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van den Berg, M

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On boson condensation into an infinite number of low-lying levels

M. van den Berg
Institute for Theoretical Physics, State University of Groningen, P. O. Box 800, Groningen, The Netherlands

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The complicated structure of the condensate of a free boson gas in two dimensions with mixed boundary conditions is examined.

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I. INTRODUCTION AND THEOREM

It has been shown in recent papers[1,2] that there exist three types of condensation in the free boson gas:

(I) Macroscopic occupation of a finite number of single-particle levels.

(II) Macroscopic occupation of an infinite number of single-particle levels.

(III) Nonextensive condensation (no levels macroscopically occupied).

In this paper we will present an example of type II. Let B_L be a finite region in R^d with volume L^d and let $E_1 < E_2^L < E_3^L \cdots$ be the spectrum of the single-particle Hamiltonian H_L; then [if we assume that $\exp(-\beta H_L)$ is trace-class] the mean number $\langle n_k \rangle_L$ of particles per volume in the kth state for a free boson gas is given by (in the grand canonical ensemble[3])

$$\langle n_k \rangle_L = \frac{1}{L^d} \frac{\zeta(L)}{e^{\eta_k^L} - \zeta(L)}, \tag{1}$$

where $\eta_k^L = E_k^L - E_1^L$ and $\zeta(L)$ is the positive solution of

$$\sum_k \langle n_k \rangle_L = \rho; \tag{2}$$

ρ is the mean number of particles per unit volume. The thermodynamic limit is the limit in which $L \to \infty$ and the number density ρ is kept fixed. If the spectrum of H_L is such that the critical density ρ_c, defined by

$$\rho_c = \lim_{\zeta \uparrow 1} \lim_{L \to \infty} \frac{1}{L^d} \sum_k (e^{\eta_k^L} - \zeta)^{-1}, \tag{3}$$

is finite, then condensation of type I, II, or III takes place if $\rho > \rho_c$. In the case when $H_L = -\Delta/2$ (with Dirichlet or Neuman conditions on the boundary ∂B_L of B_L) the critical density ρ_c is finite only for $d > 2$. However, if we impose attractive boundary on the eigenfunctions, then ρ_c is finite for all dimensions $d = 1,2,\cdots$. This was noticed by Robinson[4] and discussed in detail by Landau and Wilde.[5] The reason that ρ_c is finite in this case is that the attractive boundary conditions cause a gap in the single-particle spectrum:

$$E_j^L - E_1^L > g, \quad \text{for some } j > 1 \text{ and all } L > L_0. \tag{4}$$

It was noticed before by Bijl, De Boer, and Michels[6] that a gap in the spectrum will change the thermodynamical properties.

In this paper we will take $H_L = -\Delta/2$ and impose position-dependent boundary conditions. We will see that they lead to condensation of type II for $d = 2$ and of type I for $d = 1, d = 3, \cdots$. If the boundary conditions are position-independent, then there is condensation for $\rho > \rho_c$ of type I only (as in Ref. 4). Let us take for B_L the cuboid

$$B_L = \{x \in R^d : 0 < x_1 < L, \ldots, 0 < x_d < L\} \tag{5}$$

and let the boundary conditions be

$$\frac{\partial \phi}{\partial x_1} = -\sigma \phi \quad \text{for } x_1 = L, 0 < x_2 < L, \ldots, 0 < x_d < L, \tag{6}$$

$\phi = 0$ for any other point of the boundary.

The boundary conditions are said to be attractive if $\sigma < 0$. We have expressed all lengths in units $(\beta \hbar^2/m)^{1/2}$, where β is the inverse of the temperature times Boltzmann's constant. Let $\{\Phi_k^L\}$ be the eigenfunction of the Laplacian in B_L with boundary conditions (6) so that

$$-\tfrac{1}{2}\Delta \Phi_k^L = E_k^L \Phi_k^L. \tag{7}$$

Then

$$\Phi_k^L = \left(\frac{2}{L}\right)^{d/2} \left(1 - \frac{\sin 2L (2\epsilon_{k_1})^{1/2}}{2L (2\epsilon_{k_1})^{1/2}}\right)^{-1/2} \times \sin x_1 (2\epsilon_{k_1})^{1/2} \prod_{i=2}^{d} \sin \frac{\pi k_i x_i}{L},$$

$$E_k^L = \epsilon_{k_1} + \sum_{i=2}^{d} \frac{\pi^2 k_i^2}{2L^2}$$

$$k = (k_1, \ldots, k_d),$$

$$k_i = 1,2,3,\cdots \quad (i = 1,\ldots,d), \tag{8}$$

and $\{\epsilon_{k_1}\}$ are the positive solutions for ϵ of

$$\tan L (2\epsilon)^{1/2} = -(2\epsilon)^{1/2}/\sigma, \tag{9}$$

ordered so that $\epsilon_1 < \epsilon_2 < \epsilon_3 \cdots$. For $\sigma < -1/L$ and $L \gg 1$, the spectrum is approximately given by

$$\epsilon_{k_1} \sim (\pi^2/2L^2)(k_1 - 1)^2, \quad k_1 = 2,3,\cdots, \tag{10}$$

while there is a bound state with energy

$$\epsilon_1 \sim -\sigma^2/2. \tag{11}$$

Our main result is the following:

Theorem: For $\rho < \rho_c$, $\zeta(L)$ tends to the positive solution of

$$\rho = \sum_{n=1}^{\infty} \frac{\zeta^n}{(2\pi n)^{d/2}} e^{-n\sigma^2/2}. \tag{12}$$

For $\rho > \rho_c$, $\zeta(L)$ tends to 1 as follows:

$$\zeta(L) \sim 1 - 1/AL^2, \quad d = 2,$$

$$\zeta(L) \sim 1 - 1/(\rho - \rho_c)L^d, \quad d = 1,3,\cdots,$$

$$\rho_c = \sum_{n=1}^{\infty} \frac{e^{-n\sigma^2/2}}{(2\pi n)^{d/2}}, \tag{13}$$

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and A is the unique solution of

$$\sum_{k_2=1}^{\infty}\left(\frac{\pi^2}{2}(k_2^2-1)+\frac{1}{A}\right)^{-1}=\rho-\rho_c. \quad (14)$$

We see that due to (13) and (1)

$$\lim_{L\to\infty}\langle n_k\rangle_L=\begin{cases}[(\pi^2/2)(k_2^2-1)+1/A\,]^{-1} & k_1=1,\ k_2=1,2,3,\cdots\\ 0, & k_1=2,3,\cdots,\ k_2=1,2,\cdots\end{cases}\ d=2, \quad (15)$$

$$\lim_{L\to\infty}\langle n_k\rangle_L=\begin{cases}\rho-\rho_c, & k=(1,\ldots,1)\\ 0, & k\neq(1,\ldots,1)\end{cases}\ d\neq 2.$$

It follows that in two dimensions there is macroscopic occupation of an infinite set of low-lying single-particle states (condensation of type II) whereas in 1,3,4,$\cdots$ dimensions only the ground state is macroscopically occupied (type I).

This can also be seen by looking at the scaled spatial particle density ν_L defined by

$$\nu_L(u)=\sum_k\frac{\zeta(L)}{e^{\eta_k^L}-\zeta(L)}\,[\Phi_k^L(Lu)]^2. \quad (16)$$

One finds that

$$\lim_{L\to\infty}\nu_L(u)=\begin{cases}(\rho-\rho_c)\delta(1-u_1)+\rho_c, & d=1,\ \rho>\rho_c,\\ \delta(1-u_1)\displaystyle\sum_{j=1}^{\infty}\frac{2\sin^2\pi u_2}{(j^2-1)\pi^2/2+1/A}+\rho_c, & d=2,\ \rho>\rho_c,\\ (\rho-\rho_c)\delta(1-u_1)\displaystyle\prod_{m=2}^{d}2\sin^2\pi u_m+\rho_c, & d\geqslant 3,\ \rho>\rho_c,\\ \rho, & d\geqslant 1,\rho<\rho_c,\end{cases} \quad (17)$$

where $u\in B_1$ and $\delta(1-u_1)$ is the Dirac delta function supported on the hyperplane $u_1=1$. We see that the expressions [apart from (12) and (13)] are identical to the corresponding expressions for the free boson gas in the presence of an external field of power form in one direction (see Ref. 1). This is for the following reason: The attractive boundary condition causes a gap in the spectrum and forces the wavefunction to have a maximum near the attractive boundary. The same is true for one-particle Hamiltonian with an external potential with an absolute minimum at the boundary (and Dirichlet boundary conditions). We will give a sketch of the proof using the ideas of Lewis and Pulè.[7]

II. SKETCH OF THE PROOF

Let $f_L(z)$ be defined by

$$f_L(z)=\frac{1}{L^d}\sum_{n=1}^{\infty}z^n\sum_{\{k:k_1=1\}}e^{-n\eta_k^L}. \quad (18)$$

The first step is to show that for $z\in[0,1]$ we have

$$\lim_{L\to\infty}f_L(z)=\sum_{n=1}^{\infty}\frac{z^n}{(2\pi n)^{d/2}}e^{-n\sigma^2/2}. \quad (19)$$

This can be done using the asymptotic behavior of the E_k^L for large L given by (8),...,(11). Since it follows from (1) and (2) that for each $L>0$ and $\rho>0$ there is always a unique $\zeta(L)\in[0,1)$ we find that if $\zeta(L)$ tends to $\zeta\in[0,1)$ for $L\to\infty$, then

$$\rho=\sum_{n=1}^{\infty}\frac{\zeta^n}{(2\pi n)^{d/2}}e^{-n\sigma^2/2}+\lim_{L\to\infty}\frac{1}{L^d}\sum_{n=1}^{\infty}\zeta^n\sum_{\{k:k_1=1\}}e^{-n\eta_k^L}. \quad (20)$$

Since

$$\lim_{L\to\infty}\frac{1}{L^d}\sum_{n=1}^{\infty}\zeta^n\left[\sum_{k=1}^{\infty}\exp\frac{-n\pi^2}{2L^2}(k^2-1)\right]^{d-1}\leqslant\lim_{L\to\infty}\frac{1}{L^d}\sum_{n=1}^{\infty}\zeta^n\left(1+\frac{L}{(2\pi n)^{1/2}}\right)^{d-1}=0,$$

We arrive at Eq. (12). Suppose now that $\zeta(L)\to 1$; then

$$\frac{1}{L^d}\sum_{n=1}^{\infty}[\zeta(L)]^n\sum_{\{k:k_1=1\}}e^{-n\eta_k^L}\to\rho-\rho_c. \quad (21)$$

Equation (21) implies that for $d=1$ we have macroscopic occupation of the ground state. So for $d=2$ we have

$$\frac{1}{L^d}\sum_{k=1}^{\infty}\frac{\zeta(L)}{e^{\pi^2(k^2-1)/2}-\zeta(L)}\to\rho-\rho_c, \quad (22)$$

from which it follows that $\zeta(L)\sim 1-1/AL^2$, where A is the solution of (14). For $d\geqslant 3$ we have the following estimate:

$$\begin{aligned}&\frac{1}{L^d}\sum_{\{k:k_1=1\}}\frac{\zeta(L)}{e^{\eta_k^L}-\zeta(L)}-\frac{\zeta(L)}{1-\zeta(L)}\\ &=\frac{1}{L^d}\sum_{\substack{k:k_1=1\\ k\neq(1,\ldots,1)}}\frac{\zeta(L)}{e^{\eta_k^L}-\zeta(L)}\\ &\leqslant\frac{1}{L^d}\sum_{\substack{k:k_1=1\\ k\neq(1,\ldots,1)}}\frac{1}{e^{\eta_k^L}-1}\\ &\leqslant\frac{d}{L^d}\sum_{n=1}^{\infty}\sum_{k=2}^{\infty}\exp\left(-\frac{n\pi^2}{2L^2}(k^2-1)\right)\times\left[\sum_{k=1}^{\infty}\exp\left(-\frac{n\pi^2}{2L^2}(k^2-1)\right)\right]^{d-2}\\ &\leqslant\frac{d}{L^d}\sum_{n=1}^{\infty}e^{-n\pi^2/L^2}\frac{L}{(2\pi n)^{1/2}}\left(1+\frac{L}{(2\pi n)^{1/2}}\right)^{d-2}\\ &\leqslant\frac{d\,2^d}{L^d}\sum_{n=1}^{\infty}e^{-n\pi^2/L^2}\frac{L}{(2\pi n)^{1/2}}\left(1+\frac{L^{d-2}}{(2\pi n)^{(d-2)/2}}\right),\end{aligned} \quad (23)$$

which goes to zero as $L\to\infty$. So for $\rho>\rho_c$

$$\frac{1}{L^d}\frac{\zeta(L)}{1-\zeta(L)}\to\rho-\rho_c, \quad (24)$$

and we have macroscopic occupation of the ground state only (condensation of type I).

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