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THE LARGE DEVIATION PRINCIPLE FOR THE KAC DISTRIBUTION

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Abstact: We prove that the Large Deviation Principle holds for the distribution of the particle number density (the Kac distribution) whenever the free energy density exists in the thermodynamic limit. We use this result to give a new proof of the Large Deviation Principle for the Kac distribution of the free Boson gas. In the case of mean-field models, non-convex rate functions can arise; this is illustrated in a model previously studied by E.B. Davies.

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§ 1. Introduction

In 1971, Kac discovered that, for the free boson gas, the canonical and grand canonical ensembles are not strictly equivalent although they give rise to the same equation of state. This manifests itself in the fact that, above the critical density, the grand canonical distribution of the particle number density is not asymptotically degenerate ; in the standard example (where the single-particle hamiltonian is a constant multiple of the Laplacian with Dirichlet boundary conditions in a star-shaped region and the thermodynamic limit is taken by dilating the region about an interior point, holding the mean number density fixed) the distribution is exponential ; in general, when the distribution converges, it converges to an infinitely-divisible distribution.
For a full discussion of these aspects of the free boson gas, see [1] and [2] ; using their terminology, we shall refer to the grand canonical distribution of the number density as the Kac distribution.

Kac conjectured that the lack of equivalence of ensembles in the strict sense was a pathology of the free gas which would disappear in the presence of a repulsive interaction, however weak. To test this idea, Davies [3] studied in great detail a mean-field model of an interacting boson gas. He proved that, if the mean-field potential is strictly convex, the Kac distribution is asymptotically degenerate. In [4], a general result was proved, from which it was deduced that the Kac density is asymptotically degenerate whenever the free-energy exists and is strictly convex. It is often useful to enquire about the rate at which the asymptotic distribution is approached ; this is referred to as the problem of large deviations. In statistical mechanics, it has proved valuable to do this in the framework of Varadhan [5] where a powerful generalization of Laplace's method is available ; this framework is described in § 2 of this paper ; applications to classical lattice systems are surveyed in Ellis [6], to models of an interacting boson gas are given in [7], to quantum spin systems in [8]. In § 2 of this paper, we adapt the arguments of [4] to prove that the Kac distribution satisfies Varadhan's Large Deviation Principle whenever the free-energy density exists in the thermodynamic limit ; in § 3, we provide an alternative proof to that given in [7] of the result that the Kac distribution for the free boson gas satisfies Varadhan's Large Deviation Principle. The result proved in § 2 applies also to mean-field models, even when the mean-field potential is non-convex ; in such cases, it is possible for the free-energy density in the thermodynamic to be non-convex ; nevertheless the Kac density satisfies the Large Deviation Principle, albeit with a non-convex rate function (examples of such rate-functions were given by Ellis [6], see also [9].)

To illustrate the situation which can arise with a non-convex rate-function, we investigate in § 3 of this paper the model discussed by Davies in [3]. In § 4, we describe in detail possible asymptotic distributions for the Kac distribution in this example.

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§2. A Large Deviation Result

Varadhan's Theorem [5] concerns the asymptotic behaviour of integrals with respect to a sequence of probability measures satisfying the Large Deviation Principle and extends Laplace's Method to infinite dimensional spaces. Even in the case of a one-dimensional space, it has advantages over Laplace's Method : it applies to a wider class of measures and to a wider class of integrands.

Let E be a complete separable metric space and $\{K_\ell : \ell = 1,2, \ldots\}$ a sequence of probability measures on the Borel subsets of E : let $\{V_\ell : \ell = 1,2, \ldots\}$ be a sequence of positive constants such that $V_\ell \to \infty$. We say that $\{K_\ell\}$ obeys the Large Deviation Principle with constants $\{V_\ell\}$ and rate-function $I(\cdot)$ if there exists a function $I : E \to [0,\infty]$ satisfying :

(LD1) : $I(\cdot)$ is lower semi-continuous on E.

(LD2) : For each $m < \infty$, the set $\{x : I(x) \leq m\}$ is compact.

(LD3) : For each closed subset C of E ,

$$\limsup_{\ell \to \infty} \frac{1}{V_\ell} \ln K_\ell[C] \leq - \inf_C I(x) .$$

(LD4) : For each open subset G of E ,

$$\liminf_{\ell \to \infty} \frac{1}{V_\ell} \ln K_\ell[G] \geq - \inf_G I(x) .$$

A version of Varadhan's Theorem adequate for many applications in statistical mechanics is the following :

Varadhan's Theorem

Let $\{K_\ell\}$ be a sequence of probability measures on E satisfying the Large Deviation Principle with constants $\{V_\ell\}$ and rate -function $I(\cdot)$. Let $G : E \to R$ be a continuous function which is bounded above on the set $\bigcup_{\ell \geq 1} \operatorname{supp} K_\ell$. Then

$$\lim_{\ell \to \infty} \frac{1}{V_\ell} \ln \int_E e^{V_\ell G(x)} K_\ell[dx] = \sup_E \{G(x) - I(x)\} .$$

In [4], we proved a large deviation result whose main hypothesis was the existence of the free-energy in the thermodynamic limit ; at the time we were not aware of Varadhan's work and so our result was not formulated within the frame-work which we have just sketched. Here we reorganize the proof given in [4] to establish a result within the Varadhan scheme ; this enables us to give a simpler proof of the free-boson gas result proved in [7].

Let $\{f_\ell : \ell = 1,2, \ldots\}$ be a sequence of functions $f_\ell : [0,\infty) \to R$ satisfying $f_\ell(0) = 0$; the <u>grand canonical pressure</u> $p_\ell(\mu)$ <u>determined</u> by f_ℓ is defined by

$$p_\ell(\mu) = \frac{1}{\beta V_\ell} \ln \int_{[0,\infty)} e^{\beta V_\ell \{\mu x - f_\ell(x)\}} m_\ell[dx]$$

where, for each Borel subset A of $[0,\infty)$,

$$m_\ell[A] = \sum_{n \geq 0} \delta_{\frac{n}{V_\ell}}[A]$$

and

$$\delta_x[A] = \begin{cases} 1, & x \in A, \\ 0, & x \in A^c \end{cases}$$

and $\{V_\ell\}$ is a sequence of positive constants, $V_\ell \to \infty$.

For each μ for which $p_\ell(\mu)$ is finite, the <u>Kac distribution</u> K^μ_ℓ <u>determined by</u> f_ℓ is defined on the Borel subsets of $[0,\infty)$ by

$$K^\mu_\ell[A] = e^{-\beta V_\ell p_\ell(\mu)} \int_A e^{\beta V_\ell \{\mu x - f_\ell(x)\}} m_\ell[dx] .$$

We prove the following theorem :

<u>Theorem</u> 1

<u>Suppose that, on each compact, the sequence</u> $\{f_\ell : \ell = 1,2, \ldots\}$ <u>is bounded below and converges uniformly to a lower semi-continuous function</u> f . <u>Let</u> μ_∞ <u>be defined by</u>

$$\mu_\infty = \lim_{\ell \uparrow \infty} \left(\liminf_{x \uparrow \infty} \left(\frac{1}{x} \inf_{k \geq \ell} f_k(x) \right) \right) .$$

Then for each $\mu<\mu$ the grand canonical pressure $p(\mu) = \lim_{\ell\to\infty} p_\ell(\mu)$ exists and is given by the Legendre-Fenchel transform of f :

$$p(\mu) = f^*(\mu) \overset{\text{def}}{=} \sup_{x\geq o} \{ \mu x - f(x) \} .$$

Moreover, the sequence $\{K^\mu_\ell : \ell = 1,2, \ldots \}$ satisfies the Large Deviation Principle with constants $\{ V_\ell \}$ and rate-function $I^\mu(\cdot)$ given by

$$I^\mu(x) = p(\mu) + f(x) - \mu x .$$

Proof :

Put $g_\ell(x) = \mu x - f_\ell(x)$ and $g(x) = \mu x - f(x)$,

so that we can write

$$p_\ell(\mu) = \frac{1}{\beta V_\ell} \ln \int_{[o,\infty)} e^{\beta V_\ell g_\ell(x)} m_\ell [dx] .$$

Choose A such that $\mu < A < \mu_\infty$; choose m such that

$$\liminf_{x\uparrow\infty} \left(\frac{1}{x} \inf_{k\geq m} f_k(x)\right) > A ;$$

then there exists x_1 such that $f(x) > A x$

for all $x > x_1$ and all $\ell > m$; hence

$g_\ell(x) < -(A - \mu)x$ for all $x > x_1$ and $\ell > m$, and $g(x) \leq -(A - \mu) x$

for all $x > x_1$. But $g(0) = 0$ so that

$$\sup_{[0,\infty)} g(x) = \sup_{[0,x_1]} g(x) .$$

Now g is upper semi-continuous and bounded above on compacts, so that the supremum of g on $[0,x_1]$ is attained at some point x_0 in $[0, x_1]$:

hence

$$f^*(\mu) = \sup_{[0,\infty)} g(x) = g(x_o) < \infty .$$

Furthermore, given $\varepsilon > 0$, there exists $\delta > 0$ such that $g(x_o) - g(x) < \frac{\varepsilon}{2}$ for x in $[x_o - \delta, x_o + \delta]$; by the uniformity of convergence on compacts which was postulated for $\{ f_\ell \}$, there exists m' such that, for all $\ell > m'$, $g(x) - g_\ell(x) < \frac{\varepsilon}{2}$ for all x in $[x_o - \delta, x_o + \delta]$.

Thus we have, for all ℓ sufficiently large,

$$\int_{[0,\infty)} e^{\beta V_\ell g_\ell(x)}\, m_\ell\,[dx] > \int_{[x-\delta,\, x+\delta]} e^{\beta V_\ell\, g_\ell\,(x)}\, m_\ell[dx] > e^{\beta V_\ell (g(x_0)-\varepsilon)} ,$$

since eventually $[x_o - \delta,\ x_o + \delta]$ contains at least one point of $\{\frac{n}{V_\ell} : n = 0, 1, 2, \dots\}$. Since $\varepsilon > 0$ was arbitrary, we have

$$\liminf_{\ell\to\infty} \frac{1}{\beta V_\ell} \ln \int_{[o,\infty)} e^{\beta V_\ell\, g_\ell\,(x)}\, m_\ell\,[dx] \geq g(x_o) .$$

On the other hand,

$$\int_{[o,\infty)} e^{\beta V_\ell\, g_\ell(x)}\, m_\ell\,[dx] < e^{\beta V_\ell \{g(x_o)+\varepsilon\}} \int_{[0,x_1]} m_\ell[dx] + \int_{(x_1,\infty)} e^{-\beta V_\ell (A-\mu)x}\, m_\ell[dx]$$

$$\leq e^{\beta V_\ell \{g(x_o)+\varepsilon\}} \left\{ (V_\ell x_1 + 1) + \frac{e^{-\beta V_\ell \{(A-\mu)x_1 + g(x_o) + \varepsilon\}}}{1 - e^{-\beta(A-\mu)}} \right\}$$

for all ℓ sufficiently large ; hence, since $g(x_0) \geq 0$ and $(A-\mu)x_1 > 0$,

we have

$$\limsup_{\ell\to\infty} \frac{1}{\beta V_\ell} \ln \int_{[0,\infty)} e^{\beta V_\ell g_\ell(x)}\, m_\ell[dx] = g(x_o) + \varepsilon$$

and the statement concerning the pressure is proved, since $\varepsilon>0$ was arbitrary.

We turn to the proof of the assertion concerning the sequence $\{K^\mu_\ell : \ell = 1,2, \dots\}$:

(LD1) holds by the hypothesis that x f(x) is lower semi-continuous. It follows that, for each $m < \infty$, the set $L_m = \{ x : I^\mu_x \leq m \}$ is closed ; for $x \in L_m$, we have

$$f\,(x) \leq m - p\,(\mu) + \mu\, x ;$$

on the other hand, we have shown that, for $x>x_1$, $f(x) \geq Ax$. Hence, either $x \leq x_1$ or $x \leq \dfrac{m - p(\mu)}{A - \mu}$ so that L_m is bounded and (LD2) holds.

For a closed set C, we have, given $\varepsilon > 0$,

$$K_\ell \,[C] \leq e^{-\beta V_\ell p_\ell(\mu)} \exp \beta V_\ell \{\sup_{C\cap[0,x_2]} g(x) + \varepsilon\} \int_{C\cap[0,x_2]} m_\ell[dx]$$

$$+ \int_{C\cap[x_2,\,\infty)} e^{-\beta V_\ell (A - \mu)x} \, m_\ell[dx]$$

for all ℓ sufficiently large and all x_2 in $(0, \infty)$.

Since $\sup_{C\cap[0,x_1]} g(x) \leq \sup_C g(x)$, we have

$$K_\ell^\mu \,[C] \leq e^{\beta V_\ell \{p_\ell(\mu) + \sup_C g(x) + \varepsilon\}} \left\{ (V_\ell x_2 + 1) + \frac{e^{-\beta V_\ell \{\sup_C g(x) + \varepsilon + (A - \mu) x_2\}}}{1 - e^{-\beta(A - \mu)}} \right\}$$

for all ℓ sufficiently large. Now choose $x_2 \geq x_1$ such that

$$\sup_C g(x) + (A - \mu)\, x_2 \geq 0 \;.$$

Hence

$$\limsup_{\ell \uparrow \infty} \frac{1}{\beta V_\ell} \ln K_\ell^\mu \,[C] \leq -\, p(\mu) + \sup_C g(x) = -\inf_C I^\mu (x)$$

and (LD3) holds.

Let G be an arbitary open subset of $[0, \infty)$; given $\varepsilon > 0$ and γ in G, choose δ such that $(\gamma - \delta, \gamma + \delta) = B_\gamma^\delta \subset G$ and $g(\gamma) - g(x) < \frac{\varepsilon}{2}$ for all x in B_γ^δ (this is possible since g is upper semi-continuous) . Thus, for ℓ sufficiently large,

$$K_\ell^\mu \,[G] \geq K_\ell^\mu \,[B_\gamma^\delta] = e^{-\beta V_\ell p_\ell(\mu)} \int_{B_\gamma^\delta} e^{\beta V_\ell g_\ell(x)} \, m\,[dx]$$

$$\geq e^{-\beta V_\ell p_\ell(\mu)} \, e^{\beta V_\ell (g(\gamma) - \varepsilon)} \, m_\ell[\, B_\gamma^\delta\,] \,.$$

But eventually B_γ^δ contains at least one point of $\{\frac{n}{V_\ell} : n = 0,1,2, \ldots\}$ so that $m_\ell\,[B_\gamma^\delta] \geq 1$ and hence

$$\liminf_{\ell \to \infty} \frac{1}{\beta V_\ell} \ln K_\ell^\mu [G] \geq - p(\mu) + g(\gamma) = - I^\mu (\gamma) ;$$

since this inequality holds for each point of G,

we have

$$\liminf_{\ell \to \infty} \frac{1}{\beta V_\ell} \ln K_\ell^\mu [G] \geq \sup_G (- I^\mu (\gamma)) = - \inf_G I^\mu (\gamma)$$

and (LD4) holds.

§ 3. Mean-Field Model of Davies

The basic probability space for the class of models of boson systems which we consider in this paper is the space Ω of terminating sequences of non-negative integers :

$$\Omega = \{\omega : \omega = (\omega_1, \omega_2, \dots), \ \omega_j \in N, \sum_{j\geq 1} \omega_j < \infty\}.$$

The basic random variabales are the occupation numbers $\{\sigma_j ; : j = 1,2, \dots\}$ defined by $\sigma_j(\omega) = \omega_j$; the Hamiltonian H_ℓ associated with a region Λ_ℓ is given by

$$H_\ell(\omega) = \sum_{j\geq 1} \lambda_\ell(j) \sigma_j(\omega) \qquad (3.1)$$

where $\{\lambda_\ell(j) : j = 1,2, \dots\}$ are the energy levels, labelled in ascending order with the lowest taken to be zero : $0 = \lambda_\ell(1) \leq \lambda_\ell(2) \leq \dots$. The volume of the region Λ_ℓ is denoted by V_ℓ ; it is assumed that the sequence $\{V_\ell\}$ diverges to $+\infty$. To state the conditions placed on the double sequence $\{\lambda_\ell(j)\}$, we define

$$\Phi_\ell(\beta) = \frac{1}{V_\ell} \sum_{j\geq 1} e^{-\beta\lambda_\ell(j)} ;$$

we shall assume that the following conditions hold :

(S1) <u>The limit</u> $\Phi(\beta) = \lim_{\ell\to\infty} \Phi_\ell(\beta)$ <u>exists for all</u> β <u>in</u> $(0, \infty)$.

(S2) <u>There exists</u> β_0 <u>in</u> $(0, \infty)$ <u>such that</u> $\Phi(\beta_0) \neq 0$.

It then follows that the sequence of distribution functions

$\{F_\ell : \ell = 1,2, \dots\}$ defined by

$$F_\ell(\lambda) = \frac{1}{V_\ell} \# \{ j : \lambda_\ell(j) \leq \lambda \} \qquad (3.2)$$

converges to F, the integrated density states (at least at the points of continuity of F) which is determined uniquely by its Laplace transform $\Phi(\beta) = \int_{[0,\infty)} e^{-\beta\lambda} dF(\lambda)$. The critical denisty ρ_c is defined by

$$\rho_c = \begin{cases} \int_{[0,\infty)} (e^{\beta\lambda} - 1)^{-1} dF(\lambda) , & \text{if } \lambda \to (e^{\beta\lambda} - 1)^{-1} \text{ is integrable.} \\ \infty, & \text{otherwise.} \end{cases}$$

Let $N(\omega) = \sum_{j\geq 1} \sigma_j(\omega)$ denote the total number of particles in the configuration ω ; then the canonical partition function $Z_\ell(n)$ is defined by

$$Z_\ell(n) = \begin{cases} 1 & , n = 0 , \\ \sum_{\{\omega \in \Omega : N(\omega) = n\}} e^{-\beta H_\ell(\omega)} & , n \geq 1 . \end{cases} \qquad (3.3)$$

The free-energy density $f_\ell : [0, \infty) \to R$ is defined first on the set $\{ \frac{n}{V_\ell} : n = 0,1, \ldots\}$ by $f_\ell(\frac{n}{V_\ell}) = \frac{-1}{\beta V_\ell} \ln Z_\ell(n)$, then extended to the whole of $[0, \infty)$ by linear interpolation. Using the methods of [10] and the results of [1] one may prove (see the Appendix).

Theorem 2

Suppose that (S 1) and (S 2) hold ; then on each compact subset of $[0, \infty)$ the sequence $\{f_\ell\}$ is bounded and converges uniformly on compacts to a convex function f satisfying $f(0) = 0$; moreover, $\mu_\infty = 0$.

Putting together this result with Theorem 1 of the previous section, we have

Corollary

Suppose that (S 1) and (S 2) hold ; then, for each $\mu < 0$, the sequence $\{K_\ell^\mu : 1 = 1,2, \ldots\}$ satisfies the Large Deviation Principle with constants $\{V_\ell\}$ and rate-function $I^\mu(\cdot)$ given by

$$I^\mu(x) = f^*(\mu) + f(x) - \mu x , \qquad (3.4)$$

and $p(\mu) = f^*(\mu)$.

It may seem surprising that no use appears to have been made of the special features of the free boson gas, while the earlier proof of this result [7] made fairly delicate use of the fact that the occupation numbers $\{ \sigma_j : j = 1,2, \ldots \}$, in the grand canonical ensemble, are independent geometrically distributed random variables. It is worthwhile, perhaps, to examine this point further. The grand canonical measure P^{μ}_{ℓ} is defined by $P^{\mu}[\omega] = e^{-\beta V_{\ell} p_{\ell}(\mu)} \cdot e^{\beta\{\mu N(\omega) - H_{\ell}(\omega)\}}$ for each $\mu < 0$; an easy calculation, see [1] for instance, yields

$$P^{\mu}_{\ell}[\sigma_j \geq m] = e^{m\beta(\mu - \lambda_{\ell}(j))} . \tag{3.5}$$

By expressing N as $\sigma_1 + (N - \sigma_1)$ and using (3.5) a lower bound was obtained for $P^{\mu}_{\ell}[X_{\ell} \epsilon B^{\sigma}_{y}]$, where $X = N/V_{\ell}$ and $y = E^{\mu}_{\ell}[X_{\ell}]$; this was required for the proof in [7] that (LD4) holds. However, the use of (3.5) can be detected in the proof of Theorem 2 :

the convexity of the functions $x \to f_{\ell}(x)$ was used to prove the uniform convergence of the sequence f_{ℓ} on compacts ; the proposition that f_{ℓ} is convex is equivalent to the proposition that the inequality $Z_{\ell}(n)^2 \geq Z_{\ell}(n + 1)\ Z_{\ell}(n - 1)$ for each $n \geq 1$, but this is equivalent to the proposition that $n \to P^{\mu}_{\ell}[\sigma_j \geq m | N = n]$ is an increasing function in view of the result, proved in [9] , that

$$P^{\mu}_{\ell}[\sigma_j \geq m \mid N = n] = \begin{cases} e^{-m\beta\lambda_{\ell}(j)} \dfrac{Z_{\ell}(n-m)}{Z_{\ell}(n)} , & m \leq n , \\ 0 , & m > n . \end{cases}$$

Following Davies [3] , we consider the hamiltonian

$$\tilde{H}_{\ell} = H_{\ell} + V_{\ell}\, w(X_{\ell}) , \tag{3.6}$$

where H_{ℓ} is the free-gas hamiltonian of (3.1) and $X_{\ell} = N/V_{\ell}$ is the particle number denisty ; unlike Davies, we require only that $w : [0,\infty) \to \mathbb{R}$ be lower semi-continuous and satisfy

$$w(0) = 0 , \liminf_{x \to \infty} \frac{w(x)}{x} = +\infty . \tag{3.7}$$

Define $\tilde{f}_{\ell}$ by $\tilde{f}_{\ell}(x) = f_{\ell}(x) + w(x)$;

it then follows that

$$\tilde{f}_{\ell}\left(\frac{n}{V_{\ell}}\right) = -\frac{1}{\beta V_{\ell}} \ln \sum_{\{\omega : N(\omega) = n\}} e^{-\beta \tilde{H}_{\ell}(\omega)} . \tag{3.8}$$

Using Theorem 2 and (3.7), we verify that $\{\tilde{f}_\ell : \ell = 1,2, \ldots\}$ satisfies the conditions of Theorem 1 with $\mu_\infty = +\infty$; we conclude that the following result follows from Theorem 1 :

Theorem 3

Suppose that (S 1) and (S 2) hold and that the mean-field hamiltonian (3.6) satisfies (3.7) ; then for each $\mu < \infty$ the grand canonical pressure $\tilde{p}(\mu) = \lim_{\ell \to \infty} \tilde{p}_\ell(\mu)$ exists and is given by the Legendre-Fenchel transform

$\tilde{f}^*$ of $\tilde{f}$, where

$$\tilde{f}(x) = f(x) + w(x) \tag{3.9}$$

and f is the free-energy density of the free boson gas, and the sequence $\{\tilde{K}^\mu_\ell : l = 1,2, \ldots\}$ of Kac distributions determined by $\{\tilde{f}_\ell : l = 1,2, \ldots\}$ satisfies the Large Deviation Principle with constants $\{V_\ell\}$ and rate-function $\tilde{I}^\mu(\cdot)$ given by

$$\tilde{I}^\mu(x) = \tilde{p}(\mu) + \tilde{f}(x) - \mu x . \tag{3.10}$$

It follows that $\tilde{p}^* = \tilde{f}^{**} = \operatorname{conv} \tilde{f}$, where conv g denotes the convex envelope of g ; hence the intervals $[\tilde{p}'_-(\mu), \tilde{p}'_+(\mu)]$ of discontinuity of the derivative of $\tilde{p}$ correspond to the linear segments in the convex envelope of $\tilde{f}$. We conclude once more that $\{\tilde{K}^\mu_\ell\}$ is asymptotically degenerate whenever w is strictly convex.

§ 4 The Asymptotics of the Kac Distribution

In this section we examine the consequences of the non-convexity of $\tilde{f}$ for the asymptotics of the Kac distribution. We consider the case where conv $\tilde{f}$ has precisely one linear segment $[\rho_-, \rho_+]$ and $\tilde{f}(x) > \text{conv}\,\tilde{f}(x)$ for x in (ρ_-, ρ_+) ; the general situation should be clear from this discussion. We recall that the asymptotic Kac distribution $K^\mu = \lim_{l\to\infty} K^\mu_\ell$ gives the decomposition of the grand canonical limiting state $\langle\cdot\rangle^\mu$ into extremal (canonical) limiting states $\langle\cdot\rangle_\rho$:

$$\langle\cdot\rangle^\mu = \int_{[0,\infty)} \langle\cdot\rangle_\rho \; K^\mu\,[d\rho] \;. \tag{4.1}$$

In general, if $K^\mu = \lim_{l\to\infty} K^\mu_\ell$ exists its support is contained in the set $\{x : I^\mu(x) = 0\}$; however, if this set consists of more than one point there is no guarantee that the sequence $\{K^\mu{}_\ell : \ell = 1.2. \ldots\}$ converges. Nevertheless, by the Helly selection principle, $\{K^\mu{}_\ell : \ell = 1,2, \ldots\}$ contains at least one convergent subsequence ; in the case under consideration, where conv $\tilde{f}$ has precisely one linear segment $[\rho_-, \rho_+]$ and $\tilde{f}$ is non-convex, we have three cases determined by μ_c which is defined by $\tilde{p}'_-(\mu_c) = \rho_-$ (and hence $\tilde{p}'_+(\mu_c) = \rho_+$) so that μ_c is the slope of the linear segment of conv $\tilde{f}$:

I : $\mu < \mu_c$; $\tilde{K}^\mu_\ell \to \tilde{K}^\mu = \delta_{\rho(\mu)}$, $\rho(\mu) = \tilde{p}'(\mu)$. (4.2)

II : $\mu = \mu_c$; there exists $\{\ell_j : j = 1,2, \ldots\}$ such that $\lim_{j\to\infty} \tilde{K}^\mu_{\ell_j} = \tilde{K}^\mu$ exists and

$$\tilde{K}^\mu = \alpha\,\delta_{\rho_-} + (1-\alpha)\,\delta_{\rho_+} \;, \quad 0 \le \alpha \le 1 \;. \tag{4.3}$$

III : $\mu > \mu_c$; $\tilde{K}^\mu_\ell \to \tilde{K}^\mu = \delta_{\rho(\mu)}$, $\rho(\mu) = \tilde{p}'(\mu)$. (4.4)

We sketch the proof of II ; the proof of the remaining cases should then be clear. Choose ρ_0 such that $\rho_- < \rho_0 < \rho_+$;

Let $A_- = [0,\rho_0)$ and $A_+ = [\rho_0,\infty)$.

Then

$\left\{\tilde{K}^{\mu_c}_{\ell}[A_-]\right\}$ is a bounded sequence of real numbers and hence contains a convergent subsequence $\left\{\tilde{K}^{\mu_c}_{\ell_k}\ [A_-]\ :\ k = 1,2\ \ldots\right\}$

Consider the case in which

$$\lim_{k\to\infty} \tilde{K}^{\mu_c}_{\ell_k}\ [A_-] = \alpha\ ,\quad 0 < \alpha < 1.$$

Then

$$\int_{[0,\infty)} e^{-tx}\,\tilde{K}^{\mu_c}_{\ell_k}[dx] = \tilde{K}^{\mu_c}_{\ell_k}\ [A_-]\int_{A_-} e^{-tx}\,L_k^-[dx]$$

$$+\ (1-\tilde{K}^{\mu_c}_{\ell_k}\ [A_-])\int_{A_+} e^{-tx}\,L_k^+\ [d\mu]$$

where $L_k^-\ [A] = \dfrac{\tilde{K}^{\mu_c}_{\ell_k}\ [A\cap A_-]}{\tilde{K}^{\mu_c}_{\ell_k}\ [A_-]}$, $L_k^+\ [A] = \dfrac{\tilde{K}^{\mu_c}_{\ell_k}\ [A\cap A_+]}{\tilde{K}^{\mu_c}_{\ell_k}\ [A_+]}$

Now $\{L_k^-\}$ and $\{L_k^+\}$ satisfy the large deviation principle with rate-functions I^- and I^+ respectively, where $\tilde{I}^-$ $(\tilde{I}^+)$ is the restriction of $\tilde{I}$ to A^- (A^+) . Now $\tilde{I}^-$ has a unique minimum at ρ_- and $\tilde{I}^+$ has a unique minimum at ρ_+,

hence

$$\int_{[0,\infty)} e^{-t\eta}\,\tilde{K}^{\mu_c}_{\ell_k}\ [d\eta] \to \alpha\ e^{-t\rho_-} + (1-\alpha)\ e^{-t\rho_+}\ .$$

So that $\left\{\tilde{K}^{\mu_c}_{\ell_k}\right\}$ converges weakly to

$$\alpha\ \delta_{\rho_-} + (1-\alpha)\ \delta_{\rho_+}\ .$$

The remaining cases are clear.

It remains to consider case II in more detail : we investigate the possible dependence of α on the subsequence $\{l_j : j = 1,2, \dots\}$. We remark, in passing, that if we adopt the quasi-average approach of Bogoliubov [11], we get

$$\lim_{\mu\uparrow\mu_c} \lim_{\ell\to\infty} \tilde{K}^{\mu}_{\ell} = \delta_{\rho_-} , \quad \lim_{\mu\downarrow\mu_c} \lim_{\ell\to\infty} \tilde{K}^{\mu}_{\ell} = \delta_{\rho_+} ; \tag{4.5}$$

On the other hand, the generalized quasi-average procedure [12] enables us to scan the whole interval $0 \leq \alpha \leq 1$: here we put

$\mu_\ell = \mu_c + \dfrac{\delta}{\beta V_\ell^{\gamma}}$, $\gamma \geq 1$, and get the following limiting values

$$\tilde{K}^{\mu_c}_{\gamma,\delta} = \lim_{k\to\infty} \tilde{K}^{\mu_{\ell k}}_{\ell_k} :$$

$$\gamma = 1 : \quad \tilde{K}^{\mu_c}_{\gamma,\delta} = \lambda_\delta \, \delta_{\rho_-} + (1 - \lambda_\delta) \, \delta_{\rho_+} , \tag{4.6}$$

$$\text{where } \lambda_\delta = \frac{e^{\delta\rho_-} \alpha}{\alpha e^{\delta\rho_-} + (1 - \alpha) e^{\delta\rho_+}} . \tag{4.7}$$

$$\gamma > 1 : \quad K^{\mu_c}_{\gamma,\delta} = \lambda_o \, \delta_{\rho_-} + (1 - \lambda_o) \, \delta_{\rho_+} . \tag{4.8}$$

Note that

$$\int_{[0,\infty)} e^{-tx} K^{\mu_\ell}_{\ell} [dx] = \frac{\int_{[0,\infty)} e^{-(t - \delta V_\ell^{(1-\gamma)})x} \tilde{K}^{\mu_c}_{\ell} [dx]}{\int_{[0,\infty)} e^{\delta V_\ell^{(1-\gamma)} x} K^{\mu_c}_{\ell} [dx]} .$$

Now we can choose B and ℓ_0 sufficiently large so that

$$\frac{\delta}{V_\ell^{\gamma-1}} x + \beta V_\ell \{\mu_c x - w(x) - f_\ell(x)\} < -\beta V_\ell x$$

for $x \geq B$ and $\ell \geq \ell_0$. This follows from the fact that

$\lim_{x\to\infty} \frac{w(x)}{x} = \infty$ and the fact that $f_\ell(x) > -x$ for $x > B$ and $\ell > \ell_0$.

Then for $t \geq 0$,

$$\int_{[B,\infty)} e^{-(t-\delta V_\ell^{(1-\gamma)})x} \tilde{K}_\ell^{\mu_c}[dx] =$$

$$e^{-\beta V_\ell \tilde{P}_\ell(\mu_c)} \int_{[B,\infty)} e^{-(t-\delta V_\gamma^{(1-\gamma)})x} e^{\beta V_\ell \{\mu_c x - w(x) - f_\ell(x)\}} m_\ell[dx]$$

$$\leq \int_{[B,\infty)} e^{-\beta V_\ell x} m_\ell[dx] < \frac{e^{-\beta V_\ell B}}{1-e^{-\beta}} \text{ for } \ell \geq \ell_0 .$$

Therefore

$$\lim_{k\to\infty} \int_{[0,\infty)} e^{-(t\,\delta V_{\ell_k}^{(1-\gamma)})x} \tilde{K}_\ell^{\mu_c}[dx] =$$

$$\lim_{k\to\infty} \int_{[0,B)} e^{-(t-\delta V_{\ell_k}^{(1-\gamma)})x} \tilde{K}_\ell^{\mu_c}[dx]$$

and the proof of (4.7) and (4.8) follows as for (4.2), (4.3) and (4.4).

We end with some remarks on boson condensation in this situation ; it is only necessary to comment on the case in which the Bose-Einstein critical density ρ_c lies between ρ_- and ρ_+ . In this case we have, in the standard example described in the introduction perturbed by the mean-field term $V_\ell\, w(X_\ell)$, the following result for the occupation of the ground state.

$$\lim_{\ell\to\infty} \tilde{E}^{\mu}_{\ell}\left[\frac{\sigma_1}{V_\ell}\right] = \begin{cases} 0 & , \mu < \mu_c , \\ \rho_+ - \rho_c & , \mu = \mu_c , \\ \rho(\mu) - \rho_c & , \mu > \mu_c . \end{cases} \qquad (4.9)$$

Appendix : The free-energy density of the free boson gas

Here we prove the results about the free-energy density of the free boson gas which we used in the body of the paper. First, we remark that, as $\lambda_\ell(1) = 0$, $_\ell(\mu) > -(\beta V_\ell)^{-1} \ln(1 - e^{-\beta V})$ so that $_\ell(\mu) \to \infty$ as μ increases to zero. Moreover, it was proved in [1] that when (S1) and (S2) hold we have $p(\mu) = \lim_{\ell\to\infty} p_\ell(\mu)$ exists

for $\mu < 0$ and is given by $p(\mu) = \int_{[0,\infty)} p(\mu \mid \lambda) \quad F(\lambda)$

where $p(\mu \mid \lambda) = \beta^{-1} \ln(1 - e^{-\beta(\lambda-\mu)})^{-1}$.

It was proved also that

$$p^*(x) = \sup_{\mu<0} \{ \mu x - p(\mu) \}$$

is given by

$$p^*(x) = x\mu(x) - p(\mu(x))$$

where $\mu(x) = 0$ for $x > \rho_c$ and $\mu(x)$ is the unique real root of $x = p'(\mu)$ for $x < \rho_c$; the function $p(\mu)$, defined on $(-\infty, 0)$; is extended defining $p(0) = \lim_{\mu\uparrow 0} p(\mu) = \int_{[0,\infty)} p(0 \mid \lambda)\, d F(\lambda)$.

Lemma 1

The function $x \to f_\ell(x)$ is convex.

Proof : It is enough to prove that, for each n ,

$$f_\ell\left(\frac{n}{V_\ell}\right) \leq \frac{1}{2} f_\ell\left(\frac{n-1}{V_\ell}\right) + \frac{1}{2} f_\ell\left(\frac{n+1}{V_\ell}\right) \quad ;$$

that is, that

$$Z_\ell(n)^2 \geq Z_\ell(n-1)\, Z_\ell(n+1) \quad , \qquad (*)$$

where

$$Z_\ell(n) = \sum_{\{\omega\ :\ N(\omega) = n\}} e^{-\beta\{\lambda_\ell(1)\,\omega_1 + \lambda_\ell(2)\,\omega_2 + \ldots\}}$$

We proceed by induction on the number of levels ; Let

$$Z_\ell^k(n) = \sum_{\{\omega\ :\ N(\omega) = n\}} e^{-\beta\{\lambda_\ell(1)\omega_1 + \ldots + \lambda_\ell(k)\omega_k\}} .$$

For $k = 1$, the result (*) holds trivially.

Assume that

$$Z_\ell^k(n)^2 \geq Z_\ell^k(n-1)\; Z_\ell^k(n+1) \quad \text{for all } n \geq 1 ,$$

so that

$$Z_\ell^k(n)\; Z_\ell^k(m) \geq Z_\ell^k(n+1)\; Z_\ell^k(m-1)$$

Now $$Z_\ell^{k+1}(n) = \sum_{m=0}^{n} z^{n-m}\, Z_\ell^k(m)$$

where

$$z = e^{-\beta\lambda_\ell(k+1)} \quad , \quad \text{so that}$$

$$(Z_\ell^{k+1}(n))^2 = S + Z_\ell^k(n)\sum_{m=0}^{n} z^{n-m} Z_\ell^k(m) ,$$

where

$$S = \sum_{m_1=0}^{n-1}\sum_{m_2=0}^{n} z^{2n-m_1-m_2} Z_\ell^k(m_1) Z_\ell^k(m_2) ,$$

while

$$(Z_\ell^{k+1}(n-1))(Z_\ell^{k+1}(n+1)) = S + Z_\ell^k(n+1)\sum_{m=1}^{n} z^{n-m} Z_\ell^k(m-1)$$

Thus

$$(Z_\ell^{k+1}(n))^2 - (Z_\ell^{k+1}(n-1))(Z_\ell^{k+1}(n+1))$$

$$= z^n Z_\ell^k(n) + \sum_{m=1}^{n} z^{n-m}\{ Z_\ell^k(n) Z_\ell^k(m) - Z_\ell^k(n+1) Z_\ell^k(m-1)\}$$

$$\geq 0$$

■

Lemma 2

For the free boson gas, the finite-volume free-energy density is a decreasing function :

$$f_\ell(x) \leq f_\ell(y) \quad \text{for all} \quad x \geq y \ .$$

Proof :

Since $x \to f_\ell(x)$ is convex, it has a line of support at each point : for each y, there exists $a_\ell(y)$ such that

$$f_\ell(x) - f_\ell(y) \geq a_\ell(y)\ (x - y) \quad \text{for all } x \ .$$

Suppose there exists a point x_0 where $a(x_0) > 0$;

then, for each $\mu < 0$, we have

$$e^{\beta V_\ell\, p_\ell(\mu)} = \int_{[0,\infty)} e^{-\beta V_\ell \{f_\ell(x) - \mu x\}}\, m_\ell[dx]$$

$$\leq \int_{[0,x_0)} e^{-\beta V_\ell\, f_\ell(x)}\, m_\ell[dx] + e^{-\beta V_\ell\, f_\ell(x_0)} \int_{[x_0,\infty)} e^{-\beta V_\ell a_\ell(x_0)(x-x_0)}\, m_\ell dx]$$

$$< \infty, \quad \text{since } a_\ell(x_0) > 0 \ .$$

But $p_\ell(\mu) \to \infty$ as $\mu \uparrow 0$; contradiction. Hence $a_\ell(y) \leq 0$ for all y and

$$f_\ell(x) - f_\ell(y) \leq 0 \quad \text{for all} \quad x \geq y$$

<u>Lemma 3</u>

For all $x \geq 0$, $\liminf_{\ell \to \infty} f_\ell(x) \geq p\ (x) = \sup_{\mu<0} \{\mu x - p(\mu)\}$

<u>Proof</u> : We have

$$e^{\beta V_\ell p_\ell(\mu)} = \int_{[0,\infty)} e^{-\beta V_\ell \{f_\ell(x) - \mu x\}} m_\ell[dx]$$

$$\geq e^{-\beta V_\ell \{f_\ell(x) - \mu x\}} \quad \text{for } 0 < x < \infty .$$

$$e^{\beta V_\ell p_\ell(\mu)} = \sum_{n \geq 0} e^{-\beta V_\ell \{f_\ell(\frac{n}{V_\ell}) - \mu \frac{n}{V_\ell}\}} .$$

Thus $p_\ell(\mu) \geq - f_\rho (\frac{n}{V_\ell}) + \frac{n}{V_\ell}$ for each n .

Since $f_\ell(x)$ is defined for all x in $(0,\infty)$ by linear interpolation it follows that

$$p_\ell(\mu) \geq - f_\ell(x) + \mu x \quad \text{for all } x \text{ in } (0,\infty) ;$$

thus $f_\ell(x) \geq \mu x - p_\ell(\mu)$

so that $\liminf_{\ell \to \infty} f_\ell(x) \geq \mu x - p(\mu)$.

Hence $\liminf_{\ell \to \infty} f_\ell(x) \geq \sup_\mu \{\mu x - p(\mu)$

$$= p^*(x) .$$

■

Lemma 4 For all $x < \rho_c$,

$$\limsup_{\ell \to \infty} f_\ell(x) \leq p^*(x)$$

Proof : For the measure K_ℓ^μ defined in § 2 we have

$$\int_{[0,\infty)} e^{-sx} K_\ell^\mu [dx] = \exp\left[- s\frac{\{ p_\ell(\mu) - p_\ell(\mu-\delta_\ell)\}}{\delta_\ell}\right]$$

where $\delta_\ell = s/V_\ell$.

Now for the free boson gas if $\mu < 0$, (see [1]) ,

$$\lim_{\ell \to \infty} \frac{p_\ell(\mu) - p_\ell(\mu-\delta_\ell)}{\delta_\ell} = p'(\mu) .$$

Therefore K_ℓ^μ converges weakly to $\delta_{p'(\mu)}$.

Let $x \in [0,\rho_c]$ and $\delta \in (0,\infty)$

then $\lim_{\ell \to \infty} K_\ell^{\mu(x)-\delta} (p'(\mu(x) - 2\delta), x] = 1$

But by Lemma 2

$$\frac{1}{\beta V_\ell} \ln K_\ell^{(\mu(x) - \delta)}(p'(\mu(x) - 2\delta), x] \leq \frac{1}{\beta V_\ell} \ln V_\ell(x-p'(\mu(x)-2\delta)+1)$$

$$- f_\ell(x) + (\mu(x) - \delta)\, p'(\mu(x) - 2\delta) - p_\ell(\mu(x) - \delta) .$$

Thus $\limsup_{\ell \to \infty} f_\ell(x) \leq (\mu(x) - \delta)\, p'(\mu(x) - 2\delta) - p(\mu(x) - \delta)$.

Since p and p′ are continuous ([1]) and δ is arbitrary

this proves the lemma.

<u>Lemma 5</u> For all $x \geq \rho_c$,

$$\limsup_{\ell\to\infty} f_\ell(x) \leq p^*(\rho_c) .$$

<u>Proof</u> : By Lemma 2, for every $\varepsilon > 0$ and $x \geq \rho_c$, we have

$$f_\ell(x) \leq f_\ell(\rho_c - \varepsilon) ;$$

hence

$$\limsup_{\ell\to\infty} f_\ell(x) \leq \limsup_{\ell\to\infty} f_\ell(\rho_c - \varepsilon) .$$

But, by Lemma 4, we have

$$\limsup_{\ell\to\infty} f_\ell (\rho_c - \varepsilon) \leq p^*(\rho_c - \varepsilon) ,$$

so that

$$\limsup_{\ell\to\infty} f_\ell(x) \leq p^*(\rho_c) ,$$

since ε is arbitrary and p is continuous . ■

Since $p^* (x) = p^* (\rho_c)$ for $x \geq \rho_c$,
we have by Lemma 4 and Lemma 5 that

$$\limsup_{\ell\to\infty} f_\ell(x) \leq p^* (x) \quad \text{for } x \geq 0 .$$

Combining this with Lemma 3, we establish Theorem 2 : $\lim_{\ell\to\infty} f_\ell (x) = p^*(x)$.

$\{f_\ell\}$ is bounded on compacts by Lemma 2.

Since $f_\ell(x) \leq 0$, $\mu_\infty \leq 0$. From the inequality

$f_\ell(x) \geq \mu x - p_\ell(\mu)$ for $\mu < 0$ in Lemma 3 we get $\mu_\infty \geq 0$.

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