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The statistics of the grand canonical number density for interacting bosons.

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Abstract: It is shown that the weak law of large numbers holds for the grand canonical number density in a system of bosons interacting through a pair potential which is superstable. An estimate of the probability of large deviations is obtained in terms of the canonical free energy density.

1 Introduction

In a manuscript circulated privately in 1971 Kac showed that in the two-phase region of the free Boson gas the canonical ensemble and the grand canonical give rise to distinct states. Kac gave an integral decomposition of grand canonical expectations $\langle \quad \rangle_{\rho}^{g}$ at mean particle density ρ in terms of canonical expectations $\langle \quad \rangle_{x}$ at particle density x :

$$\langle \quad \rangle_{\rho}^{g} = \int_{0}^{\infty} \langle \quad \rangle_{x} \, K(x;\rho) \, dx . \tag{1.1}$$

The details of the proof were supplied by Cannon [1] , Pule [2] , and Lewis and Pule [3] . Kac calculated $K(x;\rho)$ (now called the Kac density) for the free Boson gas by computing the grand canonical characteristic function of the particle number density. He found that in the one-phase region the Kac density is a delta-function: the grand canonical state coincides with the canonical state in that region. On the other hand, in the two-phase region the Kac density corresponds to an exponential distribution of x with mean-value ρ . The consequences of this result were discussed in detail by Ziff, Uhlenbeck and Kac [4] ; the case was made that in the two-phase region the grand canonical ensemble does not represent a physical system. The relationship of the integral decomposition (1.1) to the work of Araki and Woods [5] was discussed by Lewis in [6] . The Kac density for bosons with spin was computed by Critchley and Lewis [7] , for bosons in a rotating bucket by Lewis and Pule [8] and for bosons in an external potential by van den Berg and Lewis [9] .

However, it has been conjectured by Kac [10] that in the presence of a repulsive interaction, no matter how small, the Kac density will be a delta-function. At first sight the results of Davies [11] on a mean-field model of an imperfect boson gas lend support to this conjecture: he showed that when the mean-field interaction is super-stable the Kac density is a delta-function. (See also Fannes and Verbeure [12] .) On closer examination we find that Davies's result can be separated into two propositions:

1. At points of continuity of the density (as a function of the chemical potential) the weak law of large numbers holds for a super-stable mean-field model of an interacting boson gas.

2. The first-order character of the phase-transition (discontinuity of the density as a function of the chemical potential) in the free boson gas is unstable with respect to mean-field perturbations.

The main purpose of this paper is to prove that the weak law of large numbers holds for bosons interacting through a super-stable pair potential at points of continuity of the density, and to point out that, since every first-order phase transition is unstable with respect to a mean-field perturbation, what is surprising about condensation in the free boson gas is that macroscopic occupation of the ground state is stable with respect to a mean-field perturbation. This can be shown [13] using ideas of Cannon [1] , or by means of correlation inequalities [12] . It is known that the first-order phase transition in the two-dimensional lattice gas is stable if [14] and only if [15,16] the perturbing potential is short-range (in a precise sense). The range of a mean field is infinite; could it be that macroscopic occupation of the ground state is stable under arbitrary superstable perturbations, or only for those which are sufficiently long range? As far as we know, this is an open question.

Our main result, the weak law of large numbers for the particle number density (Theorem 2) is stated and proved for bosons with a superstable pair potential; it holds in other cases and it is not difficult to modify the proof to cover these. The condition of superstability is imposed in the boson case to ensure that the grand canonical partition function exists for all values of the chemical potential; with the weaker condition of stability on the potential, it holds for those values of the chemical potential for which the grand canonical partition function exists. For classical statistics, and for the Maxwell-Boltzmann and Fermi quantum statistics, it holds for stable pair potentials.

2 The Weak Law of Large Numbers

Consider a system of identical bosons, each of mass m , contained in a bounded open connected subset Λ of Euclidean space $\mathbb{R}^d$; let V be the volume of Λ . Let λ be the thermal wavelength: $\lambda^2 = (2\pi\hbar^2/kTm)$. Suppose that the bosons interact through a pair potential ϕ satisfying the following conditions [17,18,19] :

(A) ϕ is a real even function of the difference of the positions of the two interacting particles, locally square-integrable on the complement of the origin (the case in which ϕ has a hard core is excluded).

(B) ϕ is superstable: there exist constants $A>0$ and $B\geq 0$ such that for any family $(x_1, \ldots, x_n)$ of n points in Λ the following inequality holds:

$$U_n(x_1, \ldots, x_n) \stackrel{\text{def}}{=} \sum_{i<j} \phi(x_i - x_j) \geq \frac{A}{V} n^2 - Bn \quad , \tag{2.1}$$

where A is independent of V for a given shape of Λ .

(C) ϕ is weakly tempered: there exist constants $R>0$, $c>d$, and $\phi_0 \geq 0$ such that

$$\phi(x) \leq \phi_0 |x|^{-c} \quad \text{whenever} \quad |x| > R \quad .$$

For each positive integer n we define a self-adjoint operator H_n in the symmetric Hilbert space $L^2_{symm}(\Lambda^n)$ by the Friedrich extension, as in [19] , so that

$$H_n = T_n + U_n \tag{2.2}$$

where T_n is the kinetic energy operator

$$T_n = -\frac{\hbar^2}{2m} \sum_{j=1}^{n} \Delta_j \tag{2.3}$$

and U_n is the potential energy operator which acts by multiplication by $U_n(x_1,\dots,x_n)$.

Next we describe the bulk limit: we take a sequence $\{\Lambda^l : l=1,2,..\}$ of regions, each satisfying the conditions set out above. The volume of Λ^l is denoted by V^l. In order that the constant A in condition (B) be independent of l, we follow Ginibre [19] in assuming that the regions satisfy a shape condition. To each region Λ^l we associate a sequence $\{H_n^l = T_n^l + U_n^l : n=1,2,..\}$ of self-adjoint Hamiltonians; it follows from condition (B) and Peierl's inequality (see Lemma 3 of Ruelle [17]) that, for all n and l, the operators $\exp(-\beta H_n^l)$ have finite trace. Define the canonical partition function $Z^l(n)$ by

$$Z^l(n) \quad = \quad \text{trace}\,(e^{-\beta H_n^l})\ ,\ l=1,2,\dots,\ n=1,2,\dots\ , \tag{2.4}$$

and the canonical free energy density $f^l(s)$ by

$$f^l\left(\frac{n}{V^l}\right) = \frac{-1}{\beta V^l}\log Z^l(n) \tag{2.5}$$

with $f^l(s)$ given for each s in $[0,\infty)$ by linear interpolation. We make use of the following theorem which holds under the above assumptions:

Theorem 1 (Ruelle [17] , Fisher [18])

For each s in $[0,\infty)$ the limit $\lim_{l\to\infty} f^l(s) = f(s)$ exists and the function f is convex and continuous. Moreover, the convergence is uniform on compacts.

The Ruelle-Fisher Theorem holds for Maxwell-Boltzmann and Fermi statistics, as well as for Bose statistics. In the Bose case, because of the upperbound to the grand canonical pressure for the free boson gas, we have the following bound for f^l :

Lemma 1 For a system of bosons interacting through a superstable pair-potential the free-energy density f^{ℓ} in the region Λ^{ℓ} satisfies

$$f^{\ell}(s) \geq As^2 - Bs - p_c \tag{2.6}$$

where $p_c = \lambda^{-d}\sum_{n=1}^{\infty} n^{-(\frac{d}{2}+1)}$ is the critical pressure of the free boson gas.

Proof: Using condition (B) and the Peierl's inequality (see Lemma 3 of [17]), we have

$$\begin{aligned} \text{trace } e^{-\beta H_n^{\ell}} &\leq \exp\beta(Bn - \frac{A}{V^{\ell}}n^2) \quad \text{trace } e^{-\beta T_n^{\ell}} \\ &\leq \exp\beta(Bn - \frac{A}{V^{\ell}}n^2) \quad \text{trace } (\sum_{m=1}^{\infty} e^{-\beta T_m^{\ell}}) \end{aligned}$$

so that

$$\begin{aligned} f^{\ell}(s) &= -\frac{1}{\beta V^{\ell}} \log \text{trace } e^{-\beta H_n^{\ell}} \\ &\geq As^2 - Bs - \frac{1}{\beta V^{\ell}} \log \text{trace}(\sum_{m=1}^{\infty} e^{-\beta T_m^{\ell}}) . \end{aligned}$$

But $\frac{1}{\beta V^{\ell}} \log \text{trace}(\sum_{m=1}^{\infty} e^{-\beta T_m^{\ell}})$ is the grand canonical pressure of the free boson gas in volume V^{ℓ} evaluated at zero chemical potential, and hence is bounded above by the critical pressure p_c (see, for example, Ruelle [17]).

The grand canonical ensemble for the superstable interacting system in region Λ^{ℓ} defines a probability measure $\mathbb{P}_{\mu}^{\ell}$ for each value of the chemical potential μ in $\mathbb{R}$, which assigns to the random variable N^{ℓ} describing the number of particles in region Λ^{ℓ} the probability distribution

$$\mathbb{P}_{\mu}^{\ell}[N^{\ell} = n] = k_{\mu}^{\ell} \exp\beta V^{\ell}(\mu\frac{n}{V^{\ell}} - f^{\ell}(\frac{n}{V^{\ell}})) , \tag{2.7}$$

where $(k_{\mu}^{\ell})^{-1}$ is the grand canonical partition function

$$(k_{\mu}^{\ell})^{-1} = \sum_{m=1}^{\infty} \exp\beta V^{\ell}(\mu\frac{n}{V^{\ell}} - f^{\ell}(\frac{n}{V^{\ell}})) . \tag{2.8}$$

We expect that the distribution will be sharply peaked around the maximum of the function $n \mapsto \mu \frac{n}{V\ell} - f^\ell(\frac{n}{V\ell})$. This leads us to define $\rho(\mu)$ to be the smallest value of s for which the function $s \mapsto \mu s - f(s)$ attains its maximum value

$$f^*(\mu) = \sup_{s \in \mathbb{R}^+} (\mu s - f(s)) . \tag{2.9}$$

(The function f^* is the conjugate of the convex function f .) Because of the convexity of f the maximum value is attained either at a unique point or on a closed interval; because $f(s)$ is bounded below by $As^2 - Bs - p_c$ the interval on which the maximum is attained must be bounded. In the first case the function $\mu \mapsto \rho(\mu)$ is continuous; in the second, it has a finite jump. Because of the convexity of f , the set of values of μ at which $\mu \mapsto \rho(\mu)$ jumps is at most countable. We consider first the case in which μ is a point of continuity.

Theorem 2 Let μ be a point of continuity of the function $\mu \mapsto \rho(\mu)$; then

$$\lim_{\ell \to 0} \mathbb{E}^\ell_\mu \frac{N^\ell}{V\ell} = \rho(\mu), \tag{2.10}$$

and the weak law of large numbers holds: for each $\epsilon > 0$,

$$\lim_{\ell \to 0} \mathbb{P}^\ell_\mu [| \frac{N^\ell}{V\ell} - \mathbb{E}^\ell_\mu \frac{N^\ell}{V\ell} | > \epsilon] = 0 . \tag{2.11}$$

Proof: The theorem follows from Chebyshev's inequality and the following Lemma.

Lemma 2 Let μ be a point of continuity of the function $\mu \mapsto \rho(\mu)$; then

$$\lim_{\ell \to 0} \mathbb{E}^\ell_\mu [(\frac{N^\ell}{V\ell} - \rho(\mu))^2] = 0 . \tag{2.12}$$

Proof: Given $\epsilon > 0$, let δ be defined by

$$\frac{\delta}{2} = \inf \{ f(s) - \mu s + f^*(\mu) : |s - \rho(\mu)| > \left(\frac{\epsilon}{3}\right)^{1/2} \}. \tag{2.13}$$

By continuity of f, there exists $\eta > 0$ such that

$$\mu s - f(s) \geqslant f^*(\mu) - \frac{\delta}{4} \tag{2.14}$$

for $|s - \rho(\mu)| \leqslant \eta$;

hence, by the uniformity of the convergence of the sequence $\{f^l\}$,

$$\mu s - f^l(s) \geqslant f^*(\mu) - \frac{\delta}{2} \tag{2.15}$$

for l sufficiently large and $|s - \rho(\mu)| \leqslant \eta$.

Thus we have

$$\mathbb{P}^l_\mu [| \frac{N^l}{V^l} - \rho(\mu)| \leqslant \eta] \geqslant k^l_\mu \sum_{\{n : |\frac{n}{V^l} - \rho(\mu)| \leqslant \eta\}} e^{\beta V^l (f^*(\mu) - \frac{\delta}{2})}$$

$$\geqslant k^l_\mu V^l \eta \, e^{\beta V^l (f^*(\mu) - \frac{\delta}{2})} .$$

Since the left hand side cannot exceed unity, for l sufficiently large we have

$$k^l_\mu \leqslant \frac{1}{\eta V^l} e^{\beta V^l (\frac{\delta}{2} - f^*(\mu))} , \tag{2.16}$$

Choose $a(\mu) > \rho(\mu)$ so that

$$\frac{A}{2} s^2 - (B + \mu) s - p_c > - f^*(\mu) + \delta \tag{2.17}$$

for $s > a(\mu)$. Then, by (6), we have

$$f^l(s) - \mu s \geqslant - f^*(\mu) + \delta + \frac{A}{2} a(\mu) s \tag{2.18}$$

for $s > a(\mu)$.

By the choice of δ and the uniformity of convergence of $\{f^l\}$ we have

$$f^l(s) - \mu s \geqslant - f^*(\mu) + \delta \tag{2.19}$$

for $|s - \rho(\mu)| \geqslant \left(\frac{\epsilon}{3}\right)^{1/2}$ and s in $[0, a(\mu)]$.

To estimate the mean-square deviation from $\rho(\mu)$ put

$$\mathbb{E}^{\ell}_{\mu}[(\frac{N^{\ell}}{V^{\ell}}-\rho(\mu))^2] = S_1+S_2+S_3 \tag{2.20}$$

where

$$S_j = k^{\ell}_{\mu}\sum_{n\in I^{\ell}_j}(\frac{n}{V^{\ell}}-\rho(\mu))^2 e^{\beta V^{\ell}(\mu\frac{n}{V^{\ell}}-f^{\ell}(\frac{n}{V^{\ell}}))} \tag{2.21}$$

and

$$I^{\ell}_1 = \{n : |\frac{n}{V^{\ell}}-\rho(\mu)| < (\frac{\epsilon}{3})^{1/2}\} ,$$

$$I^{\ell}_2 = \{n : \frac{n}{V^{\ell}} \in [0,a]\} \setminus I^{\ell}_1 ,$$

$$I^{\ell}_3 = \{n : \frac{n}{V^{\ell}} \in (a,\infty)\} .$$

Then we have the following estimates which follow easily from (2.16) and (2.21):

$S_1 < \frac{\epsilon}{3}$ by (2.15);

$S_2 < \frac{a^3}{\eta} e^{-\beta V^{\ell}\delta/2}$ by (2.19);

$S_3 < \frac{1}{\eta(V^{\ell})^3} e^{-\beta V^{\ell}\delta/2} \frac{e^{-b}(3-e^{-b})}{(1-e^{-b})^3}$, with $b=\frac{\beta A a}{2}$, by (2.18).

Holding μ fixed, choose ℓ sufficiently large to make $S_1+S_2+S_3<\epsilon$; the result follows.

The bulk limit at fixed mean density $\bar{\rho}$ is taken as follows: for each ℓ, $\mu \mapsto \mathbb{E}^{\ell}_{\mu}[\frac{N^{\ell}}{V^{\ell}}]$ is a continuous function which is strictly increasing (since $\mathbb{E}^{\ell}_{\mu}(N^{\ell})^2 - (\mathbb{E}^{\ell}_{\mu}N^{\ell})^2$ is strictly positive) so that there is a unique $\mu(\ell)$ such that $\mathbb{E}^{\ell}_{\mu(\ell)}[\frac{N^{\ell}}{V^{\ell}}]=\bar{\rho}$; since the sequence $\{\mu(\ell)\}$ is bounded, there is at least one convergent subsequence $\{\mu(\ell^*)\}$ with limit μ^* ; if μ^* is a point of continuity of $\mu\mapsto\rho(\mu)$ then it follows easily that $\rho(\mu^*)=\bar{\rho}$ and, for each $\epsilon>0$,

$$\lim_{\ell^*\to\infty} \mathbb{P}^{\ell^*}_{\mu(\ell^*)}[\,|\frac{N^{\ell}}{V^{\ell}}-\bar{\rho}|>\epsilon] = 0 . \tag{2.22}$$

If μ^* is not a point of continuity then the limit distribution of $\frac{N^\ell}{V^\ell}$ in $[\rho(\mu_-), \rho(\mu_+)]$ will depend on the sequence $\{\mu(\ell^*)\}$; that is to say, it will depend on how the bulk limit is approached (being sensitive to boundary conditions, for example).

3 Large Deviations

The traditional statement of thermodynamical equivalence of ensembles is a weaker result. It states that the grand canonical pressure $p(\mu)$, defined by

$$p(\mu) = \lim_{l\to\infty} \frac{1}{\beta V^l} \log k^l_\mu , \tag{3.1}$$

exists and is equal to the Legendre transform $f^*(\mu)$ of the canonical free energy density:

$$p(\mu) = f^*(\mu) = \sup_{s\in\mathbb{R}^+} (\mu s - f(s)) . \tag{3.2}$$

(For a review, see Griffiths [20] .)

This result holds for a system of bosons interacting through a superstable pair potential; we prove a mild generalization of this which enables us to give a result about the probability of large deviations of $\frac{N^l}{V^l}$. Define the conditional grand canonical pressure $p(\mu|I)$ given that the number density is in the interval I :

$$p(\mu|I) = - \lim_{l\to\infty} \frac{1}{\beta V^l} \log \Xi^l_\mu(I) \tag{3.3}$$

where

$$\Xi^l_\mu(I) = \sum_{\{n:\frac{n}{V^l}\in I\}} e^{n\beta\mu} Z^l(n) , \tag{3.4}$$

Define the restricted Legendre transform $f^*_I(\mu)$:

$$f^*_I(\mu) = \sup_{s\in I} (\mu s - f(s)) . \tag{3.5}$$

Theorem 3 For a system of bosons interacting through a superstable pair potential, we have

$$p(\mu|I) = f^*_I(\mu) \tag{3.6}$$

for each μ in $\mathbb{R}$ and each interval I contained in $\mathbb{R}$.

In particular,

$$p(\mu) = f^*(\mu) . \tag{3.7}$$

Proof: We have

$$\Xi_\mu^l(I) = \sum_{\{n: \frac{n}{V^l} \in I\}} \exp \beta V^l (\mu \tfrac{n}{V^l} - f^l(\tfrac{n}{V^l}))$$

$$< V^l |I| \exp \beta V^l (f_I^*(\mu) + \epsilon) \tag{3.8}$$

for $\epsilon > 0$ and l sufficiently large. (Here $|I|$ denotes the length of the interval I .) By continuity of $s \mapsto f(s)$ there exists a sub-interval J contained in I such that

$$f(s) - \mu s < -f_I^*(\mu) + \frac{\epsilon}{2} \tag{3.9}$$

for s in J ; hence by uniformity

$$f^l(s) - \mu s < -f_I^*(\mu) + \epsilon \tag{3.10}$$

for s in J and l sufficiently large, so that

$$\Xi_\mu^l(I) > \frac{V^l}{2} |J| \exp \beta V^l (f_I^*(\mu) - \epsilon) \tag{3.11}$$

for l sufficiently large. It follows that

$$\lim_{l \to \infty} \frac{1}{\beta V^l} \log \Xi_\mu^l(I) = f_I^*(\mu) . \tag{3.12}$$

Corollary

$$\lim_{l \to \infty} \frac{1}{\beta V^l} \log \mathbb{P}_\mu^l [\tfrac{N^l}{V^l} \in I] = f_I^*(\mu) - f^*(\mu). \tag{3.13}$$

Proof: This is a direct consequence of the definition

$$\mathbb{P}_\mu^l [\tfrac{N^l}{V^l} \in I] = \Xi_\mu^l(I) / \Xi_\mu^l(\mathbb{R}) . \tag{3.14}$$

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