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On Condensation in the Free-Boson Gas and the Spectrum of the Laplacian

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We prove the convergence of the thermodynamic functions of a free boson gas for a d-dimensional ($d = 3, 4, \ldots$) van Hove sequence of convex regions. The thermodynamic functions behave singularly at a critical density ρ_c which is independent of the geometrical details of the sequence. We are led to define a second critical density ρ_m depending on the geometrical details of the sequence. For densities between ρ_c and ρ_m none of the single particle states is macroscopically occupied. We derive a sufficient condition on the sequence such that $\rho_m = \rho_c$.

KEY WORDS: Free boson gas; Laplacian; second critical density.

1. INTRODUCTION AND SUMMARY

In this paper we investigate the behavior in the thermodynamic limit of a free boson gas confined in a region of d-dimensional Euclidean space ($d = 3, 4, \ldots$) by a container with hard walls. Singularities in the thermodynamic functions occur at the well-known critical density ρ_c; to discuss macroscopic occupation of single-particle levels we are led to define a second critical density ρ_m which is not necessarily equal to ρ_c. This is discussed in a wider context in van den Berg, Lewis, and Pulè,[1] which generalizes the work of Lewis and Pulè,[2] van den Berg and Lewis,[3,4] and Landau and Wilde.[5]

In the second part of this paper we derive the equation of state for convex containers with Dirichlet boundary conditions. We consider a sequence of convex regions $B_1 \subset B_2 \subset \cdots \subset B_L \subset \cdots$ with volume V_L and surface area S_L. We prove that in the van Hove limit in which $V_L \to \infty$

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and $S_L/V_L \to 0$ the equation of state in the grand canonical ensemble converges to the well-known one (p. 214 in Ref. 7).

It was pointed out in Refs. 3 and 4 that there exist various types of condensation into low-lying single-particle states depending on the relative behavior of the bottom part of the spectrum with respect to V_L^{-1} as $V_L \to \infty$. Unfortunately that behavior is not known for general convex domains, so we restrict ourselves to the case of a rectangular parallelepiped with sides $L_1 \geqslant L_2 \geqslant L_3 \geqslant \cdots \geqslant L_d$, where the spectrum of $-\Delta/2$ is known exactly. This is the case described by Bratteli and Robinson in Ref. 6. They claim in Theorem 5.2.30 of Ref. 6 that the density of the condensate in the ground state is $\rho - \rho_c$ provided that $\rho > \rho_c$ and $(L_2 \ldots L_d)/L_1 \to \infty$ as the thermodynamic limit is taken. This is false, as can be seen by a counterexample: take $d = 3$ and take $L_1 = L_2 = e^L$, $L_3 = L$ [so that $(L_2 L_3)/L_1 \to \infty$ as $L \to \infty$]; then we will prove that the density of the ground state is zero in the limit $L \to \infty$ for all densities between ρ_c and $\rho_c + 1/\pi$. {Their error occurs on p. 68: $1 - z_L^2 \exp[-\beta\epsilon_m(\Lambda_L)]$ is not necessarily positive for $z_L < \exp[\beta\epsilon_0(\Lambda)]$. This is also used in their proof of Theorem 5.2.32 concerning the Gibbs grand canonical state, which is incorrect as it stands.} Our main result is the following: For a sequence of parallelepipeds such that $(L_2 \ldots L_d)/L_1$ converges to A and $\log L_2/(L_3 \ldots L_d)$ converges to B as $L_d \to \infty$, macroscopic occupation of single-particle states occurs if and only if A is strictly positive and ρ is greater than the second critical density ρ_m given by $\rho_m = \rho_c + B/\pi$. Moreover if ρ is greater than ρ_m and A is infinite the ground state alone is macroscopically occupied with density $\rho - \rho_m$. If ρ is greater than ρ_m and A is finite and positive then there is an infinite set of single-particle states with positive densities $\rho_1 \geqslant \rho_2 \geqslant \rho_3 \geqslant \cdots$ such that $\sum_{i=1}^{\infty} \rho_i = \rho - \rho_m$. We have shown elsewhere[4] that generalized condensation occurs whenever ρ is greater than ρ_c; we show here that macroscopic occupation of single-particle states is only possible if ρ is greater than ρ_m. This clarifies a remark by Ziff, Uhlenbeck, and Kac (p. 245 in Ref. 7) concerning the absence of large fluctuations and off-diagonal long-range order in a two-dimensional film with thickness L_3: if we approximate this system by taking a sequence of three-dimensional parallelepipeds in which we take L_1 and L_2 to infinity first then ρ_m is infinite and none of the single-particle states will become macroscopically occupied, so that the large fluctuations will not appear.

In the final section we consider again a general sequence of convex regions. We prove that for a wide class of sequences (and ρ greater than ρ_c) condensation into the ground state alone occurs with density $\rho - \rho_c$. This class is much larger than the one which obeys Fisher's uniform regularity condition[8] but smaller than the one which obeys Fisher's asymptotic regularity condition[8] which coincides with the van Hove condition (see Ref. 9).

2. THE THERMODYNAMIC FUNCTIONS

Let $B_1 \subset B_2 \subset B_3 \subset \cdots B_L \subset \cdots$ be a nested sequence of convex regions in d-dimensional Euclidean space ($d = 3, 4, \ldots$) with volume $V_1 \leqslant V_2 \leqslant \cdots V_L \leqslant \cdots$ and surface area $S_1 \leqslant S_2 \leqslant \cdots \leqslant S_L \leqslant \cdots$ (see Theorem 12.6 of Ref. 15). We denote by $E_1^L < E_2^L \leqslant E_3^L \leqslant \cdots$ the spectrum of the single-particle Hamiltonian $H_L = -\Delta/2$ with Dirichlet boundary conditions on ∂B_L. In the grand canonical ensemble for noninteracting bosons in the region B_L the mean occupation number $\langle n_k \rangle_L$ of single-particle level k is given by

$$\langle n_k \rangle_L = \xi(L)\left[e^{\eta_k^L} - \xi(L) \right]^{-1} \tag{1}$$

where $\eta_k^L = E_k^L - E_1^L$ and $\xi(L)$ is determined by the condition that the mean number $\langle N \rangle_L$ of bosons is given by

$$\sum_{k=1}^{\infty} \langle n_k \rangle_L = \langle N \rangle_L \tag{2}$$

The thermodynamic functions in the grand canonical ensemble can be expressed in terms of the spectrum of H_L and $\xi(L)$. For instance the pressure p_L is given by

$$p_L = -\frac{1}{V_L} \sum_{k=1}^{\infty} \log\left[1 - \xi(L) e^{-\eta_k^L} \right] \tag{3}$$

The thermodynamic limit in the sense of van Hove[9] is the limit in which V_L increases without bound while S_L / V_L becomes arbitrarily small and the mean density $\rho = \langle N \rangle_L / V_L$ is kept fixed. Our main result is the following theorem.

Theorem 1. The thermodynamic limit $\lim_{L \to \infty} \xi(L)$ exists for all values of ρ. For $\rho < \rho_c$ it is the unique root of

$$\rho = \sum_{n=1}^{\infty} \frac{\xi^n}{(2\pi n)^{d/2}} \tag{4}$$

while for $\rho > \rho_c$ we have $\lim_{L \to \infty} \xi(L) = 1$. The critical density

$$\rho_c = \sum_{n=1}^{\infty} \frac{1}{(2\pi n)^{d/2}} \tag{5}$$

In order to prove this result we need to solve the equation

$$\rho = \frac{1}{V_L} \sum_{n=1}^{\infty} \left[\xi(L) \right]^n \sum_{k=1}^{\infty} e^{-n\eta_k^L} \tag{6}$$

This can be done using estimates on the single-particle partition function which we state in the following lemma.

Lemma 1. For $t > 0$ and ∂B_L regular (in particular, B_L convex)

$$\sum_{k=1}^{\infty} e^{-tE_k^L} \leqslant \frac{V_L}{(2\pi t)^{d/2}} \tag{7}$$

and for $t > 0$ and B_L convex

$$\left| \sum_{k=1}^{\infty} e^{-tE_k^L} - \frac{V_L}{(2\pi t)^{d/2}} \right| \leqslant \frac{e^{d/2} S_L}{2 \cdot (2\pi t)^{(d-1)/2}} \tag{8}$$

Ray[10] has proved inequality (7) and Angelescu and Nenciu (pp. 25 and 26 of Ref. 14) have proved (8).

Lemma 2.

$$E_1^L \leqslant \frac{\pi^2 d^2 S_L^2}{8 V_L^2} \tag{9}$$

Proof. Let r_L denote the radius of the largest sphere inside the region; then (see Theorem 12 of Ref. 11)

$$r_L > \frac{V_L}{S_L} \tag{10}$$

So the largest d-dimensional cube in the region has sides greater than $d^{-1/2} \cdot 2r_L$. We obtain (9) by comparison. ■

Proof of Theorem 1. For $\rho \geqslant \rho_c$ we obtain a lower bound on $\xi(L)$ using (7):

$$\begin{aligned} \rho_c = \sum_{n=1}^{\infty} \frac{1}{(2\pi n)^{d/2}} \leqslant \rho &= \frac{1}{V_L} \sum_{n=1}^{\infty} \left[\xi(L) e^{E_1^L}\right]^n \sum_{k=1}^{\infty} e^{-nE_k^L} \\ &\leqslant \sum_{n=1}^{\infty} \frac{\left[\xi(L) e^{E_1^L}\right]^n}{(2\pi n)^{d/2}} \end{aligned} \tag{11}$$

and by Lemma 2 we have

$$\xi(L) \geqslant e^{-E_1^L} \geqslant 1 - E_1^L \geqslant 1 - \frac{\pi^2 d^2 S_L^2}{8 V_L^2} \tag{12}$$

Since $\xi(L) \leqslant 1$ we established $\lim_{L\to\infty} \xi(L) = 1$ because $S_L / V_L \to 0$ as $L \to \infty$. For $\rho < \rho_c$ we obtain similarly

$$\xi(L) \geqslant \xi\left(1 - \frac{\pi^2 d^2 S_L^2}{8 V_L^2}\right) \tag{13}$$

Let $T(L)$ be the greatest integer less or equal than $(V_L/S_L)^2$. Using (8) we have the estimate

$$\begin{aligned}\rho=\sum_{n=1}^{\infty}\frac{\xi^n}{(2\pi n)^{d/2}}&>\frac{1}{V_L}\sum_{n=1}^{T(L)}\left[\xi(L)\right]^n\sum_{k=1}^{\infty}e^{-nE_k^L}\\ &\geqslant\sum_{n=1}^{T(L)}\left[\xi(L)\right]^n\left[\frac{1}{(2\pi n)^{d/2}}-\frac{e^{d/2}S_L}{2V_L\cdot(2\pi n)^{(d-1)/2}}\right]\\ &\geqslant\sum_{n=1}^{\infty}\frac{\left[\xi(L)\right]^n}{(2\pi n)^{d/2}}-\sum_{n=T(L)+1}^{\infty}\frac{1}{(2\pi n)^{d/2}}-\sum_{n=1}^{T(L)}\frac{e^{d/2}S_L}{2\cdot(2\pi n)^{(d-1)/2}V_L}\\ &\geqslant\sum_{n=1}^{\infty}\frac{\left[\xi(L)\right]^n}{(2\pi n)^{d/2}}-\frac{2S_L}{V_L}\left(1+\log\frac{V_L}{S_L}\right)\end{aligned}\tag{14}$$

for $d=3,4,\ldots$. Hence

$$\xi(L)\leqslant\xi+\frac{2\cdot(2\pi)^{d/2}S_L}{V_L}\left(1+\log\frac{V_L}{S_L}\right)\tag{15}$$

and both the right-hand sides of (13) and (15) converge to ξ as $L\to\infty$. ■

Theorem 2. $\lim_{L\to\infty}p_L$ exists and is given by

$$p=\lim_{L\to\infty}p_L=\begin{cases}\displaystyle\sum_{n=1}^{\infty}\frac{\xi^n}{n\cdot(2\pi n)^{d/2}}, & \rho\leqslant\rho_c\\ \displaystyle\sum_{n=1}^{\infty}\frac{1}{n\cdot(2\pi n)^{d/2}}, & \rho>\rho_c\end{cases}\tag{16}$$

Proof.

$$\begin{aligned}|p-p_L|\leqslant&\left|\sum_{n=1}^{\infty}\left\{\frac{\left[\xi(L)\right]^n}{n\cdot(2\pi n)^{d/2}}-\frac{\xi^n}{n\cdot(2\pi n)^{d/2}}\right\}\right|\\ &+\sum_{n=1}^{\infty}\frac{\left[\xi(L)\right]^n}{n}\left(e^{nE_1^L}-1\right)\sum_{k=1}^{\infty}e^{-nE_k^L}\\ &+\sum_{n=1}^{\infty}\frac{\left[\xi(L)\right]^n}{n}\left|\frac{1}{V_L}\sum_{k=1}^{\infty}e^{-nE_k^L}-\frac{1}{(2\pi n)^{d/2}}\right|\equiv\mathrm{I}+\mathrm{II}+\mathrm{III}\end{aligned}\tag{17}$$

Term I becomes small by Theorem 1. Term III becomes small by (8) and for II we have

$$\mathrm{II} \leqslant \sum_{n=1}^{A(L)} \frac{E_1^L e^{A(L)E_1^L}}{(2\pi n)^{d/2}} + \sum_{n=A(L)+1}^{\infty} \frac{[\xi(L)]^n}{n} \cdot \frac{1}{V_L} \sum_{k=1}^{\infty} e^{-n\eta_k^L}$$

$$\leqslant E_1^L(e\rho_c + \rho) \tag{18}$$

where $A(L)$ is the greatest integer less or equal than $(E_1^L)^{-1}$. ■

Notice that the other thermodynamic functions like the entropy density, etc., converge in the infinite volume limit in a similar way.

3. THE OCCUPATION NUMBERS

From Theorem 1 it is clear that for $\rho < \rho_c \lim_{L\to\infty}\langle n_k\rangle_L / V_L = 0$ for all k since $\lim_{L\to\infty}\xi(L) = \xi < 1$. For $\rho > \rho_c$ we restrict ourselves to the case where the convex region is a rectangular parallelepiped with sides $L_1 \geqslant L_2 \cdots \geqslant L_d$. The spectrum of $-\Delta/2$ with Dirichlet (zero) boundary conditions is then given by

$$\eta_k^L = \frac{\pi^2}{2} \sum_{i=1}^{d} \frac{k_i^2 - 1}{L_i^2} \tag{19}$$

where k denotes herein the multi-index $(k_1, \ldots, k_d)$ and $k_i = 1, 2, \ldots$ for $i = 1, \ldots, d$.

Theorem 3. Let the infinite volume limit $(L \to \infty)$ be such that the mean density ρ is kept fixed and

1. $$L_1 \geqslant L_2 \cdots \geqslant L_d \to \infty$$
2. $$\lim_{\{L_1\to\infty, \ldots, L_d\to\infty\}} \frac{L_2 \ldots L_d}{L_1} = A$$
3. $$\lim_{\{L_1\to\infty, \ldots, L_d\to\infty\}} \frac{\log L_2}{L_3 \ldots L_d} = B$$

then for $\rho \leqslant \rho_m \equiv \rho_c + B/\pi$ none of the single-particle states are macroscopically occupied. For $\rho > \rho_m$ we have

$$\rho_k \equiv \lim_{L\to\infty} \frac{1}{V_L} \langle n_{k_1,1,\ldots,1}\rangle_L = \left[\frac{\pi^2}{2}(k_1^2 - 1) + C\right]^{-1}, \qquad 0 < A < \infty \tag{20}$$

and

$$\rho_{(1,\ldots,1)} \equiv \lim_{L\to\infty} \frac{1}{V_L} \langle n_{1,1,\ldots,1}\rangle_L = \rho - \rho_m \qquad \text{if} \quad A = \infty \tag{21}$$

and

$$\rho_k \equiv \lim_{L\to\infty} \frac{1}{V_L} \langle n_k\rangle_L = 0 \tag{22}$$

for $k \neq (k_1, 1, \ldots, 1)$ if $0 < A < \infty$ and for $k \neq (1, \ldots, 1)$ if $A = \infty$ and for all k if $A = 0$. C is the positive solution of

$$\sum_{k=1}^{\infty} \left[(k^2 - 1)\pi^2/2 + C \right]^{-1} = A(\rho - \rho_m) \tag{23}$$

The following Lemma is the key to the proof of Theorem 3.

Lemma 3. For $z \in [0, 1]$

$$\lim_{L\to\infty} \sum_{\{k\,:\,k\neq(k_1,k_2,1,1,\ldots,1)} \frac{1}{V_L} \cdot \frac{z}{e^{\eta_k^L} - z} = \sum_{n=1}^{\infty} \frac{z^n}{(2\pi n)^{d/2}} \tag{24}$$

Proof. Let us define for $n > 0$

$$a(L,n) = \sum_{k=2}^{\infty} \exp\left[-\frac{n\pi^2}{2L^2}(k^2 - 1) \right] \tag{25}$$

then

$$a(L,n) \leqslant \frac{L}{(2\pi n)^{1/2}} \exp\left(-\frac{n\pi^2}{L^2} \right) \tag{26}$$

$$a(L,n) \geqslant \left[\frac{L}{(2\pi n)^{1/2}} - 2 \right] \exp\left(-\frac{3n\pi^2}{2L^2} \right) \tag{27}$$

hence

$$\left| a(L,n) - \frac{L}{(2\pi n)^{1/2}} \exp\left(-\frac{n\pi^2}{L^2} \right) \right| \leqslant 2\left(\frac{n^{1/2}}{L} + 1 \right) \exp\left(-\frac{n\pi^2}{L^2} \right) \tag{28}$$

$$\left| a(L,n) - \frac{L}{(2\pi n)^{1/2}} \right| \leqslant 6\left(\frac{n^{1/2}}{L} \right) + 2 \tag{29}$$

We have the expansion

$$\begin{aligned} &\frac{1}{V_L} \sum_{\{k\,:\,k\neq(k_1,k_2,1,\ldots,1)\}} z\left(e^{\eta_k^L} - z\right)^{-1} \\ &= \frac{1}{V_L} \sum_{n=1}^{\infty} z^n \Bigg[\sum_{i=3}^{d} a(L_i, n) + \sum_{\substack{1\leqslant i<j\leqslant d \\ (i,j)\neq(1,2)}} a(L_i, n)a(L_j, n) + \sum_{1\leqslant i<j<l\leqslant d} \\ &\qquad a(L_i, n)a(L_j, n)a(L_l, n) + \cdots + \prod_{i=1}^{d} a(L_i, n) \Bigg] \end{aligned} \tag{30}$$

By (26)

$$\frac{1}{V_L}\sum_{n=1}^{\infty} z^n \sum_{i=3}^{d} a(L_i,n) \leqslant \frac{1}{V_L}\sum_{i=3}^{d}\int_0^{\infty}\frac{L_i}{(2\pi n)^{1/2}}\exp\left(-\frac{n\pi^2}{L_i^2}\right)dn$$

$$\leqslant (d-2)\prod_{i=3}^{d}(L_i)^{-1} \tag{31}$$

$$\frac{1}{V_L}\sum_{n=1}^{\infty} z^n \sum_{\substack{1\leqslant i<j\leqslant d\\(i,j)\neq(1,2)}} a(L_i,n)a(L_j,n)$$

$$\leqslant -\frac{1}{V_L}\sum_{\substack{1\leqslant i<j\leqslant d\\(i,j)\neq(1,2)}}\frac{L_iL_j}{2\pi}\log\left[1-\exp\left(-\frac{\pi^2}{L_j^2}\right)\right]$$

$$\leqslant \frac{1}{V_L}\sum_{\substack{1\leqslant i<j\leqslant d\\(i,j)\neq(1,2)}} L_iL_j\left(\frac{\pi^2}{L_j^2}+2\log L_j\right) \tag{32}$$

The right-hand sides of (31) and (32) go to zero as $L_d\to\infty$. Each of the terms in expansion (29) with $3,4,\ldots,d-1$ a's are easily shown to be bounded from above by

$$\frac{1}{L_d}\sum_{n=1}^{\infty}\frac{1}{(2\pi n)^{3/2}}$$

for $L_d > 1$. Moreover by (26) and (27)

$$\frac{1}{V_L}\sum_{n=1}^{\infty} z^n \prod_{i=1}^{d} a(L_i,n) \leqslant \sum_{n=1}^{\infty}\frac{z^n}{(2\pi n)^{d/2}} \tag{33}$$

$$\frac{1}{V_L}\sum_{n=1}^{\infty} z^n \prod_{i=1}^{d} a(L_i,n) \geqslant \frac{1}{V_L}\sum_{n=1}^{\infty} z^n\exp\left(-\frac{3dn\pi^2}{2L_d^2}\right)\prod_{i=1}^{d}\left(\frac{L_i}{(2\pi n)^{i/2}}-2\right)$$

$$\geqslant \sum_{n=1}^{\infty}\frac{z^n}{(2\pi n)^{d/2}}\exp\left(-\frac{3dn\pi^2}{2L_d^2}\right)-\frac{1}{V_L}\sum_{n=1}^{\infty}$$

$$\times\exp\left(-\frac{3dn\pi^2}{2L_d^2}\right)\sum_{i=1}^{d-1}\frac{L_1\ldots L_i}{(2\pi n)^{i/2}}\binom{d}{i}2^{d-i}$$

$$\geqslant \sum_{n=1}^{\infty}\frac{z^n}{(2\pi n)^{d/2}}\exp\left(-\frac{3dn\pi^2}{2L_d^2}\right)-\frac{c_1L_1L_d}{V_L}-\frac{c_2L_1L_2}{V_L}$$

$$\times\log\left[1-\exp\left(-\frac{3d\pi^2}{2L_d^2}\right)\right]-\sum_{j=3}^{d-1}c_j\frac{L_1\ldots L_j}{V_L}$$

where $c_1, \ldots, c_{d-1}$ are positive numbers independent of $L_1, \ldots, L_d$. So the lower bound increases to the upper bound as $L_d \to \infty$. ■

Proof of Theorem 3. Since $L_d \to \infty$ we have $S_L / V_L \to 0$ so that by Theorem 1 $\xi(L)\uparrow 1$ for $\rho \geqslant \rho_c$. By Lemma 3 it follows that for any $\epsilon_1 > 0$ there exists an L_d large enough such that

$$\left| \frac{1}{V_L} \sum_{n=1}^{\infty} [\xi(L)]^n [1 + a(L_1, n) + a(L_2, n) + a(L_1, n) a(L_2, n)] - (\rho - \rho_c) \right| < \epsilon_1 \tag{34}$$

Moreover from (26), ..., (29) one has

$$\frac{1}{V_L} \sum_{n=1}^{\infty} a(L_2, n) \leqslant \frac{L_2^2}{V_L} \tag{35}$$

$$\begin{aligned} &\left| \frac{1}{V_L} \sum_{n=1}^{\infty} [\xi(L)]^n a(L_1, n) a(L_2, n) + \frac{L_1 L_2}{2\pi V_L} \log\left[1 - \xi(L) \exp\left(-\frac{\pi^2}{L_2^2} \right) \right] \right| \\ &\leqslant \frac{1}{V_L} \sum_{n=1}^{\infty} \left[a(L_1, n) \left| a(L_2, n) - \frac{L_2}{(2\pi n)^{1/2}} \exp\left(-\frac{n\pi^2}{L_2^2} \right) \right| \right. \\ &\qquad \left. + \frac{L_2}{(2\pi n)^{1/2}} \exp\left(-\frac{n\pi^2}{L_2^2} \right) \left| a(L_1, n) - \frac{L_1}{(2\pi n)^{1/2}} \right| \right] \\ &\leqslant \frac{1}{V_L} \left(L_1 L_2 + \frac{L_2^3}{L_1} + L_2^2 \right) \end{aligned} \tag{36}$$

For L_d large enough we have for any $\epsilon_1 > 0$ (34) replaced by

$$\begin{aligned} &\left| \frac{1}{V_L} \sum_{n=1}^{\infty} [\xi(L)]^n [1 + a(L_1, n)] - \frac{\rho_m - \rho_c}{2 \log L_2} \right. \\ &\qquad \left. \times \log\left[1 - \xi(L) \exp\left(-\frac{\pi^2}{L_2^2} \right) \right] - (\rho - \rho_c) \right| < 2\epsilon_1 \end{aligned} \tag{37}$$

We consider two cases:

(1) $\rho_c < \rho < \rho_m$. Choose $\epsilon_1 = (\rho_m - \rho)/4$. It follows that

$$-\frac{\rho_m - \rho_c}{2 \log L_2} \log\left[1 - \xi(L) \exp\left(-\frac{\pi^2}{L_2^2} \right) \right] \leqslant \rho - \rho_c + 2\epsilon_1 = \frac{(\rho_m + \rho - 2\rho_c)}{2} \tag{38}$$

so that for L_2 large enough

$$\xi(L) \leqslant \exp\left(\frac{\pi^2}{L_2^2}\right)\left(1 - L_2^{-(\rho_m+\rho-2\rho_c)/(\rho_m-\rho_c)}\right)$$

$$\leqslant \exp\left(-\frac{1}{2}\cdot L_2^{-(\rho_m+\rho-2\rho_c)/(\rho_m-\rho_c)}\right) \tag{39}$$

Using this upper bound and (25), (26) we obtain

$$\frac{1}{V_L}\sum_{n=1}^{\infty}\left[\xi(L)\right]^n\left[1 + a(L_1, n)\right]$$

$$\leqslant \frac{2}{V_L}\cdot L_2^{(\rho_m+\rho-2\rho_c)/(\rho_m-\rho_c)} + \frac{1}{V_L}\cdot L_2^{(\rho_m+\rho-2\rho_c)/(2\rho_m-2\rho_c)} \tag{40}$$

which goes to zero as $L\to\infty$. Combining this result with (37) we have proved that for $\rho_c < \rho < \rho_m$

$$\xi(L) \sim 1 - L_2^{-2(\rho-\rho_c)/(\rho_m-\rho_c)} \tag{41}$$

and all the occupation numbers ρ_k converge to zero.

(2) $\rho > \rho_m$. Instead of deriving an upper bound on $\xi(L)$ we derive a lower bound on $\xi(L)$ using (37) and (26). For L large enough

$$\frac{1}{V_L}\left[\frac{\xi(L)}{1-\xi(L)} + \frac{L_1}{\{2[1-\xi(L)]\}^{1/2}}\right]$$

$$\geqslant \sum_{n=1}^{\infty}\left[\xi(L)\right]^n\left[1 + a(L_1, n)\right] \geqslant \rho - \rho_c - (\rho_m - \rho_c) - 3\epsilon_1 \tag{42}$$

If we choose $\epsilon_1 = (\rho - \rho_m)/6$ we have for L large enough

$$1 - \xi(L) \leqslant 4\left[\frac{L_1^2}{(\rho-\rho_m)^2 V_L^2} + \frac{1}{(\rho-\rho_m)V_L}\right]$$

$$\leqslant \frac{4}{L_2^2}\left[(\rho-\rho_m)^{-2} + (\rho-\rho_m)^{-1}\right] \tag{43}$$

Combining (37) and (43) we get for $\rho > \rho_m$ and $L\to\infty$

$$\frac{1}{V_L}\sum_{n=1}^{\infty}\left[\xi(L)\right]^n\left[1 + a(L_1, n)\right] \to \rho - \rho_m \tag{44}$$

If $A = \infty$ then (26) implies

$$\frac{1}{V_L}\sum_{n=1}^{\infty}\left[\xi(L)\right]^n a(L_1, n) \leqslant \frac{1}{V_L}\sum_{n=1}^{\infty}\frac{L_1}{(2\pi n)^{1/2}}\exp\left(-\frac{n\pi^2}{L_1^2}\right) \leqslant \frac{L_1^2}{V_L} \to 0 \tag{45}$$

so that

$$\xi(L) \sim 1 - \frac{1}{(\rho - \rho_m) V_L} \tag{46}$$

which proves (21).

If $0 < A < \infty$ (20) follows from (44) and the following inequality:

$$\frac{1}{V_L}\left| \sum_{n=1}^{\infty} z^n a(L_1, n) - \sum_{k=2}^{\infty} z \left\{ \exp\left[\frac{\pi^2}{2L_1^2}(k^2 - 1) \right] - z \right\}^{-1} \right| \leqslant \frac{L_1}{V_L} \cdot \exp\left(\frac{\pi^2}{2} \right) \tag{47}$$

for $L_1 \geqslant 1$ and $z \in [0, 1]$.

If $A = 0$ one has from (44) and (27) that for L large enough

$$\frac{1}{V_L} \sum_{n=1}^{\infty} [\xi(L)]^n \left(\frac{L_1}{(2\pi n)^{1/2}} - 2 \right) \exp\left(- \frac{3n\pi^2}{2L_1^2} \right)$$

$$\leqslant \frac{1}{V_L} \sum_{n=1}^{\infty} [\xi(L)]^n a(L_1, n) \leqslant 2\rho \tag{48}$$

$$\frac{1}{V_L} \sum_{n=1}^{\infty} [\xi(L)]^n \frac{L_1}{(2\pi n)^{1/2}} \left[1 - \left(\frac{3n\pi^2}{2L_1^2} \right)^{1/2} \right] \leqslant 4\rho \tag{49}$$

So that

$$\xi(L) \leqslant \exp\left[-(1 + 6\rho V_L / L_1)^{-2} \right] \tag{50}$$

and therefore

$$\frac{1}{V_L} \frac{\xi(L)}{1 - \xi(L)} \leqslant \frac{1}{V_L} \left(1 + \frac{6\rho V_L}{L_1} \right)^2 \tag{51}$$

goes to zero. Using this result we obtain with (26) and (27)

$$\xi(L) \sim 1 - \frac{1}{2(\rho - \rho_m)^2} \left(\frac{L_1}{V_L} \right)^2 \tag{52}$$

which completes the proof of Theorem 3 in the case $\rho > \rho_m$, $A = 0$. ∎

If we want to discuss the fluctuations in the grand canonical ensemble it is convenient to calculate the grand canonical average of e^{-zN/V_L} in the limit $L \to \infty$. For the parallelepiped we have the following:

Theorem 4.

$$\lim_{L\to\infty}\langle e^{-zN/V_L}\rangle_L = \begin{cases} e^{-z\rho}, & \rho<\rho_m,\ \ \rho>\rho_m,\ \ A=0\\ e^{-z\rho}\cdot\left[1+z(\rho-\rho_m)\right]^{-1}, & \rho>\rho_m,\ \ A=\infty \\ e^{-z\rho_m}\dfrac{(2z-\pi^2+2C)^{1/2}}{(2C-\pi^2)^{1/2}} & \\ \quad\cdot\dfrac{\sinh(2C-\pi^2)^{1/2}}{\sinh(2z-\pi^2+2C)^{1/2}}, & \rho>\rho_m,\ \ 0<A<\infty \end{cases} \tag{53}$$

where $z>0$ and C, A, and ρ_m are as in Theorem 3.

We will not prove this theorem but if we compare the given expression with the corresponding ones in Refs. 3 and 4 we notice that the ρ_c in Refs. 3 and 4 has been replaced by ρ_m.

4. A SUFFICIENT CONDITION ON CONDENSATION INTO THE GROUND STATE ALONE

Theorem 5. If the sequence of convex regions $B_1\subset B_2\subset\cdots\subset B_L\subset\cdots$ is such that

$$\frac{S_L}{V_L}\left(E_2^L-E_1^L\right)^{-1/d}\to 0 \tag{54}$$

as $L\to\infty$ then for $\rho>\rho_c$

$$\rho_1\equiv\lim_{L\to\infty}\frac{1}{V_L}\frac{\xi(L)}{1-\xi(L)}=\rho-\rho_c \tag{55}$$

and

$$\rho_k\equiv\lim_{L\to\infty}\frac{1}{V_L}\xi(L)\left[e^{\eta_k^L}-\xi(L)\right]^{-1}=0,\qquad k=2,3,\ldots \tag{56}$$

Proof. By the classical isoperimetric inequality [see (1.1) in Ref. 13]

$$S_L\geqslant d\pi^{1/2}\left[\Gamma(d/2+1)\right]^{-1/d}V_L^{1-1/d} \tag{57}$$

we have with (54)

$$V_L\left(E_2^L - E_1^L\right) \to \infty \tag{58}$$

so that

$$\frac{1}{V_L}\frac{\xi(L)}{e^{\eta_k^L} - \xi(L)} \leqslant \frac{1}{V_L}\cdot\frac{1}{e^{\eta_k^L} - 1} \leqslant \frac{1}{V_L\left(E_2^L - E_1^L\right)} \to 0 \tag{59}$$

which proves (56). In order to prove (55) we have the following lower bound:

$$\frac{1}{V_L}\sum_{k=2}^{\infty}\frac{\xi(L)}{e^{\eta_k^L} - \xi(L)} \geqslant \frac{1}{V_L}\sum_{k=2}^{\infty}\frac{1}{e^{E_k^L} - 1} \geqslant \frac{1}{V_L}\sum_{k=1}^{\infty}\left(\frac{1}{e^{E_k^L} - 1}\right) - \frac{1}{V_L E_1^L}$$

$$\geqslant \rho_c - \frac{2S_L}{V_L}\left(1 + \log\frac{V_L}{S_L}\right) - \frac{1}{V_L E_1^L} \tag{60}$$

where we have used (11) and an inequality similar to (14). For E_1^L we use the d-dimensional Rayleigh–Faber–Krahn inequality (see Theorem 3.4 of Ref. 13)

$$E_1^L \geqslant \frac{1}{\pi} j_{(d/2-1)}^2 \cdot \left[V_L \Gamma\left(\frac{d}{2} + 1\right)\right]^{-2/d} \tag{61}$$

so that the lower bound (60) converges to ρ_c for $d = 3, 4, \ldots$. (The first positive zero of the Bessel function $J_n(x)$ is denoted by j_n.) To complete the proof of (55) we derive an upper bound using (7):

$$\frac{1}{V_L}\sum_{k=2}^{\infty}\frac{\xi(L)}{e^{\eta_k^L} - \xi(L)} \leqslant \frac{1}{V_L}\sum_{k=2}^{\infty}\frac{1}{e^{\eta_k^L} - 1} \leqslant \frac{1}{V_L}\sum_{n=1}^{\infty}\sum_{k=2}^{\infty} e^{-n(E_k^L - E_1^L)}$$

$$\leqslant \rho_c + \frac{1}{V_L}\sum_{n=1}^{A(L)}\left(e^{nE_1^L} - 1\right)\sum_{k=2}^{\infty} e^{-nE_k^L} + \frac{1}{V_L}\sum_{n=A(L)+1}^{\infty}\sum_{k=2}^{\infty} e^{n(E_1^L - E_k^L)}$$

$$\equiv \rho_c + I + II \tag{62}$$

where $A(L)$ is the greatest integer less or equal than $(E_1^L)^{-1}$. Furthermore

$$I \leqslant \sum_{n=1}^{A(L)} e^{nE_1^L} \cdot \frac{nE_1^L}{(2\pi n)^{d/2}} \leqslant \begin{cases} e^{A(L)E_1^L}\cdot 2\left(E_1^L\right)^{1/2} \leqslant 2e\left(E_1^L\right)^{1/2}, & d = 3 \\ e^{A(L)E_1^L}\cdot E_1^L\left(1 - \log E_1^L\right), & d = 4 \\ e^{A(L)E_1^L}\cdot E_1^L \sum_{n=1}^{\infty} n^{-3/2}, & d \geqslant 5 \end{cases} \tag{63}$$

Since $A(L)E_1^L \leqslant 1$ and $E_1^L \to 0$ by Lemma 2 we have $I \to 0$ as $L \to \infty$. Moreover by Lemma 1 and Lemma 2

$$II = \frac{1}{V_L} \sum_{k=2}^{\infty} \frac{\exp\left[A(L)(E_1^L - E_k^L)\right]}{1 - \exp(E_1^L - E_k^L)}$$

$$\leqslant \frac{\exp\left[A(L)E_1^L\right]}{1 - \exp(E_1^L - E_2^L)} \sum_{k=2}^{\infty} \exp(-E_k^L/E_1^L)$$

$$\leqslant \frac{e^{1+E_2^L}}{(2\pi)^{d/2}} \cdot \frac{(E_1^L)^{d/2}}{E_2^L - E_1^L} \leqslant e^{1+E_2^L} \cdot \left(\frac{\pi d^2}{16}\right)^{d/2} \cdot \left(\frac{S_L}{V_L}\right)^d \cdot (E_2^L - E_1^L)^{-1} \tag{64}$$

The right-hand side of (64) goes to zero by condition (54). ■

Since $E_2^L - E_1^L \to 0$ it follows that condition (54) is stronger than van Hove's condition[9] or Fisher's asymptotic regularity condition.[8] For many convex regions B (e.g., all parallelepipeds)

$$E_2^B - E_1^B \geqslant \frac{3\pi^2}{2} \cdot (D_B)^{-2} \tag{65}$$

(where D_B is the diameter of B). If we combine (54) and (65) we obtain

$$\frac{S_L}{V_L} \cdot (D_L)^{2/d} \to 0 \tag{66}$$

which is weaker than Fisher's uniform regularity condition if $d = 3, 4, \ldots$. Unfortunately only for Neumann boundary conditions an inequality similar to (65) has been proven (Theorem 3.24 of Ref. 13 or 12).

Corollary. If B_L is the dilation of a convex region B_1 then for $\rho > \rho_c$ the ground state is macroscopically occupied with density $\rho - \rho_c$ in the limit $L \to \infty$.

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REFERENCES

1. M. van den Berg, J. T. Lewis, and J. V. Pulè, in preparation.
2. J. T. Lewis and J. V. Pulè, The Equilibrium States of the Free Boson Gas, *Commun. Math. Phys.* **36**:1–18 (1974).
3. M. van den Berg and J. T. Lewis, On the Boson Gas in a Weak External Potential, *Commun. Math. Phys.* **81**:475–494 (1981).

4. M. van den Berg and J. T. Lewis, On Generalized Condensation in the Free Boson Gas, *Physica* **110A**:550–564 (1982).
5. L. J. Landau and I. F. Wilde, On Bose–Einstein Condensation of an Ideal Gas, *Commun. Math. Phys.* **70**:43–51 (1979).
6. O. Bratteli and D. W. Robinson, *Operator Algebras and Quantum Statistical Mechanics II* (Springer-Verlag, Berlin, 1981).
7. R. M. Ziff, G. M. Uhlenbeck, and M. Kac, The Ideal Bose–Einstein Gas, Revisited, *Phys. Lett.* **32C**:171–248 (1977).
8. M. E. Fisher, The Free Energy of a Macroscopic System, *Arch. Rat. Mech. Anal.* **17**:377–410 (1964).
9. D. Ruelle, *Statistical Mechanics. Rigorous Results* (W. A. Benjamin, Inc., New York, 1969).
10. D. B. Ray, Spectra of Second-Order Differential Operators, *Trans. Am. Math. Soc.* **77**:299–321 (1954).
11. R. Osserman, Bonnesen-Style Isoperimetric Inequalities, *Bull. Am. Math. Soc.* **84**:1182–1238 (1978).
12. L. E. Payne and H. F. Weinberger, An Optimal Poincaré Inequality for Convex Domains, *Arch. Rat. Mech. Anal.* **5**:286–292 (1960).
13. C. Bandle, *Isoperimetric Inequalities and Applications* (Pitman Advanced Publishing Program, Boston, 1980).
14. N. Angelescu and G. Nenciu, On the Independence of the Thermodynamic Limit on the Boundary Conditions in Quantum Statistical Mechanics, *Commun. Math. Phys.* **29**:15–30 (1973).
15. F. A. Valentine, *Convex Sets*. (R. E. Krieger Publishing Company, Huntington, New York, 1976).