Equilibrium states for the Bose gas

Lieselot Vandevenne ¹, André Verbeure ²
and
Valentin A. Zagrebnov ³

Instituut voor Theoretische Fysica, Katholieke Universiteit Leuven,
Celestijnenlaan 200D, B-3001 Leuven, Belgium
Université de la Méditerranée et Centre de Physique Théorique - CNRS,
Campus de Luminy-Case 907, F-13288 Marseille, Cedex 09, France

Abstract

The generating functional of the cyclic representation of the CCR (Canonical Commutation Relations) representation for the thermodynamic limit of the grand canonical ensemble of the free Bose gas with attractive boundary conditions is rigorously computed. We use it to study the condensate localization as a function of the homothety point for the thermodynamic limit using a sequence of growing convex containers. The Kac function is explicitly obtained proving non-equivalence of ensembles in the condensate region in spite of the condensate density being zero locally.

Keywords: Cyclic Representations of CCR, Bose-Einstein Condensation, Equivalence of Ensembles, Condensate Localization.

PACS: 05.30.Jp, 03.75.Fi, 67.40.-w.

¹KULeuven, lieselot.vandevenne@fys.kuleuven.ac.be
²KULeuven, andre.verbeure@fys.kuleuven.ac.be
³U II – Marseille, zagrebnov@cpt.univ-mrs.fr
1 Introduction

The interest in the phenomenon of standard Bose Einstein Condensation (BEC) revived in recent years due to the spectacular experimental work on Bosons in traps. We refer, e.g., to [9] and [12] for experimental and theoretical state of affairs. A renewed interest in old problems connected with the phase transition accompanying BEC is at order. The generic model for BEC is the free Bose gas as already was pointed out by Bose and Einstein in 1925. On the level of mathematical physics, the understanding of the phase transition started with the well known paper of Araki and Woods [1], where the generating functionals of the cyclic representations of the canonical commutation relations corresponding to the equilibrium states of the free Bose gas are computed for periodic boundary conditions. Lewis and Pulé [7, 8, 11] computed the grand canonical equilibrium states for a set of boundary conditions including the Dirichlet and Neumann boundary conditions but not the attractive boundary conditions. They are using the Kac method. An important consequence of their result is the explicit computation of a non-trivial Kac density showing non-equivalence of the canonical and grand-canonical ensembles in the condensate region. The next result is found in [3], where the same conclusion was obtained for generalized condensations in some models of imperfect gases with diagonal interactions.

In the present paper we complete this computation of the equilibrium states for the free Bose gas with attractive boundary conditions. About the relevance of this type of boundary conditions, see e.g. [4, 10]. This model has a particular type of condensation namely condensation in quantum states corresponding to isolated points in the spectrum. It is well known [10], [5] that in this case the condensate is situated at the "boundary" and not uniformly spread out everywhere in space. We give a precise formulation of the generating functional in the frame of the theory of generating functionals on the CCR in order to catch up the condensate. Finally we derive also that there is non-equivalence of ensembles, something which was unclear until now because of the fact that the quantum fluctuations show a pattern [6] completely different from the free Bose gas with Dirichlet or Neumann boundary conditions. The intuition behind this fact is related to a wondering peculiarity of the free Bose gas with attractive boundary conditions [10], [5]. If one takes the thermodynamic limit using a sequence of growing convex domains with the point of homothety at the origin of the coordinates, then locally the condensation density is always equal to zero. As a byproduct, our computations imply that the condensate is spatially situated in a region logarithmically close to the boundary of these increasing domains. In the present paper we take different positions of the homothety point for cubic containers to show that the density of this logarithmic stratum of condensate inherits also a spatial anisotropy due to the choice of cubic containers. Finally remark that for the rotating bucket case [11], one has also the effect of the condensate being increased at the boundary. But this is an effect of large angular momentum and not of the boundary conditions as in our case.
2 CCR-Representations and the generating functional

For details about the CCR algebra, we refer to [2].

Let $h$ be a complex pre-Hilbert space with inner product $(\cdot, \cdot)$. A representation of the CCR over $h$ on a Hilbert space $H$ is a map $f \mapsto W(f)$ of $h$ into the group $U(H)$ of unitary operators on a Hilbert space $H$ satisfying the Weyl relations:

$$W(f_1)W(f_2) = \exp \left\{ -\frac{i}{2} \text{Im}(f_1, f_2) \right\} W(f_1 + f_2)$$  \hspace{1cm} (2.1)

such that for each $f \in h$ the map $\lambda \mapsto W(\lambda f)$ of $\mathbb{R}$ into $U(H)$ is strongly continuous. By Stone’s theorem, this continuity condition implies the existence of self-adjoint operators $\Phi(f)$ such that

$$W(f) = \exp\{i\Phi(f)\}$$ \hspace{1cm} (2.2)

These $\Phi(f)$ are called field operators. The map $f \mapsto \Phi(f)$ is linear over $\mathbb{R}$, but not linear over $\mathbb{C}$. Using the $\Phi(f)$ we can now define the creation and annihilation operators $a^*(f)$ and $a(f)$ for $f \in h$ by:

$$a^*(f) = 2^{-1/2}\{\Phi(f) - i\Phi(if)\}$$ \hspace{1cm} (2.3)

$$a(f) = 2^{-1/2}\{\Phi(f) + i\Phi(if)\}$$ \hspace{1cm} (2.4)

A state on the CCR-algebra is a linear functional $\omega : h \to \mathbb{C}$ with the properties:

$$\omega(A^*A) \geq 0, \quad \omega(1) = 1, \quad \text{for } A \text{ linear combinations of the } W(f), \ f \in h$$

A representation $(W, H, \Omega)$ is called a cyclic representation if $\Omega$ is a cyclic vector. A vector $\Omega$ is cyclic if the set $\{W(f)\Omega\}_{f \in h}$ is dense in $H$. To each cyclic representation $(W, H, \Omega)$ of the CCR corresponds a generating functional $E : h \to \mathbb{C}$ given by:

$$E(f) = \omega(W(f)) = (\Omega, W(f)\Omega)$$ \hspace{1cm} (2.5)

**Proposition 2.1.** A functional $E : h \to \mathbb{C}$ is the generating functional of a cyclic representation of the CCR if and only if it satisfies the following conditions:

(i) $E(0) = 1$,

(ii) $\forall f \in h : \lambda \mapsto E(\lambda f)$ is continuous,

(iii) $\forall$ finite sets of complex numbers $c_1, \ldots, c_n$ and elements $f_1, \ldots, f_n \in h : \sum_i \sum_j E(f_i - f_j) e^{\pm \text{Im}(f_i, f_j)} c_i c_j \geq 0$. 

3
3 Kac-density and equivalence of ensembles

3.1 Concrete setup

Let $\Lambda_\nu^L = [-L/2, L/2]^\nu$ be a bounded region in $\mathbb{R}^\nu$ with volume $V = L^\nu$. We put $h_L = L^2(\Lambda_\nu^L)$ for the Hilbert space of the wave-functions in $\Lambda_\nu^L$ with the scalar product $(f, g)_{h_L} := \int_{\Lambda_\nu^L} dx^\nu f(x) g(x)$. Then $\Lambda_\nu^L \subseteq \Lambda_\nu^{L'}$, and $h_L \subseteq h_{L'}$ whenever $L \leq L'$ via natural imbedding.

Let $t^\sigma_L$ be the self-adjoint extension of the operator $-\Delta_L$ (with domain $\text{dom}(-\Delta_L) = C_0^\infty(\Lambda_\nu^L)$) determined by the boundary conditions $\partial_n \phi + \sigma \phi = 0$ on $\partial \Lambda_\nu^L$. Here $\partial_n$ is the directional derivative in the direction of the outward normal $n$ to $\partial \Lambda_\nu^L$. If the parameter $\sigma \leq 0$, we say that the boundary $\partial \Lambda_\nu^L$ is attractive.

First we have to solve the one-dimensional one-body eigenvalue problem on $\Lambda_L = [-L/2, L/2]$

$$(t^\sigma_L \phi)(x) = \lambda \phi(x)$$

with boundary conditions ($\sigma < 0$):

$$\begin{cases}
\left( \frac{d\phi}{dx} - \sigma \phi \right)_{x=-L/2} = 0, \\
\left( \frac{d\phi}{dx} + \sigma \phi \right)_{x=L/2} = 0.
\end{cases}$$

Due to these attractive boundary conditions, there are two negative eigenvalues tending to the same limit $-\sigma^2$ (when $L \to \infty$) and an infinite number of positive eigenvalues (for $L|\sigma| > 2$):

$$\epsilon_L(0) < \epsilon_L(1) < 0 < \epsilon_L(2) < \epsilon_L(3) < \ldots,$$

$$\epsilon_L(0) = -\sigma^2 - O(e^{-L|\sigma|})$$

$$\epsilon_L(1) = -\sigma^2 + O(e^{-L|\sigma|}),$$

$$k \geq 2: \left( \frac{(k-1)\pi}{L} \right)^2 < \epsilon_L(k) < \left( \frac{k\pi}{L} \right)^2.$$ (3.1)

The corresponding eigenfunctions $\{\phi_k^L\}_{k \in \mathbb{Z}^+}$ form a basis in $h_L$ and are given by

$$\phi_0^L(x) = \sqrt{\frac{2}{L}} \left( 1 + \frac{\sinh(L|\sigma|)}{L|\sigma|} \right)^{-1/2} \cosh(-|\sigma|x),$$

$$\phi_1^L(x) = \sqrt{\frac{2}{L}} \left( -1 + \frac{\sinh(L|\sigma|)}{L|\sigma|} \right)^{-1/2} \sinh(-|\sigma|x),$$

$$\phi_k^L(x) = \begin{cases} 
\sqrt{\frac{2}{L}} \left( 1 + \frac{\sin(\sqrt{\epsilon_L(k)}L)}{\sqrt{\epsilon_L(k)}L} \right)^{-1/2} \cos(\sqrt{\epsilon_L(k)}x), & \text{for } k \text{ even}, \\
\sqrt{\frac{2}{L}} \left( 1 - \frac{\sin(\sqrt{\epsilon_L(k)}L)}{\sqrt{\epsilon_L(k)}L} \right)^{-1/2} \sin(\sqrt{\epsilon_L(k)}x), & \text{for } k \text{ odd}.
\end{cases}$$
The eigenvalues and the wave functions of the corresponding multi-dimensional case have the form:

\[ E_L(k) = \sum_{i=1}^{\nu} \epsilon_L(k_i), \]

\[ \psi_L^k(x) = \prod_{i=1}^{\nu} \phi_L^k(x_i), \]

where \( k = \{k_i\}_{i=1}^{\nu} \in \mathbb{Z}_+^\nu \) and \( x = \{x_i\}_{i=1}^{\nu} \in \Lambda_L^\nu. \)

### 3.2 Kac density

The Kac density relates expectation values of observables in the canonical ensemble and those in the grand canonical ensemble. The canonical equilibrium state for a free Bose gas in a cube \( \Lambda_L^\nu \) of volume \( V = L^\nu \) with total particle density \( \rho \) and inverse temperature \( \beta \) is given by

\[
\omega_{\text{can}}^{\beta,\rho}(A) = \frac{\text{Tr}_{\mathcal{H}_{L,\beta}^{(n)}} A(n) e^{-\beta T_L^{\sigma,(n)}}}{\text{Tr}_{\mathcal{H}_{L,\beta}^{(n)}} e^{-\beta T_L^{\sigma,(n)}}}, \quad \text{where } n = [V \rho], \quad \text{dom}(A(n)) \subset \mathcal{H}_L^{(n)}, \tag{3.2}
\]

and \( T_L^{\sigma,(n)} \) is the \( n \)–particle free Bose gas Hamiltonian in the cube \( \Lambda_L^\nu \) with boundary conditions defined by \( \sigma \). Now we consider the grand canonical equilibrium state at chemical potential \( \mu \) and inverse temperature \( \beta \):

\[
\omega_{\text{g.c.}}^{\beta,\mu}(A) = \frac{\text{Tr}_{\mathcal{F}_{\beta,\mu}} A \exp\{-\beta (T_L^{\sigma} - \mu N_L)\}}{\text{Tr}_{\mathcal{F}_{\beta,\mu}} \exp\{-\beta (T_L^{\sigma} - \mu N_L)\}}, \quad \text{dom}(A) \subset \mathcal{F}_{L,B}. \tag{3.3}
\]

Here \( T_L^{\sigma} = \sum_{k \in \mathbb{Z}_+^\nu} E_L(k) a^*(\psi_k^L)a(\psi_k^L) \) is the free Bose gas Hamiltonian and \( N_L = \sum_{k \in \mathbb{Z}_+^\nu} N_{L,k} = \sum_{k \in \mathbb{Z}_+^\nu} a^*(\psi_k^L)a(\psi_k^L) \), is the particle number operator in \( \mathcal{F}_{L,B} \), the boson Fock space over \( L^2(\Lambda_L^\nu) \):

\[
\mathcal{F}_{L,B} = \mathcal{F}_B(L^2(\Lambda_L^\nu)) = \bigoplus_{n=0}^{\infty} \mathcal{H}_{L,B}^{(n)} \tag{3.4}
\]

with \( \mathcal{H}_{L,B}^{(n)} \) the symmetrized \( n \)–particle Hilbert space appropriate for bosons and \( \mathcal{H}_{L,B}^{(0)} = \mathbb{C} \). Notice that in the thermodynamic limit \( L \to \infty \) the canonical ensemble state \( \omega_{\text{can}}^{\beta,\rho}(\cdot) \) may not coincide with the equilibrium state of the grand canonical ensemble state \( \omega_{\text{g.c.}}^{\beta,\mu}(\cdot) \) for the corresponding particle density \( \rho \). Here \( \overline{\pi}(\beta, \rho) = \lim_{L \to \infty} \overline{\pi}_L(\beta, \rho) \) and \( \overline{\pi}_L(\beta, \rho) \) is a solution of the grand canonical particle density equation (see also (3.22))

\[
\rho = \omega_{\text{g.c.}}^{\beta,\mu}(N_L/V). \tag{3.5}
\]
By virtue of (3.4) the states (3.2) and (3.3) are related by
\[
\omega_{g.c.}^{L,\beta,\mu}(A) = \int_{\mathbb{R}^+} K_{g.c.}^{L,\beta,\mu}(d\xi) \omega_{can}^{L,\beta,\xi}(A([V\xi])),
\]  
(3.6)
where \( A^{(n)} = A[H_{L,B}^{(n)}] \) is a restriction of the operator \( A \) on the subspace \( H_{L,B}^{(n)} \) and
\[
K_{g.c.}^{L,\beta,\mu}(\xi) = \frac{\sum_{n=0}^{\infty} \exp(n\beta\mu) \text{Tr}_{H_{L,B}^{(n)}}(\exp(-\beta T_{L}^{(n)}))}{\text{Tr}_{H_{L,B}}(\exp(-\beta(T_{L} - \mu N_{L})))}. 
\]  
(3.7)
For a given grand canonical density (3.5), the measure (3.7) takes the form :
\[
K_{L,\beta,\rho}(d\xi) := K_{g.c.}^{L,\beta,\mu}(\xi) = d\xi K_{L,\beta}(\xi;\rho),
\]  
(3.8)
and the limit \( K_{\beta}(x;\rho) = \lim_{L \to \infty} K_{L,\beta}(x;\rho) \) is known as the Kac density, see e.g. [8]. If the Kac density happens to be a \( \delta \)-function with support at \( \rho \) , then clearly one has \(\text{strong equivalence of ensembles:}\)
\[
\omega_{g.c.}^{L,\beta,\mu}(A) = \omega_{can}^{L,\beta,\mu}(A), 
\]  
(3.9)
Otherwise there is only \text{weak equivalence of ensembles, see [3].}

The limit \( \rho_{c}(\beta) := \lim_{\mu \to -\nu\sigma^{2}} \lim_{L \to \infty} \omega_{g.c.}^{L,\beta,\mu}(N_{L}/V) \) is the critical density for the free Bose gas in a box with attractive boundary conditions. We shall show that in the model the canonical and the grand canonical ensembles are \text{not} equivalent in the \text{presence} of the Bose condensate, i.e. for \( \rho > \rho_{c}(\beta) \), or for \( \beta > \beta_{c}(\rho) \), where \( \rho_{c}(\beta_{c}(\rho)) = \rho \). The non-equivalence of ensembles in the case of the free Bose gas with \text{attractive} boundaries \text{is not the same phenomenon as in the case of the one with, for example Dirichlet, } \sigma = \infty, \text{or Neumann, } \sigma = 0, \text{boundary conditions. In the case of the attractive boundary conditions (} \sigma < 0)\text{, the condensation phenomenon is a surface effect (not a bulk effect as in the free Bose gas with } \sigma = \infty \text{ or } \sigma = 0): \text{the condensate is located near the walls, see Section 4.2.}

To determine the Kac density, we have to calculate (see (3.6))
\[
\omega_{g.c.}^{L,\beta,\mu}(W(f)) = \int_{\mathbb{R}^+} K_{L,\beta,\rho}(d\xi) \omega_{can}^{L,\beta,\xi}(W(f)) 
\]  
(3.10)
for any test function \( f \in C_{0}^{\infty}(\mathbb{R}^\nu) \), the \( C^{\infty} \)-functions on \( \mathbb{R}^\nu \) with compact support. Therefore we first must calculate the limit of the expectation value of the exponential function:
\[
\omega_{g.c.}^{\beta,\rho}(W(f)) := \lim_{L \to \infty} \omega_{g.c.}^{L,\beta,\mu}(W(f)) \]  
(3.11)
with \( \{\mu_{L}(\beta,\rho)\}_{L} \) solutions of the density equation (3.5).
This is possible because the states $\omega_{L,\beta,\mu}^{g.c}$, where $\mu < -\nu \sigma^2$, are quasi-free states, and these are easily obtained by using the truncated functionals $\omega_{L,\beta,\rho}(\ldots)_T$, see e.g. [2]. The functionals are defined by the recursion relations:

$$\omega_{L,\beta,\mu}^{g.c}(A_1 \ldots A_n) = \sum_{\tau \in P_n} \prod_{J \in \tau} \omega_{L,\beta,\mu}^{g.c}(A_{j(1)}, \ldots, A_{j(|J|)})_T$$

(3.12)

for all $A_i (i = 1, 2)$ creation or annihilation operators and $n \in \mathbb{N}$. The sum $\tau \in P_n$ is over all partitions $\tau$ of a set of $n$ elements into ordered subsets $J = \{j(1), \ldots, j(|J|)\} \in \tau$. One can verify that the truncated functionals associated to the equilibrium states $\omega_{L,\beta,\mu}^{g.c}$ satisfy

$$\omega_{L,\beta,\mu}^{g.c}(a^\tau(f))_T = \omega_{L,\beta,\mu}^{g.c}(a^\tau(f)) = 0,$$

$$\omega_{L,\beta,\mu}^{g.c}(a^*(f_1), a^*(f_2))_T = \omega_{L,\beta,\mu}^{g.c}(a(f_1), a(f_2))_T = 0,$$

$$\omega_{L,\beta,\mu}^{g.c}(a^*(f_1), a(f_2))_T = \left( f_2, \frac{1}{\psi_L^{(E_L(k) - \mu)} - 1} f_1 \right)_{h_L},$$

(3.13)

with $f, f_1, f_2, \ldots \in h_L$, the space of testfunctions with support in $\Lambda^\nu_L$, $a^\tau = \{a \text{ or } a^*\}$ and $t^\nu_L$ is the self-adjoint extension of the Laplacian $-\Delta_L$ corresponding to attractive boundary conditions $\sigma < 0$ on $\partial \Lambda^\nu_L$. Then the non-trivial two-point functions (3.13) are explicitly given by

$$\omega_{L,\beta,\mu}^{g.c}(a^*(f_1), a(f_2))_T = \sum_{k \in \mathbb{Z}^n} \frac{f_2(k)}{f_1(k)} \frac{1}{\psi_L^{(E_L(k) - \mu)} - 1},$$

(3.14)

where the transformation $f(x) \mapsto \hat{f}(k)$ of $f \in C_0^\infty(\mathbb{R}^n)$, is now defined by

$$\hat{f}(k) := (\psi_L^L, f)_{h_L} = \int_{\Lambda^\nu_L} dx \, \psi_L^L(x) f(x),$$

(3.15)

the Fourier transforms for the basis of $t^\nu_L$ (see section 3.1).

Now

$$\omega_{L,\beta,\mu}^{g.c}(W(f)) = \omega_{L,\beta,\mu}^{g.c}(e^{i\Phi(f)})$$

$$= \exp \sum_{n=1}^{\infty} \frac{i^n}{n!} \omega_{L,\beta,\rho}(\Phi(f), \Phi(f), \ldots, \Phi(f))_T,$$ 

(3.16)

where the $\omega_{L,\beta,\mu}^{g.c}(\Phi(f), \Phi(f), \ldots, \Phi(f))_T$ are the $n-$point truncated field correlation functions. Because of the fact that $\omega_{L,\beta,\mu}^{g.c}$ is a quasi-free state, only the two-point truncated correlation function is non-vanishing, yielding:

$$\omega_{L,\beta,\mu}^{g.c}(W(f)) = \exp \left( -\frac{1}{2} \omega_{L,\beta,\mu}^{g.c}(\Phi(f), \Phi(f))_T \right)$$

(3.17)

7
By virtue of (2.3) and (2.4) it can be rewritten in terms of the creation and annihilation operators \( a^\ast(f) \) and \( a(f) \):
\[
\omega_{L,\beta,\mu}^{g.c.}(\Phi(f), \Phi(f)) = \frac{1}{2} \langle f, f \rangle_{hl} + \omega_{L,\beta,\mu}^{g.c.}(a^\ast(f)a(f))
\]
so that the explicit form of the generating functional (3.17) becomes:
\[
\omega_{\beta,\mu}^{g.c.}(W(f)) = \lim_{L \to \infty} \omega_{L,\beta,\mu}^{g.c.}(W(f))
\]
\[
= \exp \left( -\frac{1}{4} \langle f, f \rangle_{hl} - \frac{1}{2} \lim_{L \to \infty} \omega_{L,\beta,\mu}^{g.c.}(a^\ast(f)a(f)) \right)
\]
A last remark about the thermodynamic limit. Notice that the grand-canonical ensemble for the free Bose gas exists only for \( \mu < \inf \text{spec}(t) \). Therefore, the solution of equation (3.5) verifies the inequality \( \overline{\mu}_L(\beta, \rho) < -\nu \sigma^2 \). Since the critical density
\[
\lim_{\mu \to -\nu \sigma^2} \lim_{L \to \infty} \omega_{L,\beta,\mu}^{g.c.} \left( \frac{N_L}{L^\nu} \right) = \rho_c(\beta)
\]
for the free Bose gas with attractive boundary conditions \( \sigma < 0 \) is finite for all dimensions greater than, or equal to one, [10], [5], Bose-Einstein condensation occurs for \( \rho > \rho_c(\beta) \):
\[
\rho_0(\beta) := \rho - \rho_c(\beta) = \lim_{L \to \infty} 2^\nu \omega_{L,\beta,\mu}^{g.c.} \left( \frac{N_L}{L^\nu} \right) > 0,
\]
where \( N_{L,0} \) is the number-operator on \( F_{L,B} \) of the zero mode \( k = 0 \). The factor \( 2^\nu \) is due to the asymptotic degeneracy of the inf \( \text{spec}(t) \) = \( -\nu \sigma^2 + O(e^{-L|\sigma|}) \) for \( L \to \infty \), see Section 3.1. Notice that (3.21) implies that the solution of (3.5) for \( \rho > \rho_c(\beta) \) has the asymptotics:
\[
\overline{\mu}_L(\beta, \rho) = -\nu \sigma^2 - \frac{2^\nu}{\beta(\rho - \rho_c(\beta))L^\nu} + o(L^{-\nu}).
\]
We use this result in the computations of the thermodynamic limit of the generating functional below.

We conclude this section by the following statement about the explicit form of the Kac density for the thermodynamic limit of the free Bose gas in the cubic box with attractive boundary conditions.

**Theorem 3.1.** For the free Bose gas \( T^\sigma_L \) with attractive boundary conditions \( \sigma < 0 \) the limiting Kac density has the form:

\[
K_\beta(\xi; \rho) = \begin{cases} 
\delta(\xi - \rho), & \text{for } \rho < \rho_c(\beta), \\
\frac{2^\nu \theta(\xi - \rho_c(\beta))}{(2^\nu - 1)!} \left( \frac{2^\nu(\xi - \rho_c(\beta))}{\rho - \rho_c(\beta)} \right)^{2^\nu-1} \exp \left\{ -\frac{2^\nu(\xi - \rho_c(\beta))}{\rho - \rho_c(\beta)} \right\}, & \text{for } \rho \geq \rho_c(\beta).
\end{cases}
\]

Here \( \theta(z \leq 0) = 0 \) and \( \theta(z > 0) = 1 \).
Proof: By the identity (3.10), the Kac density \( K_{\beta}(\xi; \rho) \) is related to the thermodynamic limit of the characteristic function of the particle density \( N_L/V \) for \( t \in \mathbb{R}^1 \):

\[
\lim_{L \to \infty} \omega_{L,\beta,\mu_L}(\beta,\rho)(\exp(itN_L/V)) = \int_{\mathbb{R}_+} K_{\beta,\rho}(d\xi) \omega_{\beta,\xi}^{\text{con}}(\exp(it\xi)) = \int_{\mathbb{R}_+} d\xi K_{\beta}(\xi; \rho) \exp(it\xi), \quad (3.24)
\]

To calculate the limit in the left-hand side of (3.24), we use that the state \( \omega_{L,\beta,\mu_L}(\beta,\rho) \cdot \) is quasi-free. Then

\[
\omega_{L,\beta,\mu_L}(\beta,\rho)(\exp(itN_L/V)) = \prod_{k \in \mathbb{Z}_i^\nu} \left\{ \frac{1 - \exp[-\beta(E_L(k) - \mu_L(\beta,\rho))]}{1 - \exp[-\beta(E_L(k) - \mu_L(\beta,\rho) - it/\beta L^\nu)]} \right\}. \quad (3.25)
\]

Since the \( 2^\nu \) lowest energy-levels, i.e. the levels for which \( k \in \mathbb{K}_{\leq 2^\nu} = \{ k \in \mathbb{Z}_i^\nu : k_i = 0,1; i = 1,\ldots,\nu \} \) are exponentially degenerated when \( L \to \infty : E_L(k \in \mathbb{K}_{\leq 2^\nu}) = -\nu \sigma^2 + O(e^{-L|\sigma|}) \), by virtue of (3.22) and (3.25) we get that

\[
\lim_{L \to \infty} \omega_{L,\beta,\mu_L}(\beta,\rho)(\exp(itN_L/V)) = \begin{cases} 
\exp(it\rho), & \text{for } \rho \leq \rho_c(\beta), \\
[1 - it2^{-\nu}(\rho - \rho_c(\beta))]^{-2^\nu} \exp(it\rho_c(\beta)), & \text{for } \rho > \rho_c(\beta).
\end{cases} \quad (3.26)
\]

Therefore, by (3.24), the Kac density (3.23) is the Fourier transformation of the right-hand side of (3.26). \( \square \)

4 The generating functional

4.1 Condensate and generating functional

We are interested in the thermodynamic limit of the generating functional \( \omega_{\beta,\rho}^{g,c}(W(f)) = \lim_{L \to \infty} \omega_{L,\beta,\mu_L}(\beta,\rho)(W(f)) \) for any \( f \in C_0^\infty(\mathbb{R}^\nu) \). To this end we choose the box \( \Lambda_L^\nu \) with \( L \) large enough such that the \( \Lambda_f := \text{supp}(f) \) is contained in \( \Lambda_L^\nu \). We consider here the generating functional \( \omega_{\beta,\rho}^{g,c}(W(f)) \) for \( f \) an element in \( C_0^\infty(\mathbb{R}^\nu) \).

**Theorem 4.1.** The generating functional \( \omega_{\beta,\rho}^{g,c}(W(f)) \) on \( C_0^\infty(\mathbb{R}^\nu) \) is given by:

\[
\omega_{\beta,\rho}^{g,c}(W(f)) = \exp \left( -\frac{1}{4}(f,f) \right) \exp \left( -\frac{1}{2}(f,g_\nu(\beta,\rho)f) \right), \quad (4.1)
\]
with operator \( g_\sigma(\beta, \rho) \) on \( L^2(\mathbb{R}^\nu) \) defined by

\[
(g_\sigma(\beta, \rho)f)(x) = \int_{\mathbb{R}^\nu} dy \, G_\sigma(\beta, \rho)(\|x - y\|) f(y),
\]

\[
G_\sigma(\beta, \rho)(r) = (4\pi \beta)^{-\nu/2} \sum_{n=1}^\infty e^{-r^2/4n\beta} \frac{e^{-n/r}}{n^{\nu/2}}, \tag{4.2}
\]

where \( \pi(\beta, \rho) < -\nu\sigma^2 \) for \( \rho < \rho_c(\beta) \) and \( \pi(\beta, \rho) = -\nu\sigma^2 \) for \( \rho \geq \rho_c(\beta) \) are limiting solutions of the grand canonical density equation (3.3).

**Proof**: In order to determine the generating functional \( \omega_{\beta, \rho}^c(W(f)) \), we have to compute \( \lim_{L \to \infty} \omega_{L, \beta, \pi_L(\beta, \rho)}^c(a^*(f)a(f)) \), see (3.19). Since the attractive boundary conditions \( \sigma < 0 \) create a gap in the spectrum \( \text{spec}(t_L^L) \), and respectively in \( \text{spec}(T_L^L) \), the calculations need a separation of the negative eigenvalues from the positive part of the spectrum.

We consider first the one-dimensional case, when there are only two negative eigenvalues tending to \(-\sigma^2\) for \( L \to \infty \), see Section 3.1. By virtue of (3.14) one gets for a given \( f \in C_0^\infty(\mathbb{R}^1) \) that

\[
\lim_{L \to \infty} \omega_{L, \beta, \pi_L(\beta, \rho)}^c(a^*(f)a(f)) = \lim_{L \to \infty} \sum_{k \in \mathbb{Z}} \left| \hat{f}(k) \right|^2 \frac{1}{e^{\beta(\epsilon L(k) - \pi_L(\beta, \rho))} - 1} = \lim_{L \to \infty} \left( \left| \hat{f}(0) \right|^2 \frac{1}{e^{\beta(\epsilon L(0) - \pi_L(\beta, \rho))} - 1} + \left| \hat{f}(1) \right|^2 \frac{1}{e^{\beta(\epsilon L(1) - \pi_L(\beta, \rho))} - 1} + \sum_{n=1}^\infty e^{-n\beta L(1)} \sum_{k=2}^\infty e^{-n\beta L(k)} \left| \hat{f}(k) \right|^2 \right) \tag{4.3}
\]

As mentioned before, we choose \( \Lambda_L \) large enough such that \( \text{supp} (f) = \Lambda_f \) is contained in \( \Lambda_L \). Then one estimates that \( |\hat{f}(0)|^2 \) has an asymptotics of the order of \( O(e^{-L|\sigma|}) \) for large \( L \) since

\[
|\hat{f}(0)|^2 = \left| \int_{\Lambda_f} dx \, f(x) \hat{\phi}_L^0(x) \right|^2 = 2L \left( 1 + \frac{\sinh(L|\sigma|)}{L|\sigma|} \right)^{-1} \left| \int_{\Lambda_f} dx \, f(x) \cosh(-|\sigma|x) \right|^2 = 4|\sigma| e^{-L|\sigma|} \left| \int_{\Lambda_f} dx \, f(x) \cosh(-|\sigma|x) \right|^2 + o(e^{-L|\sigma|}) \tag{4.4}
\]

The integral in the last expression is independent of \( L \), because \( \text{supp} (f) \) is finite and inside the box \( \Lambda_L \). Similarly one gets for \( L \to \infty \) that

\[
|\hat{f}(1)|^2 = 4|\sigma| e^{-L|\sigma|} \left| \int_{\Lambda_f} dx \, f(x) \sinh(-|\sigma|x) \right|^2 + o(e^{-L|\sigma|}) \tag{4.5}
\]
Consider now the coefficients of $|\hat{f}_L(0)|^2$ and of $|\hat{f}_L(1)|^2$ in (4.3). If $\rho < \rho_c(\beta)$, then $\bar{\rho}(\beta, \rho) < -\sigma^2$, i.e. $\epsilon_L(0) - \bar{\rho}(\beta, \rho) > 0$ for large $L$. Therefore, by virtue of (4.3), (4.4) and (4.5), both of those terms are of the order $O(e^{-L|\sigma|})$ for large $L$. If $\rho \geq \rho_c(\beta)$, then $\bar{\rho}(\beta, \rho) = -\sigma^2 + O(L^{-1})$, and one gets for large $L$:

\[
\left\{ \left| \hat{f}(0) \right|^2 \frac{1}{e^{\beta(\epsilon_L(0) - \bar{\rho}(\beta, \rho))}} - 1 + \left| \hat{f}(1) \right|^2 \frac{1}{e^{\beta(\epsilon_L(1) - \bar{\rho}(\beta, \rho))}} - 1 \right\} \approx \frac{1}{2} \rho_0(\beta) L \left\{ \left| \hat{f}(0) \right|^2 + \left| \hat{f}(1) \right|^2 \right\},
\]

where $\rho_0(\beta) = \rho - \rho_c(\beta)$ is the condensate density. Therefore, again by virtue of (4.4) and (4.5), these terms vanish in the limit $L \to \infty$.

Consider now the last term in the limit (4.3). By virtue of (3.15) for $\nu = 1$ (see Section 3.1) we can represent the sum over $k \geq 2$ in the following explicit form:

\[
\frac{2}{L} \sum_{\{k \geq 2: \text{even}\}} \left( 1 + \frac{\sin(\sqrt{\epsilon_L(k)}L)}{\sqrt{\epsilon_L(k)}L} \right)^{-1} \hat{F}_{\text{even}}(k) \hat{F}_{\text{even}}(k) e^{-s\epsilon_L(k)} + \frac{2}{L} \sum_{\{k \geq 2: \text{odd}\}} \left( 1 - \frac{\sin(\sqrt{\epsilon_L(k)}L)}{\sqrt{\epsilon_L(k)}L} \right)^{-1} \hat{F}_{\text{odd}}(k) \hat{F}_{\text{odd}}(k) e^{-s\epsilon_L(k)},
\]

where $s = n\beta$ and

\[
\hat{F}_{\text{even}}(k) := \int_{\Lambda_f} dx \cos(\sqrt{\epsilon_L(k)}x) f(x), \quad \hat{F}_{\text{odd}}(k) := \int_{\Lambda_f} dx \sin(\sqrt{\epsilon_L(k)}x) f(x). \quad (4.8)
\]

Since the spectrum $\{\epsilon_L(k)\}_{k \geq 2}$ verifies the conditions (3.1) and $f \in C_0^\infty(\mathbb{R}^1)$, the first and the second series of terms in (4.7) are Darboux-Riemann sums for the corresponding integrals:

\[
\lim_{L \to \infty} \left\{ \frac{2}{L} \sum_{\{k \geq 2: \text{even}\}} \left( 1 + \frac{\sin(\sqrt{\epsilon_L(k)}L)}{\sqrt{\epsilon_L(k)}L} \right)^{-1} \hat{F}_{\text{even}}(k) \hat{F}_{\text{even}}(k) e^{-s\epsilon_L(k)} + \frac{2}{L} \sum_{\{k \geq 2: \text{odd}\}} \left( 1 - \frac{\sin(\sqrt{\epsilon_L(k)}L)}{\sqrt{\epsilon_L(k)}L} \right)^{-1} \hat{F}_{\text{odd}}(k) \hat{F}_{\text{odd}}(k) e^{-s\epsilon_L(k)} \right\}
= \frac{1}{\pi} \int_0^\infty dk \Re (e^{ik \cdot \cdot \cdot} f)_{hL} \Re (e^{ik \cdot \cdot \cdot} f)_{hL} e^{-sk^2} + \frac{1}{\pi} \int_0^\infty dk \Im (e^{ik \cdot \cdot \cdot} f)_{hL} \Im (e^{ik \cdot \cdot \cdot} f)_{hL} e^{-sk^2}. \quad (4.9)
\]

The last expression of (4.9) yields:

\[
\frac{1}{2\pi} \int_{-\infty}^{\infty} dk \left( (e^{ik \cdot \cdot \cdot} f)_{hL} (e^{ik \cdot \cdot \cdot} f)_{hL} e^{-sk^2} \right)
= (4\pi s)^{-1/2} \int_{\mathbb{R}^1} dx \int_{\mathbb{R}^1} dy f(x) f(y) \exp \left\{ -\frac{|x - y|^2}{4s} \right\}. \quad (4.10)
\]
Finally, taking into account (4.4)–(4.6), (4.10), and the fact that $\overline{\mu}(\beta, \rho) \leq -\sigma^2 < 0$, we get for the limit (4.3) in the one-dimensional case:

$$\omega_{\beta, \rho}^{g.c}(a^*(f)a(f)) = (f, g_{\sigma, \nu=1}(\beta, \rho)f)_{h_L},$$  \hspace{1cm} (4.11)

where $g_{\sigma, \nu=1}(\beta, \rho)$ is the integral operator on $L^2(\mathbb{R})$ defined by

$$(g_{\sigma, \nu=1}(\beta, \rho)f)(x) = \int_{\mathbb{R}} dy \ G_{\sigma, \nu=1}(\beta, \rho)(|x-y|) f(y),$$

$G_{\sigma, \nu=1}(\beta, \rho)(r) = (4\pi\beta)^{-1/2} \sum_{n=1}^{\infty} e^{-r^2/4n\beta} \frac{e^{-n\beta\overline{\mu}(\beta, \rho)}}{n^{1/2}}.$

Using the results for the one-dimensional case, one computes the two-point correlation function $\omega_{\beta, \rho}^{g.c}(a^*(f)a(f))$ in the $\nu$-dimensional case. Since the first $2\nu$ wave functions $\{\psi^L_k(x)\}_{k \in \mathbb{Z}^\nu_+}$ have the same exponential behaviour as in the one-dimensional case and since $\inf_L \text{spec}(t^*_L) = -\nu\sigma^2$, see Section 3.1, we get:

$$\lim_{L \to \infty} \omega_{L, \beta, \overline{\mu}(\beta, \rho)}^{g.c}(a^*(f)a(f)) = \lim_{L \to \infty} \sum_{k \in \mathbb{Z}^\nu_+} |\hat{f}(k)|^2 \frac{1}{e^{\beta(E_L(k) - \overline{\mu}(\beta, \rho))} - 1}$$

$$= \sum_{n=1}^{\infty} e^{-n\beta\overline{\mu}(\beta, \rho)} (4\pi n\beta)^{-\nu/2} \int_{\mathbb{R}^\nu} dx \int_{\mathbb{R}^\nu} dy f(x) f(y) \exp \left\{ -\frac{\|x-y\|^2}{4n\beta} \right\},$$

which implies (4.2). By virtue of (3.19) this finishes the proof of (4.1) and of the theorem for any particle density $\rho$. \hfill \Box

Theorem 4.1 tells us that the condensate is not traceable by considering only strictly local observables. The characteristic functional on the CCR-C*-algebra of quasi-local observables coincides with the one without condensate. The reason for this is that the condensate is not homogeneous but located in the vicinity of the container boundary.

In order to catch up the presence of the condensate or to get a complete picture of the system, one has to extend the algebra of observables to the weak closure of the CCR-C*-algebra with respect to the limit Gibbs states. In the next paragraph we compute the limit functional on the relevant non-localised observables, and obtain a complete picture yielding the existence of sufficiently many fields in the representation of any $\ast$-limit point of Gibbs states as $L$ tends to infinity. In fact our strategy will be to make a relevant choice of the homothety point for the thermodynamic limit of convex containers, in order to catch up the condensate.

Above and below we considered only the easy shape container limit, namely cubic boxes. Because of the particular inhomogeneous spreading of the condensate in the neighbourhood of the box boundary, it is clear that this thermodynamic limit treatment can be very much shape dependent. In this paper we do not enter into the details of this specific problem.
4.2 Condensate localization

Remark 4.2. It sounds curious that in spite of the non-zero condensate density for $\rho > \rho_c(\beta)$, there is no trace of it in the generating functional (4.1). This is in contrast to the Kac density (3.23), which explicitly depends on the condensate density $\rho - \rho_c(\beta)$. To understand this difference one has to take into account that (4.1) is localized on the support of the function $f \in C_0^\infty(\mathbb{R}^n)$ whereas the Kac density is a global function, depending on the condensate even if it is localized at "infinity", stuck to the attractive boundaries.

In order to make this statement rigorous we start first with the one-dimensional case. Let the function $f \in C_0^\infty(\mathbb{R}^1)$ be such that $\text{supp}(f) = (-\delta, \delta) \subset (-L/2, L/2)$ and $\delta < (\ln L)/2|\sigma|$. Consider its shift over a distance $\gamma_L(\sigma) := L/2 - (2|\sigma|)^{-1}\ln L$:

$$f_{\gamma_L(\sigma)}(x) \equiv (\tau_{\gamma_L(\sigma)} f)(x) := f(x - [L/2 - (2|\sigma|)^{-1}\ln L]) \quad (4.12)$$

Then $f_{\gamma_L(\sigma)} \in C_0^\infty(-L/2, L/2)$.

To get the generating functional we compute now the limit of the corresponding two-point function (3.13):

$$\lim_{L \to \infty} \omega_{\beta, \rho_c(\beta)}^{L, \beta, \beta, \beta}(\tau_{\gamma_L(\sigma)} f) \equiv \alpha^{\beta, \rho_c(\beta)}(\tau_{\gamma_L(\sigma)} f)(\tau_{\gamma_L(\sigma)} f)$$

$$\begin{align*}
\lim_{L \to \infty} & \sum_{k=0}^{\infty} \left| \hat{f}_{\gamma_L(\sigma)}(k) \right|^2 \frac{1}{e^{\beta(\epsilon_L(k) - \beta, \beta)} - 1} \\
= & \lim_{L \to \infty} \left( \left| \hat{f}_{\gamma_L(\sigma)}(0) \right|^2 \frac{1}{e^{\beta(\epsilon_L(0) - \beta, \beta)} - 1} + \sum_{k=2}^{\infty} \left| \hat{f}_{\gamma_L(\sigma)}(k) \right|^2 \frac{1}{e^{\beta(\epsilon_L(k) - \beta, \beta)} - 1} \right) \quad (4.13)
\end{align*}$$

Remark 4.3. Notice that in contrast to (4.3), the shift (4.12) corresponds simply to the choice of a new point of homothety for the thermodynamic limit (4.13). In (4.3), the point of homothety coincides with the origin of coordinates $x = 0$, whereas in (4.13) this point is $L/2 - (2|\sigma|)^{-1}\ln L$.

Now, and in contrast to (4.3), $|\hat{f}_{\gamma_L(\sigma)}(0)|^2$ goes like $L^{-1}$ for large $L$. Indeed,

$$|\hat{f}_{\gamma_L(\sigma)}(0)|^2 = \left| \int_{\gamma_L(\sigma) - \delta}^{\gamma_L(\sigma) + \delta} dx f(\gamma_L(\sigma) f)(x) \phi_0^L(x) \right|^2$$

$$= |\sigma| L^{-1} \left| \int_{-\delta}^{\delta} dx f(x) e^{\sigma |x|} \right|^2 + o(L^{-1})$$

Remark that for $\rho > \rho_c(\beta)$ the first term in (4.13) remains now finite in the limit $L \to \infty$. Taking into account (3.21) and (3.22) one gets:

$$\lim_{L \to \infty} \left| \hat{f}_{\gamma_L(\sigma)}(0) \right|^2 \frac{1}{e^{\beta(\epsilon_L(0) - \beta, \beta)} - 1} = \frac{\rho_0(\beta, \rho)}{2} |\sigma| \left| \int_{-\delta}^{\delta} dx f(x) e^{\sigma |x|} \right|^2. \quad (4.14)$$
The same reasoning for the second term in formula (4.13) gives a similar result:

$$\lim_{L \to \infty} \frac{|\hat{f}_{\gamma L}(1)|^2}{e^{\beta(\epsilon_L(1)-\pi L(\beta,\rho))} - 1} = \rho_0(\beta, \rho) |\sigma| \left( \int_{-\delta}^{\delta} \frac{1}{x} \mid dx f(x) e^{\mid \sigma \mid x} \right)^2. \tag{4.15}$$

By the same computations as used in the proof of Theorem 4.1, the third term in (4.13) yields for $\rho > \rho_c(\beta)$:

$$\lim_{L \to \infty} \sum_{k=2}^{\infty} \frac{|\hat{f}_{\gamma L}(k)|^2}{e^{\beta(\epsilon_L(k)-\pi L(\beta,\rho))} - 1} = \sum_{n=1}^{\infty} \exp^{-n(\beta \sigma^2)(4\pi n \beta)^{-1/2}} \int_{\mathbb{R}^1} dx f(x) \int_{\mathbb{R}^1} dy f(y) \exp \left\{ \frac{-(x-y)^2}{4n\beta} \right\}. \tag{4.16}$$

Hence the two-point function for the one-dimensional problem becomes:

$$\lim_{L \to \infty} \omega^{g.c.}_{L, \beta, \pi L(\beta,\rho)}(a^*(\tau_{\gamma L}(\sigma)f)a(\tau_{\gamma L}(\sigma)f)) = \rho_0(\beta, \rho) |\sigma| \left( \int_{\mathbb{R}^1} \frac{1}{x} \mid dx f(x) e^{\mid \sigma \mid x} \right)^2 + (f, g_{\sigma,\nu=1}(\beta, \rho)f), \tag{4.17}$$

see (4.14) for the definition of the operator $g_{\sigma,\nu=1}(\beta, \rho)$.

It is evident that one gets the same result for the shift of $\text{supp}(f) = (-\delta, \delta)$ over a distance $-\gamma_L(\sigma) = -L/2 + (2|\sigma|)^{-1} \ln L$, i.e.:

$$\lim_{L \to \infty} \omega^{g.c.}_{L, \beta, \pi L(\beta,\rho)}(a^*(\tau_{\pm \gamma L}(\sigma)f)a(\tau_{\pm \gamma L}(\sigma)f)) = \rho_0(\beta, \rho) |\sigma| \left( \int_{\mathbb{R}^1} \frac{1}{x} \mid dx f(x) e^{\pm \mid \sigma \mid x} \right)^2 + (f, g_{\sigma,\nu=1}(\beta, \rho)f), \tag{4.18}$$

where

$$(\tau_{\pm \gamma L}(\sigma)f)(x) := f \left( x \mp \frac{L}{2} - (2|\sigma|)^{-1} \ln L \right). \tag{4.19}$$

Therefore, taking the thermodynamic limit $L \to \infty$ at one of the homothety points $\pm \gamma_L(\sigma)$, we get that the generating functional depends on the Bose-condensate density for $\rho \geq \rho_c(\beta)$:

$$\lim_{L \to \infty} \omega^{g.c.}_{L, \beta, \pi L(\beta,\rho)}(W(\tau_{\pm \gamma L}(\sigma)f)) = \exp \left( -\frac{1}{2}(f,f) \right) \exp \left( -\frac{1}{4}C_{\sigma,\nu=1}^+(f) - \frac{1}{2}(f, g_{\sigma,\nu=1}f) \right), \tag{4.20}$$

where, by virtue of (4.18), one has

$$C_{\sigma,\nu=1}^+(f) = \rho_0(\beta, \rho) |\sigma| \left( \int_{\mathbb{R}^1} \frac{1}{x} \mid dx f(x) e^{\pm \mid \sigma \mid x} \right)^2. \tag{4.21}$$
Remark 4.4. Notice that this result is due to a fine (logarithmic) tuning of the position of the homothety points \( \pm \gamma_L(\sigma) \). Indeed, take \( \pm \gamma_L(a\sigma) \), for \( 0 < a < 1 \), i.e. the homothety points are more distant from the boundary \( \pm L/2 \). Taking into account the explicit form of the eigenfunctions for \( k = 0, 1 \) one finds that now \( |\hat{f}_{x,\pm \gamma_L(\sigma)}(k = 0, 1)|^2 \) goes for large \( L \) like \( L^{-1/a} \). This implies that both limits (4.14) and (4.15), and hence (4.21), vanish. So, the generating functional (4.20) has the same form as for thermodynamic limit with the homothety point at the origin. In contrast to that, the choice \( 1 < a \) means that the homothety points are closer to the boundaries \( \pm L \). Then \( |\hat{f}_{x,\pm \gamma_L(\sigma)}(k = 0, 1)|^2 \) goes slower then \( L^{-1} \). This implies that both limits (4.14) and (4.15), and hence (4.21), becomes infinite. So, for \( \rho \geq \rho_c(\beta) \) the generating functional (4.20) is zero, whereas for \( \rho < \rho_c(\beta) \) it is nontrivial with \( C_{aL,\nu} = 1(\nu) = 0 \).

To interpret these results, consider the local particle density:

\[
\omega_{L,\beta,\rho_L(L,\beta,\rho)}^g(a^*(x)a(x)) = \sum_{k \in \mathbb{Z}^d} \frac{|\phi_k^L(x)|^2}{e^{\beta(c_k)(k - \rho(L,\beta,\rho) - 1)} - 1}. \tag{4.22}
\]

Here \( a(x) \) is the Bose-field operator such that \( a(f) = \int_{\mathbb{R}^d} df(x)a(x) \) for \( f \in C^\infty(\mathbb{R}^d) \) and \( N(x) = a^*(x)a(x) \) is the local number operator, cf. (3.14). Then by (3.25) and (3.14), the global density is:

\[
\omega_{L,\beta,\rho_L(L,\beta,\rho)}^g \left( \frac{N_L}{L} \right) = \frac{1}{L} \int_{\mathbb{R}^d} dx \omega_{L,\beta,\rho_L(L,\beta,\rho)}^g(a^*(x)a(x)) \tag{4.23}
\]

Consider the thermodynamic limit of the local particle density at the origin of the coordinates \( x = 0 \). Taking into account the explicit form of the eigenfunctions, one gets that

\[
\rho(\beta, \rho; x = 0) := \lim_{L \to \infty} \omega_{L,\beta,\rho_L(L,\beta,\rho)}^g(a^*(x = 0)a(x = 0)) = \frac{1}{\pi} \int_{\mathbb{R}^d} dk \frac{1}{e^{\beta(k^2 - \rho(L,\beta,\rho))} - 1} \tag{4.24}
\]

for \( \rho < \rho_c(\beta) \), and

\[
\rho(\beta, \rho; x = 0) = \lim_{L \to \infty} \omega_{L,\beta,\rho_L(L,\beta,\rho)}^g(a^*(x = 0)a(x = 0)) = \frac{1}{\pi} \int_{\mathbb{R}^d} dk \frac{1}{e^{\beta(k^2 + \sigma^2)} - 1} = \rho_c(\beta) \tag{4.25}\]

for \( \rho \geq \rho_c(\beta) \) by (4.22). By inspection of (4.21) and (4.25) based on the explicit formulae for the eigenfunctions one readily gets that

\[
\rho(\beta, \rho; x) = \rho(\beta, \rho; x = 0) \tag{4.26}
\]

for any \( x \) in a bounded domain \( D \), containing the origin of the coordinates \( x = 0 \). In particular we get that the limiting local density for \( x \in D \) corresponding to the first two modes \((k = 0, 1)\) is

\[
\rho_0(\beta, \rho; x) := \lim_{L \to \infty} \sum_{k = 0, 1} \frac{|\phi_k^L(x = 0)|^2}{e^{\beta(\epsilon(L,k - \rho(L,\beta,\rho))} - 1} = 0. \tag{4.27}
\]
On the other hand, the global Bose-Einstein condensation density (3.21) is also related exactly to these two modes:

$$\rho_0(\beta, \rho) = \lim_{L \to \infty} \frac{1}{L} \sum_{k=0,1} \frac{1}{e^{\beta (\epsilon_L(k) - \mu_L(\beta, \rho))} - 1} = \rho - \rho_c(\beta) > 0,$$

(4.28)

which is not present in (4.25).

Consider now the local density of the Bose-Einstein condensation (4.27) at the homothety points \(\pm \gamma_L(\sigma).\) Then taking into account the explicit form of the eigenfunctions \(\phi_{k=0,1}^L(x)\) and (3.22), we get that, in contrast to (4.27), the local condensate density is

$$\lim_{L \to \infty} \sum_{k=0,1} \frac{|\phi_k^L(x = \pm \gamma_L(\sigma))|^2}{e^{\beta (\epsilon_L(k) - \mu_L(\beta, \rho))} - 1} = \rho_0(\beta, \rho) |\sigma|.$$  

(4.29)

The same arguments as above show that this condensate local density varies from zero to infinity when the parameter \(a\) in the homothety point positions \(\pm \gamma_L(a \sigma)\) varies in the same interval.

**Remark 4.5.** These observations can be interpreted as follows: the Bose-Einstein condensate for attractive boundary conditions \(\sigma < 0\) is localized in a logarithmically narrow domain in the vicinity of the boundary. In other words this kind of condensation is a surface phenomenon. At the same time globally it is very "visible", since the Kac density indicates a non-equivalence of ensembles in the presence of the condensate, see Theorem 3.1.

For the generalization to the \(\nu\)-dimensional case, we start with the corresponding local condensate density:

$$\rho_0(\beta, \rho; x) := \lim_{L \to \infty} \sum_{k \in \{ \mathbb{Z}^\nu_+: k_\alpha = 0,1; \alpha = 1,\ldots,\nu \}} \frac{|\psi_k^L(x)|^2}{e^{\beta (\epsilon_L(k) - \mu_L(\beta, \rho))} - 1}.$$  

(4.30)

Let \(x\) belong to a bounded domain \(D^\nu,\) containing the origin of the coordinates \(x = 0.\) Then using the explicit expressions for the eigenfunctions \(\psi_k^L(x),\) see Section 3.1, and by the same arguments as above for \(\nu = 1,\) we obtain that the limit (4.30) is zero for all densities \(\rho > 0.\)

The product structure: \(\psi_k^L(x) = \prod_{i=1}^\nu \phi_{k^i}^L(x_i),\) implies that this conclusion does not change if we consider instead of \(x \in D^\nu,\) the condensate density in the vicinity of the points corresponding to the shifts where at least one among the \(\nu\) arguments remains unshifted. On the other hand, this structure and the asymptotics of \(\phi_{k=0,1}^L(x)\) for \(|x| \to \infty\) yields also that for any \(k \in \{ \mathbb{Z}^\nu_+: k_\alpha = 0, 1; \alpha = 1,\ldots,\nu \}\) one gets

$$\left( \prod_{\alpha=1}^{\nu} \tau_{\pm \gamma_L(a_\alpha \sigma)} \psi_k^L \right)(x = 0) = |\sigma|^{\nu/2} L^{-\frac{\nu}{2}(a_{1}^{-1} + a_{2}^{-1} + \ldots + a_{\nu}^{-1})} + o \left( L^{-\frac{\nu}{2}(a_{1}^{-1} + a_{2}^{-1} + \ldots + a_{\nu}^{-1})} \right)$$  

(4.31)
as $L \to \infty$. Then, by virtue of (3.22), the limit for the local condensate density becomes non-trivial:

$$
\lim_{L \to \infty} \sum_{k \in \mathbb{Z}_+^\nu : k_\alpha = 0, \ldots, 1; \alpha = 1, \ldots, \nu} \frac{\bigl| (\prod_{\alpha=1}^\nu \tau_{\pm \gamma_L(a_\alpha \sigma)} \psi_k^{(L)}) (x = 0) \bigr|^2}{e^{\beta(L) - \mu_L (\beta, \rho)}} - 1 = |\sigma| |(\rho - \rho_c(\beta))| > 0, \quad (4.32)
$$

if and only if

$$
a_1^{-1} + a_2^{-1} + \ldots + a_\nu^{-1} = \nu. \quad (4.33)
$$

This means that the condensate (up to logarithmic deviations) is localized essentially in the corners of the hypercube $\Lambda_L^\nu$, where $L \to \infty$. We proved the following statement:

**Theorem 4.6.** Let $x$ be in a bounded domain $D^\nu$, containing the origin of the coordinates $x = 0$, then the thermodynamic limit of the local particle density is

$$
\rho(\beta, \rho; x) := \lim_{L \to \infty} \sum_{k \in \mathbb{Z}_+^\nu} \frac{\bigl| \psi_k^{(L)} (x) \bigr|^2}{e^{\beta(L) - \mu_L (\beta, \rho)}} - 1 = \frac{1}{\pi^\nu} \int_{\mathbb{R}_+^\nu} \frac{1}{e^{\beta(k^2) - \mu_L (\beta, \rho)}} - 1, \quad (4.34)
$$

where $\mu_L (\beta, \rho) < -\nu \sigma^2$ for $\rho < \rho_c(\beta)$ and $\mu_L (\beta, \rho) = -\nu \sigma^2$ for $\rho \geq \rho_c(\beta)$. Thus $\rho(\beta, \rho; x) = \rho_c(\beta)$ for $\rho \geq \rho_c(\beta)$, i.e. the local condensate density $\rho_0(\beta, \rho; x) = 0$ for any $\rho > 0$. Whereas at the homothety points corresponding to the shifts $\prod_{\alpha=1}^\nu \tau_{\pm \gamma_L(a_\alpha \sigma)}$ with parameters satisfying (4.33), the local condensate density (4.32) is nontrivial. Moreover, besides being inhomogeneous it is also anisotropic and essentially localized in the directions of the corners of the hypercube $\Lambda_L^\nu$. Varying the parameters $\{a_\alpha\}_{\alpha=1}^\nu$ in the range $(0, +\infty)$ one finds this local condensate density varying from zero to infinity.

Now we extend Theorem 4.1 on the basis of our discussion above of the condensate localization and Theorem 4.6. Similar to the one-dimensional case, see Remark 4.4, our relevant localized observable in the $\nu$-dimensional case will be a function $f \in C_0^\infty(\mathbb{R}^\nu)$ such that $\text{supp}(f) = (-\delta_1, \delta_1) \times (-\delta_2, \delta_2) \times \ldots \times (-\delta_\nu, \delta_\nu) \subset \Lambda_L^\nu$ and with $\delta = \max_{\nu=1, \ldots, \nu} \delta_\nu$, such that $\delta < (\ln L)/2|\sigma|$. Consider in each coordinate the shift over a distance $\gamma_L(\sigma) = L/2 - (2|\sigma|)^{-1} \ln L$:

$$
\left( \prod_{\alpha=1}^\nu \tau_{\gamma_L(\sigma)} f \right) (x) = f \left( x_1 - (L/2 - (2|\sigma|)^{-1} \ln L), \ldots, x_\nu - (L/2 - (2|\sigma|)^{-1} \ln L) \right),
$$

then $\prod_{\alpha=1}^\nu \tau_{\gamma_L(\sigma)} f \in C_0^\infty(\Lambda_L^\nu)$.

To get the generating functional in the $\nu$-dimensional case, we compute the limit of the
corresponding two-point correlation function:

\[
\lim_{L \to \infty} \omega_{L,\beta,\tau_L(\beta,\rho)}^{\alpha,\gamma} \left( a^* \left( \prod_{\alpha=1}^\nu \tau_{\gamma_L(\sigma)} \hat{f} \right) a \left( \prod_{\alpha=1}^\nu \tau_{\gamma_L(\sigma)} \hat{f} \right) \right) \\
= \lim_{L \to \infty} \sum_{k \in \mathbb{Z}_+^\nu} \left| \prod_{\alpha=1}^\nu \left( \hat{f}_{\tau_{\gamma_L(\sigma)}}(k) \right) \right|^2 \frac{1}{e^{\beta E_L(k) - \tau_L(\beta,\rho)} - 1} \\
= \lim_{L \to \infty} \left( \sum_{k \in \{Z_+^\nu : k_\alpha = 0,1; \alpha = 1, \ldots, \nu\}} \left| \prod_{\alpha=1}^\nu \left( \hat{f}_{\tau_{\gamma_L(\sigma)}}(k) \right) \right|^2 \frac{1}{e^{\beta E_L(k) - \tau_L(\beta,\rho)} - 1} + \sum_{n=1}^\infty e^{n\beta \tau_L(\beta,\rho)} \sum_{k \in \mathbb{Z}_+^\nu \setminus \{Z_+^\nu : k_\alpha = 0,1; \alpha = 1, \ldots, \nu\}} e^{-nE_L(k)} \left| \prod_{\alpha=1}^\nu \left( \hat{f}_{\tau_{\gamma_L(\sigma)}}(k) \right) \right|^2 \right) \quad (4.35)
\]

This thermodynamic limit depends on the homothety point corresponding to the shifts \( \prod_{\alpha=1}^\nu \tau_{\gamma_L(\alpha,\sigma)} \) with parameters \( a_\alpha = 1 \). Notice that the factor \( \left| \prod_{\alpha=1}^\nu \left( \hat{f}_{\tau_{\gamma_L(\sigma)}}(k) \right) \right|^2 \) is of the order \( O(L^{-\nu}) \) for large \( L \):

\[
\left| \prod_{\alpha=1}^\nu \left( \hat{f}_{\tau_{\gamma_L(\sigma)}}(k) \right) \right|^2 = \int_{\gamma_L(\sigma) - \delta_1}^{\gamma_L(\sigma) + \delta_1} dx_1 \cdots \int_{\gamma_L(\sigma) - \delta_\nu}^{\gamma_L(\sigma) + \delta_\nu} dx_\nu \left| \prod_{\alpha=1}^\nu \left( \tau_{\gamma_L(\sigma)} \hat{f}(x) \psi^{L}(x) \right) \right|^2 \\
= |\sigma|^{\nu} L^{-\nu} \left| \int_{\text{supp}(f)} dx f(x) \prod_{\alpha=1}^\nu e^{\sigma|x_\alpha|} \right|^2 + o(L^{-\nu}) \quad (4.36)
\]

and for any \( k \in \{Z_+^\nu : k_\alpha = 0,1; \alpha = 1, \ldots, \nu\} \). Hence, by the same reasoning, which implies (4.32), the first \( 2^\nu \) terms in (4.35) give:

\[
\lim_{L \to \infty} \sum_{k \in \{Z_+^\nu : k_\alpha = 0,1; \alpha = 1, \ldots, \nu\}} \left| \prod_{\alpha=1}^\nu \left( \hat{f}_{\tau_{\gamma_L(\sigma)}}(k) \right) \right|^2 \frac{1}{e^{\beta E_L(k) - \tau_L(\beta,\rho)} - 1} \\
= \rho_0(\beta, \rho) |\sigma|^{\nu} \left| \int_{\mathbb{R}^\nu} dx f(x) \prod_{i=1}^\nu e^{\sigma|x_i|} \right|^2 \quad (4.37)
\]

For the last term in (4.35), we perform the computations as in Theorem 4.1 yielding:

\[
\lim_{L \to \infty} \sum_{k \in \mathbb{Z}_+^\nu \setminus \{Z_+^\nu : k_\alpha = 0,1; \alpha = 1, \ldots, \nu\}} \left| \prod_{\alpha=1}^\nu \left( \hat{f}_{\tau_{\gamma_L(\sigma)}}(k) \right) \right|^2 \frac{1}{e^{\beta E_L(k) - \tau_L(\beta,\rho)} - 1} \\
= \sum_{n=1}^\infty e^{-n\beta \sigma^2 (4\pi n\beta)^{-\nu/2}} \int_{\mathbb{R}^\nu} dx \int_{\mathbb{R}^\nu} dy f(x) \overline{f(y)} \exp \left\{ -\frac{\|x - y\|^2}{4n\beta} \right\} \quad (4.38)
\]
So, taking the thermodynamic limit $L \to \infty$ at one of the homothety points $\{\pm \gamma_L(\sigma)\}_{\sigma=1}^\nu$, we get now the generating functional for $\rho \geq \rho_c(\beta)$:

\[
\lim_{L \to \infty} \omega_{\beta,c}^{g,c}(L,\beta,\tau_{\pm \gamma_L(\sigma)} f) \left( \prod_{\sigma=1}^\nu W(\tau_{\pm \gamma_L(\sigma)} f) \right)
\]

\[
= \exp \left( -\frac{1}{4} (f,f) \right) \exp \left( -\frac{1}{2} C^\pm_{\sigma}(\beta,\rho)(f) - \frac{1}{2} (f,g_\sigma(\beta,\rho)f) \right)
\]

with

\[
C^\pm_{\sigma}(\beta,\rho)(f) = \rho_0(\beta,\rho)|\sigma|^{\nu} \int_{\mathbb{R}^\nu} dx \frac{f(x)}{\prod_{\sigma=1}^\nu e^{\pm |x_i|}} \chi_\nu(\alpha).
\]

Remark 4.7. Again this result is due to a fine (logarithmic) tuning of the position of the homothety points $\{\pm \gamma_L(\sigma)\}_{\sigma=1}^\nu$ in the corner directions of the hypercube $\Lambda_L^\nu$. Indeed, take as in Theorem 4.7 the shifts $\prod_{\sigma=1}^\nu \tau_{\pm \gamma_L(\sigma)}$, with $\sum_{\sigma=1}^\nu (a_\alpha)^{-1} > \nu$, i.e. the homothety points are too distant from the corners of the hypercube. Taking into account the explicit form of the eigenfunctions for $k \in \{Z_+^\nu : k_\alpha = 0, 1 : \alpha = 1, \ldots, \nu\}$, one finds now that $|\prod_{\sigma=1}^\nu \hat{f}_{\tau_{\pm \gamma_L(\sigma)}}(k)|^2$ with $k \in \{Z_+^\nu : k_\alpha = 0, 1 : \alpha = 1, \ldots, \nu\}$ goes like $L^{-\nu(a_1^{-1}+a_2^{-1}+\ldots+a_\nu^{-1})}$ for large $L$. This implies that the limits of the first $2^\nu$ terms (4.37), and hence (4.40), vanish. So, the generating functional (4.39) has the same form as for the thermodynamic limit with the homothety point at the origin $x = 0$. In contrast to that, the choice $0 < \sum_{\sigma=1}^\nu (a_\alpha)^{-1} < \nu$ means that the homothety points are too close to the corners of the hypercube $\Lambda_L^\nu$. Then $|\prod_{\sigma=1}^\nu \hat{f}_{\tau_{\pm \gamma_L(\sigma)}}(k)|^2$ with $k \in \{Z_+^\nu : k_\alpha = 0, 1 : \alpha = 1, \ldots, \nu\}$ goes to zero slower than $L^{-\nu}$. This implies that the limit (4.40) becomes infinite. So, for $\rho \geq \rho_c(\beta)$ the generating functional (4.39) is zero, whereas for $\rho < \rho_c(\beta)$ it remains nontrivial with $C^\pm_{\sigma}(f) = 0$.

Therefore, we have proved the following theorem:

Theorem 4.8. The generating functional $\lim_{L \to \infty} \omega_{\beta,c}^{g,c}(L,\beta,\tau_{\pm \gamma_L(\sigma)} f)$ on $C_0^\infty(\mathbb{R}^\nu)$ is given by

\[
\lim_{L \to \infty} \omega_{\beta,c}^{g,c}(L,\beta,\tau_{\pm \gamma_L(\sigma)} f) \left( \prod_{\sigma=1}^\nu W(\tau_{\pm \gamma_L(\sigma)} f) \right)
\]

\[
= \exp \left( -\frac{1}{4} (f,f) \right) \exp \left( -\frac{1}{2} C^\pm_{\sigma}(\beta,\rho)(f) - \frac{1}{2} (f,g_\sigma(\beta,\rho)f) \right)
\]

with

\[
C^\pm_{\sigma}(\beta,\rho)(f) = \rho_0(\beta,\rho)|\sigma|^{\nu} \int_{\mathbb{R}^\nu} dx \frac{f(x)}{\prod_{\sigma=1}^\nu e^{\pm |x_i|}} \chi_\nu(\alpha).
\]

\[
(g_\sigma(\beta,\rho)f)(x) = \int_{\mathbb{R}^\nu} dy G_\sigma(\beta,\rho)(|x - y|) f(y),
\]

\[
G_\sigma(\beta,\rho)(r) = (4\pi \nu)^{-\nu/2} \sum_{n=1}^\infty e^{-r^2/4n\beta} \frac{e^{-n\beta |\sigma|^2}}{n^{\nu/2}}.
\]
Here $\mu(\beta, \rho) < -\nu\sigma^2$ for $\rho < \rho_c(\beta)$ and $\mu(\beta, \rho) = -\nu\sigma^2$ for $\rho \geq \rho_c(\beta)$ are the limiting solutions of the grand canonical density equation (3.5), $\rho_0(\beta, \rho) = 0$ for $\rho < \rho_c(\beta)$ whereas $\rho_0(\beta, \rho) = \rho - \rho_c(\beta)$ for $\rho \geq \rho_c(\beta)$ and the function $\chi_\nu(a) = 0, 1, +\infty$, respectively for $\nu < \sum_{a=1}^{\nu} (a_\nu)^{-1}$, $\nu = \sum_{a=1}^{\nu} (a_\nu)^{-1}$, and $\nu > \sum_{a=1}^{\nu} (a_\nu)^{-1}$.

\[ \square \]

5 Concluding remarks

The main results of our analysis for the free Bose gas with attractive boundary conditions are contained in the Theorems 3.1, 4.1 and 4.8.

In Theorem 3.1 we obtain a Kac density function showing non-equivalence of the canonical and the grand canonical ensemble in the presence of the condensate even if the condensate density is locally zero.

We learn from Theorem 4.1 that the condensation is not visible in the expectation values of strictly localized observables because the Bose condensate is situated near the boundary of an "infinite container". Nevertheless one should observe the effects of condensation in the equilibrium states, i.e., in the generating functional.

Theorem 4.8 yields the answer. We make precise for which type of observables the equilibrium states show their dependence on the condensate. This completes the rigorous analysis of the problem of (non-)equivalence of ensembles for the free Bose gas with attractive boundary conditions and the inhomogeneous condensate localization.

Finally we repeat that we analyzed only the problem taking the thermodynamic limits in the sense of homothetically increasing cubes, with the consequence that the condensate is situated anisotropically in the direction of the corners of these cubes and is "localized at infinity". To prove this we tune the homothety point position at the logarithmic (in the units of the cube size) distance from the cube boundary. If instead one looks for the limit of spherical containers, this anisotropy in the positioning of the condensate should disappear. Does one expect spontaneous spherical symmetry breaking of the equilibrium states in this case?

Acknowledgements. The paper was initiated during V.A.Z.’s visit at the Instituut voor Theoretische Fysica, KU Leuven. He wishes to thank the Instituut voor Theoretische Fysica for hospitality.

References

[1] H. Araki and E.J. Woods, *Representations of the Canonical Commutation Relations Describing a Nonrelativistic Infinite Free Bose Gas*; J. Math. Phys. 4, 637-662 (1963)

[2] O. Bratteli and D.W. Robinson, *Operator Algebras and Quantum Statistical Mechanics Vol.2*; Springer-Verlag, Berlin, 1996
[3] J.-B. Bru, B. Nachtergaele, and V.A. Zagrebnov, \textit{The Equilibrium States for a Model with Two Kinds of Bose Condensation}; J. Stat. Phys. 109, 143-176 (2002)

[4] J.O. Indekeu and J.M.J. van Leeuwen, \textit{Wetting, Prewetting and Surface Transitions in Type-I Superconductors}; Physica C 251, 290-306 (1995)

[5] J. Landau and I.F. Wilde, \textit{On the Bose-Einstein Condensation of an Ideal Gas}; Commun. Math. Phys. 70, 43-51 (1979)

[6] J. Lauwers and A. Verbeure, \textit{Fluctuations in the Bose Gas with Attractive Boundary Conditions}; J. Stat. Phys. 108, 123-168 (2002)

[7] J.T. Lewis and J.V. Pulé, \textit{The Equilibrium State of the Free Boson Gas}; Commun. Math. Phys. 36, 1-18 (1974)

[8] J.T. Lewis and J.V. Pulé, \textit{The Free Boson Gas in a Rotating Bucket}; Commun. Math. Phys. 45, 115-131 (1975)

[9] L. Pitaevskii and S. Stringari, \textit{Bose-Einstein Condensation}; Oxford Univ. Press, Oxford, 2003

[10] D.W. Robinson, \textit{Bose-Einstein Condensation with Attractive Boundary Conditions}; Commun. Math. Phys. 50, 53-59 (1976)

[11] P. Tuyls, M. Van Canneyt and A. Verbeure, \textit{Angular Momentum Fluctuations of the Ideal Bose Gas in a Rotating Bucket}; J. Phys. A: Math. Gen. 28, 1-18 (1995)

[12] V.A. Zagrebnov and J.-B. Bru, \textit{The Bogoliubov Model of Weakly Imperfect Bose Gas}; Physics Reports 350, 291-442 (2001)