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On Generalized Bose-Einstein Condensation in the Almost-Ideal Boson Gas

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Abstract:

We scrutinize an interparticle interaction which can create the type-I generalized Bose-Einstein condensation in spite of other thermodynamic properties of the model coinciding with those for the free boson gas.

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1. Introduction

In a recent paper [1] we investigated the problem of equivalence of the canonical and grand canonical ensembles in connection with Bose-Einstein condensation (BEC). This problem is nontrivial already for the free boson gas, see e.g. [2-4] . That is why in our paper [1] we proposed a sequence of exactly soluable models with repulsive interactions involving an increasing number of particles. We observed the restoration of the strong equivalence of ensembles only for the model with the strongest interaction (model III of [1]) in spite of which the standard BEC persisits: One gets macroscopic occupation of the single-particle ground state above the critical density. One of the proposed models is the almost-ideal boson gas (model I of [1]) with the interaction in the ground state. As we observed for this model, BEC has a pecularity: the repulsive interaction forces the condensed particles to the first excited level. In the thermodynamic limit, this level coincides with the ground state. Therefore, from the naive point of view, BEC should coincide with that for the free boson gas. But we shall demonstrate that this is true only if the first excited level is nondegenerate. In the opposite case, BEC for model I is in fact the type-I generalized condensation (GC) in accordance with the classification proposed in [5,6]. For the reader's convenience, we recall the definition:

Type-I GC corresponds to the macroscopic occupation of a finite number of single-particle levels; type-II GC corresponds to the macroscopic occupation of an infinite number of single-particle levels; type-III GC corresponds to nonextensive BEC: no levels are macroscopically occupied on the scale of the volume.

In this paper, we prove that, in spite of their thermodynamic equivalence (coincide of their thermodynamic functions) the almost-ideal and the free boson gases have different Kac densities. Therefore, one can distinguish these two models by their different types of BEC.

2. The Model

Let $\Lambda \subset \mathbb{R}^{\nu}$ be a region in ν-dimensional Euclidean space with volume $V = |\Lambda|$, smooth boundary $\partial\Lambda$. Let $\sum(T_{\Lambda}^{\sigma}) = \{\varepsilon_k^{\sigma}(\Lambda)\}_{k=0}^{\infty}$ be the spectrum of the single-particle Hamiltonian T_{Λ}^{σ} corresponding to a self-adjoint extension of the operator $T_{\Lambda} = (-\Delta/2m)$, $D(T_{\Lambda}) = C_0^{\infty}(\Lambda)$ with σ-boundary conditions on $\partial\Lambda$. Here Δ is the ν-dimensional Laplacian and m is the particle mass. Below we consider "nonsticky" boundary conditions: $\sigma \geqslant 0$ [7] , and omit the index σ . Then, $\varepsilon_0(\Lambda) \geqslant 0$ and $\varepsilon_0(\Lambda) \searrow 0$ for $\Lambda \nearrow \mathbb{R}^{\nu}$. The thermodynamic limit (t-lim) is implemented by an isotropic dilation of the region Λ about the origin 0 which is assumed to lie inside Λ [8] .

To pass to the many-body problem. We introduce the probability space Ω of terminating sequences $\omega = \{\omega_k\}_{k \geqslant 0}$ of non-negative integers:

$$\Omega = \{\omega : \sum_{k \geqslant 0} \omega_k < \infty \ , \omega_k \in \mathbb{N}\} = \bigcup_{N \geqslant 0} \Omega^{(N)} \ ,$$

where $\Omega^{(N)} = \{\omega : \sum_{k \geqslant 0} \omega_k = N\}$. The basic dynamic (random) variables will be the occupation numbers $n_k : \omega \to \omega_k$, $k = 0, 1, 2 \ldots$.

The Hamiltonian $T_\Lambda^{(N)}$ of N free bosons in the region Λ can be written as

$$T_\Lambda^{(N)} = T_\Lambda \restriction \Omega^{(N)} \;, \quad T_\Lambda[\omega] = \sum_{k \geq 0} \varepsilon_k(\Lambda)\, n_k[\omega] \;. \tag{1}$$

Then the Hamiltonian H_Λ of the almost-ideal Bose gas (model I [1]) has the form

$$H_\Lambda[\omega] = T_\Lambda[\omega] + \frac{g}{2V}\, n_0^2[\omega] \quad , \quad g > 0 \;. \tag{2}$$

It corresponds to the switching on of the mean-field repulsive interaction between the bosons occupying the single-particle ground state.

Now we can define on the space Ω the grand canonical finite-volume Gibbs states $\langle - \rangle_{T_\Lambda}(\beta,\mu)$ and $\langle - \rangle_{H_\Lambda}(\beta,\mu)$ for the temperature $\beta^{-1} \geq 0$ and the chemical potential $\mu \leq 0$. It is clear that they correspond to the product measures. For the model (2) this measure has the form

$$P_\Lambda^\mu[\omega] = \frac{\exp\left(-\beta g\, n_0^2[\omega]/2V\right)}{\exp\left[\beta V\left(p_\Lambda(\beta,\mu) - p_\Lambda^0(\beta,\mu)\right)\right]}\, P_{\Lambda,0}^\mu[\omega] \;, \tag{3}$$

where $P_{\Lambda,0}^\mu[\omega]$ is the finite-volume free boson gas Gibbs measure:

$$P_{\Lambda,0}^\mu[\omega] = \frac{\exp\left[-\beta\left(T_\Lambda[\omega] - \mu N[\omega]\right)\right]}{\exp\left[\beta V p_\Lambda^{(0)}(\beta,\mu)\right]} \;. \tag{4}$$

Here $N[\omega]=\sum_{k\geq 0} n_k[\omega]$ is the total number of particles in the configuration ω, and

$$p_\Lambda^{(0)}(\beta,\mu)=(\beta V)^{-1}\ln\left\{\sum_{\omega\in\Omega}\exp\left[-\beta\left(T_\Lambda[\omega]-\mu N[\omega]\right)\right]\right\},$$

$$p_\Lambda(\beta,\mu)=(\beta V)^{-1}\ln\left\{\sum_{\omega\in\Omega}\exp\left[-\beta\left(H_\Lambda[\omega]-\mu N[\omega]\right)\right]\right\} \tag{5}$$

are the grand canonical pressures for the models (1) and (2). The thermodynamics potentials in the canonical ensemble (free-energy density) have the form

$$f_\Lambda^{(0)}(\beta,\rho)=-(\beta V)^{-1}\ln\left\{\sum_{\omega\in\Omega^{(N)}}\exp\left(-\beta T_\Lambda[\omega]\right)\right\},$$

$$f_\Lambda(\beta,\rho)=-(\beta V)^{-1}\ln\left\{\sum_{\omega\in\Omega^{(N)}}\exp\left(-\beta H_\Lambda[\omega]\right)\right\}. \tag{6}$$

They correspond to the finite-volume Gibbs measures in the canonical ensemble:

$$P_{\Lambda,0}^{(N)}=P_{\Lambda,0}^{\mu}\restriction\Omega^{(N)};\quad P_\Lambda^{(N)}=P_\Lambda^{\mu}\restriction\Omega^{(N)}. \tag{7}$$

Theorem 1. Let $\nu\geq 1$ and $g\geq 0$. Then, the model (2) is thermodynamically equivalent to the free boson gas (1):

(a) $t\text{-}\lim f_\Lambda(\beta,\rho)=t\text{-}\lim f_\Lambda^{(0)}(\beta,\rho)$, $\rho\geq 0$;

(b) $t\text{-}\lim p_\Lambda(\beta,\mu)=t\text{-}\lim p_\Lambda^{(0)}(\beta,\mu)$, $\mu\leq 0$.

Proof. (a) Let $\tilde{f}_\Lambda^{(0)}$ and $\tilde{p}_\Lambda^{(0)}$ be the finite-volume thermodynamic potentials of the free boson gas with the single-particle spectrum $\Sigma(T_\Lambda)\setminus\varepsilon_0(\Lambda)$. Then, one gets that $t\text{-}\lim(\tilde{f}_\Lambda^{(0)}-f_\Lambda^{(0)})=0$ and the inequalities

$$\inf_{\xi\geq 0}\left[\tfrac{1}{2}g\xi^2\rho^2+\tilde{f}_\Lambda^{(0)}(\beta,\rho(1-\xi))\right]\geq f_\Lambda(\beta,\rho)\geq$$

$$\geq-\frac{1}{\beta V}\ln(N+1)+\inf_{\xi\geq 0}\left[\tfrac{1}{2}g\xi^2\rho^2+\tilde{f}_\Lambda^{(0)}(\beta,\rho(1-\xi))\right]\quad, \tag{8}$$

where $\xi=n_0/V$ and $\rho=N/V$. Now, taking into account the monotonicity of the function $x\to f^{(0)}(\beta,x)=t\text{-}\lim f_\Lambda^{(0)}(\beta,x)$ and the inequalities (8) we obtain that $t\text{-}\lim(\tilde{f}_\Lambda^{(0)}-f_\Lambda)=0$, which provides the proof of (a).

(b) Using the explicit form of the Hamiltonian (2) one gets

$$p_\Lambda(\beta,\mu)=\tilde{p}_\Lambda^{(0)}(\beta,\mu)+$$
$$+\frac{1}{\beta V}\ln\left\{\sum_{n_0=0}^{\infty}\exp\left[\beta(\mu n_0-\varepsilon_0(\Lambda)n_0-gn_0^2/2V)\right]\right\}\quad. \tag{9}$$

Then, from the inequality $(\mu\leq 0)$

$$\sum_{n_0=0}^{\infty}\exp\left[\beta(\mu n_0-\varepsilon_0(\Lambda)n_0-gn_0^2/2V)\right]\leq c\left(\frac{V}{\beta g}\right)^{1/2}$$

and the limit $t\text{-}\lim(\tilde{p}_\Lambda^{(0)}-p_\Lambda^{(0)})=0$ we get the proof of (b). □

Corollary 1. The free-energy density $f(\beta,\rho)=t\text{-}\lim f_\Lambda(\beta,\rho)$ and the pressure $p(\beta,\mu)=t\text{-}\lim p_\Lambda(\beta,\mu)$ for the model (2) with $g\geq 0$ are related by the Legandre transform, i.e. for this model the canonical and the grand canonical ensembles are weekly equivalent.

3. Condensation and the Kac Density

The relation between thermodynamics and statistical mechanics for Bose systems has recently been scrutinized in several aspects [9-12]. In this section we show that in spite of the thermodynamic equivalence the models (1) and (2) are different.

Theorem 2. Let $g>0$ and Λ be a rectangular box with the equal edges (cuboid) and with the center at 0. Then, we get for the model (2) with $\sigma=+\infty$ (Dirichlet boundary condition) that

$$\text{(a)}\quad t\text{-}\lim\left\langle\frac{n_0}{V}\right\rangle_\Lambda(\beta,\rho)=t\text{-}\lim\left\langle\frac{n_0}{V}\right\rangle_\Lambda(\beta,\mu)=0\quad,\ \nu\geq 1\ ; \tag{10}$$

$$\text{(b)}\quad t\text{-}\lim\left\langle\frac{n_k}{V}\right\rangle_\Lambda(\beta,\rho)=t\text{-}\lim\left\langle\frac{n_k}{V}\right\rangle_\Lambda(\beta,\mu)=\begin{cases}0 & ,\ \rho<\rho_c^{(0)}\\ (\rho-\rho_c^{(0)})/\nu & ,\ \rho\geq\rho_c^{(0)}\end{cases} \tag{10b}$$

for $k=1,2,\ldots,\nu$ and $\nu>2$. Here $\langle-\rangle_\Lambda(\beta,\rho)$ and $\langle-\rangle_\Lambda(\beta,\mu)$ are the finite-volume canonical and grand canonical Gibbs states corresponding to the model (2); $\rho_c^{(0)}$ and $\mu_c^{(0)}(=0)$ are the critical parameters for the free boson gas.

Proof. (a). These two limits are the consequence of the estimate ($\mu\leq 0$)

$$\left\langle\frac{n_0}{V}\right\rangle_\Lambda(\beta,\mu)\leq\left\langle\frac{n_0}{V}\right\rangle_\Lambda(\beta,\mu=0)=$$

$$=\frac{1}{V}\sum_{\omega\in\Omega}n_0 P_\Lambda^{\mu=0}[\omega]=\frac{1}{V}\ \frac{\sum_{n_0\geq 0}n_0\exp(-\beta g n_0^2/2V)}{\sum_{n_0\geq 0}\exp(-\beta g n_0^2/2V)}\ . \tag{11}$$

(b) For the cuboid Λ the first excited level is 2ν-fold degenerate. Now, we can repeat the standard arguments about BEC to get

$$\rho = \left\langle \frac{n_0}{V} \right\rangle_\Lambda (\beta, \bar{\mu}_\Lambda(\rho)) + \nu \left\langle \frac{n_{k=1}}{V} \right\rangle_\Lambda (\beta, \bar{\mu}_\Lambda(\rho)) + + \sum_{k \geq \nu+1} \left\langle \frac{n_k}{V} \right\rangle_\Lambda (\beta, \bar{\mu}_\Lambda(\rho)) \,, \tag{12}$$

where $\mu = \bar{\mu}_\Lambda(\rho)$ is the solution of equation (11) for a fixed density ρ .

Hence, taking into account (10a) we derive from (11) that asymptotically

$$\bar{\mu}_\Lambda(\rho) \simeq \begin{cases} \bar{\mu}(\rho) + O(V^{-1}) \,, & \rho \leq \rho_c^{(0)} \\ \varepsilon_{k=1,2,\ldots,\nu}(\Lambda) - [\beta V(\rho - \rho_c^{(0)})/\nu]^{-1} + o(V^{-1}) \,, & \rho > \rho_c^{(0)} \end{cases} \tag{13}$$

where $\rho_c^{(0)} = \bar{\rho}(\beta, \mu = 0) = \partial_\mu p(\beta, \mu = 0)$ is equal to

$$t\text{-}\lim \sum_{k \geq \nu+1} \left\langle \frac{n_k}{V} \right\rangle_\Lambda (\beta, \mu = 0) = \left(\frac{m}{2\pi}\right)^{\nu/2} \frac{1}{\Gamma(\nu/2)} \int_0^\infty d\varepsilon \, \varepsilon^{\nu/2 - 1} (e^{\beta\varepsilon} - 1)^{-1} . \tag{14}$$

Collecting (12)-(14) one gets (10b). $\square$

Remark 1. The thermodynamic properties of the model (2) (including the values of the critical parameters) coincide with those for the free boson gas. If the first single-particle excited level is degenerate, then the interaction generates the type-I BEC instead of the BEC in the ground state alone. But if not (e.g. for Λ a rectangular box with different edges) the model (2) is identical to the free boson gas.

Remark 2. (A Generalized Almost-Ideal Bose Gas) From above it is clear that up to minor technical corrections the same properties are exhibited by the model

$$H_\Lambda^M = T_\Lambda + \sum_{k=0}^{M} g_k \frac{n_k^2}{2V} \quad , \ \{g_k > 0\}_{k=0}^{M} \quad . \tag{15}$$

Let $K_\Lambda^\mu = P_\Lambda^\mu \circ X_\Lambda^{-1}$ be the distribution function (the finite-volume Kac density) for the random variable $X_\Lambda(\omega) = \frac{N(\omega)}{V}$; it relates the Gibbs states of different ensembles:

$$\langle - \rangle_\Lambda(\beta,\mu) = \int_0^\infty dx\, K_\Lambda^\mu(x|\rho)\, \langle - \rangle_\Lambda(\beta,x) \quad ;$$

$$\rho = t\text{-}\lim \langle X_\Lambda \rangle_\Lambda (\beta, \bar{\mu}_\Lambda(\rho)) \; .$$

The limit distribution $K_{\beta,\mu} = t\text{-}\lim K_\Lambda^\mu$ (as the weak limit) plays an important role in analysing the ensemble equivalence [1-4] and BEC [5, 6, 8, 13]. The canonical and grand canonical ensembles are strongly (or statistically) equivalent if the limit distribution is degenerate: $K_{\beta,\mu}(x|\bar{\rho}) = \delta_{\bar{\rho}}(x)$ concentrated at $\bar{\rho}(\mu) = \partial_\mu p(\beta,\mu)$ [1].

Theorem 3. For the almost-ideal boson gas (2) with $g>0$ and isotropic dilation $\Lambda \nearrow \mathbb{R}^\nu$ of the cuboid Λ, the limit Kac density has the form $(\nu > 2)$:

$$K_{\beta,\mu}(x|\rho) = \begin{cases} \delta_\rho(x) \qquad , \quad \rho = \partial_\mu p(\beta,\mu) \leqslant \rho_c^{(0)} \; ; \\ \\ \dfrac{\nu}{(\nu-1)!} \cdot \dfrac{\theta(x-\rho_c^{(0)})}{\rho-\rho_c^{(0)}} \cdot \left[\dfrac{\nu(x-\rho_c^{(0)})}{\rho-\rho_c^{(0)}}\right]^{\nu-1} \exp\left[-\dfrac{\nu(x-\rho_c^{(0)})}{\rho-\rho_c^{(0)}}\right], \rho > \rho_c^{(0)} . \end{cases} \tag{16}$$

Proof. By definition, the Kac density $K_{\beta,\mu}(x|\rho)$ is related to the $t\text{-}\lim$ of the characteristic function of the random variable $X_\Lambda(\omega)$

$$t\text{-}\lim \langle \exp(itX_\Lambda) \rangle_\Lambda (\beta,\mu) = \int_0^\infty dx\, K_{\beta,\mu}(x|\rho) \exp(itx) \; . \tag{17}$$

To calculate the limit in the left-hand side of (17), we use the product-measure $P_\Lambda^\mu[\omega]$:

$$\langle \exp(itX_\Lambda)\rangle_\Lambda(\beta,\mu) =$$

$$= \sum_{n_0=0}^{\infty} P_\Lambda^{\mu}(n_0)\exp\left(\frac{itn_0}{V}\right)\prod_{k\geq 1}^{\infty}\left\{\frac{1-\exp[-\beta(\varepsilon_k(\Lambda)-\mu)]}{1-\exp[-\beta(\varepsilon_k(\Lambda)-\mu-it/\beta V)]}\right\} . \qquad (18)$$

Then, from the estimate (11) and the asymptotics (13) one gets

$$t\text{-}\lim\langle \exp(itX_\Lambda)\rangle_\Lambda(\beta,\mu) =$$

$$= \begin{cases} \exp(it\bar{\rho}(\mu)) & , \ \bar{\rho}(\mu) = \partial_\mu p(\beta,\mu) \leq \rho_c^{(0)}(\mu<0) \ ; \\ [1-it(\rho-\rho_c^{(0)})/\nu]^{-\nu}\exp(it\rho_c^{(0)}), & \rho = t\text{-}\lim\langle X_\Lambda\rangle_\Lambda(\beta,\bar{\mu}_\Lambda(\rho)) > \rho_c^{(0)}(\mu=0) . \end{cases} \qquad (19)$$

Expression (16) is the result of the Fourier-transform of the right-hand side of (19). □

Corollary 2. As for the free boson gas, the strong equivalence of ensembles for the model (2) is broken.

Remark 3. The dependence of the Kac density $K_{\beta,\mu}(x|\rho)$ on the parameter $g \geq 0$ is strongly nonanalytic. The deviation of $K_{\beta,\mu}(x|\rho)$ from the free boson gas Kac density

$$K_{\beta,\mu}^{(0)}(x|\rho) = \begin{cases} \delta_\rho(x) & , \ \rho = \partial_\mu p^{(0)}(\beta,\mu) \leq \rho_c^{(0)} \ (\mu < \mu_c^{(0)} = 0) \\ \dfrac{\theta(x-\rho_c^{(0)})}{\rho-\rho_c^{(0)}}\exp\left[-\dfrac{x-\rho_c^{(0)}}{\rho-\rho_c^{(0)}}\right] & , \ \rho > \rho_c^{(0)} \ (\mu = \mu_c^{(0)}) \end{cases}$$

is heavily dependent on the structure of the single-particle spectrum near the bottom. If the region Λ has a shape such that the first excited level is nondegenerate then $K_{\beta,\mu}(x|\rho) = K_{\beta,\mu}^{(0)}(x|\rho)$. In this case there is no difference between the almost-ideal and the free boson gases.

4. Conclusion

First it should be stressed that Theorem 3 and Remark 3 are valid for the model (15). The knowledge of the spectrum $\Sigma(T_\Lambda)$ and vector $\{g_k\}_{k=0}^{M}$ is sufficient to determine all possible corrections to the Kac density $K_{\beta,\mu}(x|\rho)$. As above, the result depends not on the absolute value of the $g_{k=0,1,\dots,M}$ but on their signs only.

In this connection it is interesting to consider the model (2) for $g<0$. Then, $p_\Lambda(\beta,\mu)=+\infty$ (collapse) and one has to save the situation by switching on a repulsive interaction as was done in [14]. But the free-energy density for the model (2) with $g<0$ exists and has the form

$$f(\beta,\rho)=\inf_{\xi\geq 0}\left[\frac{1}{2}g\xi^2\rho^2+f^{(0)}(\beta,\rho(1-\xi))\right] \quad . \tag{20}$$

Therefore, the weak equivalence is broken in this case.

For $\nu\geq 1$ the right-hand side of (20) reaches the infinum at $\bar{\xi}(\rho)=t\text{-}\lim\langle n_0/V\rangle_\Lambda(\beta,\rho)$:

$$\bar{\xi}(\rho)=\begin{cases} 0 & , \quad \rho\leq\rho_c(g) \\ \xi^*(\rho)>0 & , \quad \rho>\rho_c(g) \end{cases} ,$$

where $\xi^*(\rho)=\max\limits_{1,2}\{\xi_{1,2}(\rho)\}$ and $\xi_{1,2}(\rho)$ are nontrivial roots of the equation

$$g\xi\rho+\partial_x f^{(0)}(\beta,x=\rho(1-\xi))=0 \; .$$

The critical density $\rho_c(g)$ is defined by the relation

$$\rho_c(g)=\begin{cases} \rho_c^{(0)} & , \; \nu\geq 5 \, , \; -g\leq \lim\limits_{\rho\to\rho_c^{(0)}-0}\partial_\rho^2 f^{(0)}(\beta,\rho) \\ \rho^*<\rho_c^{(0)} & , \text{in the other cases} \end{cases} ,$$

where ρ^* is the solution of the equation

$$f^{(0)}(\beta,\rho)+\frac{g}{2}(\rho\cdot\xi^*(\rho))^2-f^{(0)}(\beta,\rho(1-\xi^*(\rho)))=0 \; .$$

Thus, the properties of the model (2) are very different for $g<0$ (collapse) and for $g>0$ (almost-ideal boson gas). Scrutinizing the models (2) and (15), we demonstrate how subtle BEC is: the interaction which does not change the thermodynamics can create generalized BEC.

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