverges to $-\infty$, whereas if $\rho = \rho_+$ then $\gamma_\rho = o(V) \to +\infty$. It follows that Theorem 3.3 is proven for any $\rho \in [\rho_-, \rho_+]$.

5. Appendix

In this appendix, we first give supplementary results needed in the previous section. Next, for the convenience of our reader, we shortly repeat the notion of large deviations principles.

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

$$p^{SB}(\beta,\mu,c) := \lim_{\Lambda} p_\Lambda^{SB}(\beta,\mu,c) = \inf_{\alpha \le 0} \left\{ p_0^B(\beta,\alpha,x) + \frac{(\mu-\alpha)^2}{2\lambda_0} \right\}.$$

Here $x = |c|^2 \ge 0$ and recall that $p_0^B(\beta,\alpha,x)$ is defined in (2.12), cf. also (4.5).

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 othonormal basis $\{\langle\psi_n'|\}_{n=1}^\infty$ of $\mathcal{F}_\Lambda'$,

$$\mathrm{Tr}_{\mathcal{F}_\Lambda'}\{W_\Lambda(c)\} = \sum_{n=1}^{\infty} \langle c \otimes \psi_n'|\, e^{-\beta(H_{\Lambda,\lambda_0}^{SB} - \mu N_\Lambda)}\, |c \otimes \psi_n'\rangle, \tag{5.1}$$

and so, by the Peierls-Bogoliubov inequality we get

$$\mathrm{Tr}_{\mathcal{F}_\Lambda'}\{W_\Lambda(c)\} \ge \sup_{\{\psi_n'\}_{n=1}^\infty} \left\{ \sum_{n=1}^{\infty} e^{-\beta\left\langle c\otimes\psi_n' \middle| H_{\Lambda,\lambda_0}^{SB} - \mu N_\Lambda \middle| c\otimes\psi_n' \right\rangle} \right\} = \mathrm{Tr}_{\mathcal{F}_\Lambda'}\left\{ e^{-\beta H_{\Lambda,\lambda_0}^{SB}(c,\mu)} \right\}, \tag{5.2}$$

see e.g. [16, 17], where $H_{\Lambda,\lambda_0}^{SB}(c,\mu)$ results from the Bogoliubov approximation (3.1) of $\{H_{\Lambda,\lambda_0}^{SB} - \mu N_\Lambda\}$. From [8] we already know that

$$\lim_{\Lambda} \frac{1}{\beta V} \ln \mathrm{Tr}_{\mathcal{F}_\Lambda'}\left\{ e^{-\beta H_{\Lambda,\lambda_0}^{SB}(c,\mu)} \right\} = \inf_{\alpha \le 0} \left\{ p_0^B(\beta,\alpha,|c|^2) + \frac{(\mu-\alpha)^2}{2\lambda_0} \right\}. \tag{5.3}$$

Consequently, the inequality (5.2) implies in the thermodynamic limit the lower bound

$$p^{SB}(\beta,\mu,c) \ge \inf_{\alpha \le 0} \left\{ p_0^B(\beta,\alpha,|c|^2) + \frac{(\mu-\alpha)^2}{2\lambda_0} \right\}, \tag{5.4}$$

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 [18], and use the coherent state representation of $\{H_{\Lambda,\lambda_0}^{SB}-\mu N_\Lambda\}$ given by

$$H_{\Lambda,\lambda_0}^{SB}-\mu N_\Lambda=\int_{\mathbb{C}} \mathrm{d}^2c\left\{\hat{H}_{\Lambda,\lambda_0}^{SB}(c,\mu)\left|c\right\rangle\left\langle c\right|\right\}, \tag{5.5}$$

where the Hamiltonian $\hat{H}_{\Lambda,\lambda_0}^{SB}(c,\mu)$ is defined on $\mathcal{F}'_\Lambda$ by

$$\hat{H}_{\Lambda,\lambda_0}^{SB}(c,\mu):=H_{\Lambda,\lambda_0}^{SB}(c,\mu)+\Delta, \tag{5.6}$$

with

$$\Delta:=\mu-2\lambda_0|c|^2+\frac{\lambda_0}{V}-\frac{1}{V}\sum_{k\in\Lambda^*\backslash\{0\}}(\lambda_0+\lambda_k)\,a_k^*a_k. \tag{5.7}$$

Actually, $\hat{H}_{\Lambda,\lambda_0}^{SB}(c,\mu)$ is derived by replacing the operators $a_0^*a_0$, a_0a_0, $a_0^*a_0^*$, and $a_0^*a_0^*a_0a_0$ in $\{H_{\Lambda,\lambda_0}^{SB}-\mu N_\Lambda\}$ 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 othonormal basis of eigenvectors of $\hat{H}_{\Lambda,\lambda_0}^{SB}(c,\mu)$. Since for any $z,c\in\mathbb{C}$

$$\langle z|c\rangle=e^{-\frac{1}{2}\{(\bar{z}-\bar{c})(z-c)+\bar{c}z-\bar{z}c\}}, \tag{5.8}$$

it follows that

$$\begin{aligned}
\mathrm{Tr}_{\mathcal{F}'_\Lambda}\{W_\Lambda(c)\} &= \sum_{n=1}^{\infty}\langle c\otimes\psi'_n(c)|\,e^{-\beta\int_{\mathbb{C}}\mathrm{d}^2z\hat{H}_{\Lambda,\lambda_0}^{SB}(z,\mu)|z\rangle\langle z|}\,|c\otimes\psi'_n(c)\rangle\\
&= \sum_{n=1}^{\infty}\left\{1+\sum_{m=1}^{\infty}\frac{(-\beta)^m}{m!}\int_{\mathbb{C}^m}\mathrm{d}^2z_1\cdots\mathrm{d}^2z_m e^{-\frac{V}{2}\{\mathrm{R}_m(z_1,\cdots,z_m)+i\mathrm{I}_m(z_1,\cdots,z_m)\}}\right.\\
&\qquad\left.\times\prod_{j=1}^{m}\langle\psi'_n(c)|\,\hat{H}_{\Lambda,\lambda_0}^{SB}(z_j,\mu)\,|\psi'_n(c)\rangle\right\},
\end{aligned} \tag{5.9}$$

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

$$\begin{aligned}
\mathrm{R}_m(z_1,\cdots,z_m)&:=|z_1-c|^2+\sum_{j=1}^{m}|z_{j-1}-z_j|^2+|z_m-c|^2,\\
\mathrm{I}_m(z_1,\cdots,z_m)&:=i(\bar{z}_1c-\bar{c}z_1)+i\sum_{j=1}^{m}(\bar{z}_jz_{j-1}-\bar{z}_{j-1}z_j)+i(\bar{c}z_m-\bar{z}_mc).
\end{aligned} \tag{5.10}$$

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

$$\inf_{(z_1,\cdots,z_m)\in\mathbb{C}^m}\mathrm{R}_m(z_1,\cdots,z_m)=\mathrm{R}_m(c,\cdots,c)=0, \tag{5.11}$$

by virtue of (5.9) combined with large deviations arguments, one can obtain in the thermodynamic limit that

$$p^{SB}(\beta,\mu,c)=\lim_{\Lambda}\frac{1}{\beta V}\ln\mathrm{Tr}_{\mathcal{F}'_\Lambda}\left\{e^{-\beta\hat{H}_{\Lambda,\lambda_0}^{SB}(c,\mu)}\right\}. \tag{5.12}$$

Justification of the LD technique in sums (5.9) is based on the uniform domination theorem and it follows the line of reasoning developed in [18]. Meanwhile, by using the Bogoliubov convexity inequality [14] it follows that

$$\mathrm{Tr}_{\mathcal{F}'_\Lambda}\left\{e^{-\beta\hat{H}_{\Lambda,\lambda_0}^{SB}(c,\mu)}\right\}\leq\frac{1}{\beta V}\ln\mathrm{Tr}_{\mathcal{F}'_\Lambda}\left\{e^{-\beta H_{\Lambda,\lambda_0}^{SB}(c,\mu)}\right\}-\frac{1}{V}\left\langle\Delta\right\rangle_{\hat{H}_{\Lambda,\lambda_0}^{SB}(c,\mu)}, \tag{5.13}$$

where

$$\left\langle-\right\rangle_{\hat{H}_{\Lambda,\lambda_0}^{SB}(c,\mu)}:=\frac{\mathrm{Tr}_{\mathcal{F}'_\Lambda}\left\{-e^{-\beta\hat{H}_{\Lambda,\lambda_0}^{SB}(c,\mu)}\right\}}{\mathrm{Tr}_{\mathcal{F}'_\Lambda}\left\{e^{-\beta\hat{H}_{\Lambda,\lambda_0}^{SB}(c,\mu)}\right\}}. \tag{5.14}$$

In particular, since for $k \in \mathbb{R}^3$, $0 \leq \lambda_k \leq \lambda_0$ by our assumption (B) on the interaction potential, we obtain from the inequality (5.13) together with (5.7) that

$$\begin{aligned}\frac{1}{\beta V} \ln \mathrm{Tr}_{\mathcal{F}'_\Lambda} \left\{ e^{-\beta \hat{H}^{SB}_{\Lambda,\lambda_0}(c,\mu)} \right\} \quad &\leq \quad \frac{1}{\beta V} \ln \mathrm{Tr}_{\mathcal{F}'_\Lambda} \left\{ e^{-\beta H^{SB}_{\Lambda,\lambda_0}(c,\mu)} \right\} + \frac{2|c|^2\lambda_0 - \mu}{V} - \frac{\lambda_0}{V^2} \\ &+ \frac{2\lambda_0}{V^2} \sum_{k \in \Lambda^* \backslash \{0\}} \langle a_k^* a_k \rangle_{\hat{H}^{SB}_{\Lambda,\lambda_0}(c,\mu)} . \end{aligned} \tag{5.15}$$

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

$$\frac{1}{V} \sum_{k \in \Lambda^* \backslash \{0\}} \langle a_k^* a_k \rangle_{\hat{H}^{SB}_{\Lambda,\lambda_0}(c,\mu)} = \mathcal{O}(1) \ \text{ as } \Lambda \uparrow \mathbb{R}^3. \tag{5.16}$$

Therefore, from (5.15) together with (5.3) and (5.12) one deduces that

$$p^{SB}(\beta,\mu,c) \leq \inf_{\alpha \leq 0} \left\{ p_0^B(\beta,\alpha,|c|^2) + \frac{(\mu-\alpha)^2}{2\lambda_0} \right\}. \tag{5.17}$$

Together with the lower bound (5.4), this inequality proves the lemma. $\square$

Lemma 5.2 (The free-energy density $f_\Lambda^{SB}(\beta,y,c)$ in the thermodynamic limit)
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

$$f^{SB}(\beta,y,c) := \lim_{\Lambda} f_\Lambda^{SB}(\beta,y,c) = f_0^B(\beta,y,x) + \frac{\lambda_0}{2}(y+x)^2,$$

with $x = |c|^2 \geq 0$, and $f_0^B(\beta,y,x)$ defined as the Legendre-Fenchel transform of $p_0^B(\beta,\alpha,x)$ (2.12), cf. Theorem 4.1.

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

$$p_\Lambda^{SB}(\beta,\mu,c) = \frac{1}{\beta V} \ln \int_{\mathbb{R}_+} e^{\beta V \left(\mu y - f_\Lambda^{SB}(\beta,y,c)\right)} \nu_\Lambda(\mathrm{d}y) + \mu|c|^2, \tag{5.18}$$

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

$$p^{SB}(\beta,\mu,c) = \sup_{y \geq 0} \left\{ \mu y - f^{SB}(\beta,y,c) \right\} + \mu|c|^2, \tag{5.19}$$

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 (4.5). Thus, by using the *Tauberien theorem* proven in [20], 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

$$f^{SB}(\beta,y,c) = \sup_{\mu \in \mathbb{R}} \left\{ \mu(y+|c|^2) - p^{SB}(\beta,\mu,c) \right\} \ \text{ for } y \geq 0. \tag{5.20}$$

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

$$f^{SB}(\beta,y,c) = \sup_{\alpha \leq 0} \left\{ \alpha(y+|c|^2) - p_0^B(\beta,\alpha,|c|^2) \right\} + \frac{\lambda_0}{2}(y+x)^2. \tag{5.21}$$

$\square$

5.2 Large deviations principles

Let $\mathcal{X}$ denote a topological 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 $m \geq 0$. 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 with speed a_l and rate function I if, for any closed subset $\mathcal{C}$ of $\mathcal{X}$,

$$\limsup_{l\rightarrow+\infty} \frac{1}{a_l} \ln \mathbb{P}_l \left(X_l \in \mathcal{C}\right) = \limsup_{l\rightarrow\infty} \frac{1}{a_l} \ln \mathbb{P}_l \left(\mathcal{C}\right) \leq -\inf_{\mathcal{C}} \mathrm{I}\left(x\right), \tag{5.22}$$

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

$$\liminf_{l\rightarrow+\infty} \frac{1}{a_l} \ln \mathbb{P}_l \left(X_l \in \mathcal{G}\right) = \limsup_{l\rightarrow\infty} \frac{1}{a_l} \ln \mathbb{P}_l \left(\mathcal{G}\right) \leq -\inf_{\mathcal{G}} \mathrm{I}\left(x\right). \tag{5.23}$$

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 deviations principle*. The principle is called *weak* if the upper bound in (5.22) 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 large deviations principle is Varadhan's Lemma, which says that, for any bounded and continuous function $\varphi : \mathcal{X} \rightarrow \mathbb{R}$,

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

For a comprehensive treatment of the theory of large deviations, see [19].

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 invitation to CPT.

References

[1] J.T. Lewis, J.V. Pulé and V.A. Zagrebnov, The Large Deviation Principle for the Kac Distribution, *Helv. Phys. Acta* **61**: 1063-1078 (1988).

[2] J.L. Lebowitz, M. Lenci and H. Spohn, Large Deviations for Ideal Quantum Systems, *J. Math.Phys.* **41**: 1224-1243 (2000).

[3] G. Gallavotti, J.L. Lebowitz and V. Mastropietro, Large deviations in rarefied quantum gases, *J. Stat. Phys.* **108**(5/6): 831-861 (2002).

[4] N. Angelescu, A. Verbeure and V.A. Zagrebnov, On Bogoliubov's model of superfluidity, *J. Phys. A: Math.Gen.* **25**: 3473-3491 (1992).

[5] V.A. Zagrebnov and J.-B. Bru, The Bogoliubov Model of Weakly Imperfect Bose Gas, *Phys. Rep.* **350**: 291-434 (2001).

[6] N. Angelescu, A. Verbeure and V.A. Zagrebnov, Superfluidity III, *J. Phys. A: Math.Gen.* **30**: 4895-4913 (1997).

[7] S. Adams and J.-B. Bru, Critical Analysis of the Bogoliubov Theory of Superfluidity, *Physica A* **332**: 60-78 (2004).

[8] S. Adams and J.-B. Bru, Exact solution of the AVZ-Hamiltonian in the grand canonical ensemble, *Annales Henri Poincaré* **5**: 405-434 (2004).

[9] S. Adams and J.-B. Bru, A New Microscopic Theory of Superfluidity at all Temperatures, *Annales Henri Poincaré* **5**: 435-476 (2004).

[10] J.-B. Bru, Beyond the dilute Bose gas, *Physica A* **359**: 306-344 (2006).

[11] O. Brattelli and D.W. Robinson, *Operator Algebras and Quantum Statistical Mechanics, Vol II*, 2nd ed. Springer-Verlag, New York (1996).

[12] D. Ruelle, *Statistical Mechanics: Rigorous Results*, Benjamin-Reading, New-York (1969).

[13] J.-B. Bru and V.A. Zagrebnov, On condensations in the Bogoliubov Weakly Imperfect Bose-Gas, *J. Stat. Phys.* **99**:1297 (2000).

[14] V.A. Zagrebnov and J.-B. Bru, The Bogoliubov Model of Weakly Imperfect Bose Gas, *Phys. Rep.* **350**:291 (2001).

[15] J. Ginibre, On the Asymptotic Exactness of the Bogoliubov Approximation for many Bosons Systems, *Commun. Math. Phys.* **8**: 26-51 (1968).

[16] M. Reed and B. Simon, *Methods of Modern Mathematical Physics, Vol. I: Functional Analysis,* Academic Press, New York-London (1972).

[17] B. Simon, *The Statistical Mechanics of Lattice Gases, Vol. I*, Princeton Univ. Press, Princeton (1993).

[18] E.H. Lieb, R. Seiringer, and J. Yngvason, Justification of c-Number Substitutions in Bosonic Hamiltonians, *Phys. Rev. Lett.* **94**: 080401-1-4 (2005) .

[19] A. Dembo and O. Zeitouni, *Large Deviations Techniques and Applications,* 2nd ed. Springer-Verlag, New-York (1998).

[20] R.A. Minlos and A.Ja. Povzner, Thermodynamic limit for entropy, *Trans. Moscow Math. Soc.* **17:** 269 (1967).