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Condensation in the Imperfect Boson Gas

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We prove that Bose–Einstein condensation persists in the imperfect boson gas; it is not destroyed by the mean field interaction.

KEY WORDS: Bose–Einstein condensation; mean field.

1. INTRODUCTION

In the mean field model of a system of interacting bosons, the interaction energy is represented by a term $aN^2/2V$ which is added to the Hamiltonian of the free boson gas; here a is a strictly positive constant representing the strength of the interaction, N is the total number of particles, and V is the volume of the confining region. This crude model of a system of interacting bosons is commonly called the imperfect boson gas.[1] It is of interest because the pathological aspects of the free boson gas are removed by the mean field interaction: the grand canonical partition function converges for all real values of the chemical potential[2]; the grand canonical distribution of the particle number density is asymptotically degenerate for all values of the mean density[3,4]; the fluctuations in the particle number density in the grand canonical ensemble are normal and shape independent.[5] In this paper we prove that Bose–Einstein condensation persists in the imperfect boson gas; it is not removed by the mean field interaction. Our starting point is a general theory of Bose–Einstein condensation in a noninteracting system of bosons given in Ref. 6; there a distinction was drawn between macroscopic occupation of the ground state and generalized condensation: *macroscopic*

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occupation of the ground state is said to occur when the number of particles in the ground state becomes proportional to the volume; *generalized condensation* is said to occur when the number of particles whose energy levels lie in an arbitrary small band above zero become proportional to the volume. Obviously, the first implies the second. However, the second can occur without the first; this is called *nonextensive condensation.* Macroscopic occupation of the ground state is a subtle matter; its magnitude depends strongly on the shape of the container, for example. Generalized condensation is much more robust; in the free boson gas it always occurs when the number density ρ exceeds a critical value ρ_c. It this paper we prove that generalized condensation is stable with respect to a mean field perturbation of the free-particle Hamiltonian. The proof depends on obtaining an explicit formula for the grand canonical pressure of the imperfect boson gas. In Section 2 we establish the notation and state the theorem on the existence of the pressure in the thermodynamic limit; we list some straightforward consequences of the theorem. In Section 3 we use the theorem to prove the persistence of generalized condensation. In Section 4 we give a proof of the theorem. The connection with earlier work is discussed in Section 2.

2. THE GRAND CANONICAL PRESSURE

To fix the notation we recall some facts about the grand canonical ensemble. Let $Z_V^\beta(n)$ be the canonical partition function for n particles at inverse temperature β in a region of volume V; put $Z_V^\beta(0)=1$. The grand canonical pressure $p_V(\mu)$ is defined by

$$e^{\beta V p_V(\mu)} = \sum_{n=0}^{\infty} e^{n\beta\mu} Z_V^\beta(n) \tag{2.1}$$

for all values of the chemical potential μ for which the infinite series converges. Denote by N the total number of particles in volume V; we regard N as a random variable taking values in the nonnegative integers. The probability $\mathbb{P}_V^\mu[N=n]$ that N takes the value n is given by

$$\mathbb{P}_V^\mu[N=n] = e^{n\beta\mu} Z_V^\beta(n)\, e^{-\beta V p_V(\mu)} \tag{2.2}$$

The probability distribution function $K_V^\mu(x)$ of the particle number density is defined by

$$K_V^\mu(x) = \mathbb{P}_V^\mu[N/V \leqslant x] \tag{2.3}$$

and it is determined uniquely by its Laplace transform $\mathbb{E}_V^\mu[e^{-sN/V}] = \int_{[0,\infty)} e^{-sx}\, dK_V^\mu(x)$, which can be expressed in terms of the pressure $p_V(\mu)$ as

$$\mathbb{E}_V^\mu[\exp(-sN/V)] = \exp[\beta V\{p_V(\mu - s/\beta V) - p_V(\mu)\}] \tag{2.4}$$

It follows that the mean density ρ is given by

$$\rho = \mathbb{E}_V^\mu[N/V] = p_V'(\mu) \tag{2.5}$$

Now we specialize to the case of a free boson gas. We shall go to the thermodynamic limit at fixed mean density. Let $\{(h_l, V_l): l = 1, 2,...\}$ be a sequence of pairs, each pair consisting of a self-adjoint operator h_l, the single-particle Hamiltonian of the system, and a real number V_l, the volume of the system. Let $\varepsilon_l(1) \leqslant \varepsilon_l(2) \leqslant \cdots$ be the eigenvalues of h_l and let $\lambda_l(k) = \varepsilon_l(k) - \varepsilon_l(1)$, $k = 1, 2,...$; we may take for the canonical partition function for a noninteracting bosons, each having h_l as single-particle Hamiltonian, the expression

$$Z_l^\beta(n) = \sum_{\{n(k):\, \sum n(k) = n\}} e^{-\beta \sum n(k) \lambda_l(k)} \tag{2.6}$$

It follows that the grand canonical pressure $p_l(\mu)$ is determined by the distribution function

$$F_l(\lambda) = \max\{k : \lambda_l(k) \leqslant \lambda\}/V_l \tag{2.7}$$

since, from (2.1) and (2.6),

$$\exp[\beta V_l p_l(\mu)] = \prod_k \{1 - \exp[\beta(\mu - \lambda_l(k))]\}^{-1} \tag{2.8}$$

so that

$$p_l(\mu) = \int_{[0,\infty)} p(\mu \mid \lambda)\, dF_l(\lambda) \tag{2.9}$$

where

$$p(\mu \mid \lambda) = \beta^{-1} \log(1 - e^{\beta(\mu - \lambda)})^{-1} \tag{2.10}$$

and (2.7) holds for $-\infty < \mu < 0$.

In good cases the sequence $\{F_l: l = 1, 2,...\}$ converges to a distribution function F, called the *integrated density of states*, the sequence $\{p_l(\mu):$

$l=1,2,\ldots\}$ converges pointwise to the grand canonical pressure $p(\mu)$ of the free gas, and p is determined by F through the formula

$$p(\mu)=\int_{[0,\infty)} p(\mu \mid \lambda)\, dF(\lambda) \tag{2.11}$$

valid for $-\infty<\mu<0$.

In Ref. 6 it was shown that a sufficient condition for the above to hold is

$$\text{(A):} \quad \phi(\beta)=\lim_{l\uparrow\infty} V_l^{-1} \sum_{k=1}^{\infty} e^{-\beta\lambda_l(k)}$$

exists for all β *in* $(0,\infty)$ *and is nonzero for some* β *in* $(0,\infty)$. *In this case* F *is determined uniquely by*

$$\phi(\beta)=\int_{[0,\infty)} e^{-\beta\lambda}\, dF(\lambda)$$

It follows from (2.4) and (2.8) that we can regard the random variables N as a sum

$$N=\sum_k n(k) \tag{2.12}$$

of independent random variables $n(k)$, each with a geometric thermal distribution

$$\mathbb{P}_l^\mu[n(k)\geqslant n]=\exp[n\beta(\mu-\lambda_l(k))] \tag{2.13}$$

We interpret $n(k)$ as the occupation number of the kth level. For each $\delta>0$, let

$$N_l(\delta)=\sum_{\{k:\lambda_l(k)<\delta\}} n(k) \tag{2.14}$$

In Ref. 1 we showed that generalized condensation occurs provided (A) holds, in the sense that

$$\lim_{\delta\downarrow 0}\lim_{l\uparrow\infty} \mathbb{E}_\rho[N_l(\delta)/V_l]=(\rho-\rho_c)^+ \tag{2.15}$$

the symbol $\mathbb{E}_\rho$ indicates that for each l the expectation $\mathbb{E}_l^\mu$ is taken with $\mu=\mu_l(\rho)$, the unique root in $(-\infty,0)$ of

$$\mathbb{E}_l^\mu[N/V_l]=\rho \tag{2.16}$$

and

$$\rho_c = \int_{[0,\infty)} (e^{\beta\lambda} - 1)^{-1}\, dF(\lambda) \tag{2.17}$$

In the mean-field model of a system of noninteracting bosons the interaction energy is represented by adding to the Hamiltonian a term $aN^2/2V_l$; here a is a strictly positive constant and represents the strength of the interaction. The new grand canonical pressure $p^a(\mu)$ is given by

$$e^{\beta V_l p_l^a(\mu)} = \sum_{n=0}^{\infty} e^{n\beta\mu} Z_l^n(\beta)\, e^{-\beta a n^2/2V_l} \tag{2.18}$$

where $Z_l^n(\beta)$ is the canonical partition function of the noninteracting system. As we shall see, the Gaussian factor ensures the convergence of the series, and hence the existence of $p^a(\mu)$, for all values of μ in $(-\infty, \infty)$. All our results follow from the following

Theorem. Suppose that the sequence $\{(h_l, V_l)\colon l = 1, 2,...\}$ satisfies condition (A); then for $a > 0$ the grand canonical pressure $p^a(\mu)$ of the imperfect boson gas exists for all μ in $(-\infty, \infty)$ and in given in terms of the free gas pressure $p(\mu)$ by

$$p^a(\mu) = (p - \alpha(\mu))^2/2a \ + (p \circ \alpha)(\mu) \tag{2.19}$$

where $\alpha(\mu)$ is zero for $\mu \geqslant a\rho_c$ and is the unique root in $(-\infty, 0)$ of $\alpha + ap'(\alpha) = \mu$ for $\mu < a\rho_c$.

We postpone the proof of Section 4. We list here some immediate consequences of the theorem:

1. It follows from (2.19) that $\mu \to p^a(\mu)$ is differentiable for all values of μ and its first derivative is continuous and given by

$$(p^a)'(\mu) = (\mu - \alpha(\mu))/a \tag{2.20}$$

2. Since $\mu \to (p^a)'(\mu)$ is continuous there is no first-order phase transition in the imperfect gas; the sequence $\{K_l^{a,\mu}\colon l = 1, 2,...\}$ of distribution functions for the particle number density converges to the degenerate distribution concentrated at $x = (p^a)'(\mu)$. For the details, see Lewis and Pulè.[7] This generalizes an earlier result of Davies,[3] obtained by different means; see also Fannes and Verbeure.[4] The precise order of the phase transition in the imperfect boson gas to determined by the behavior of the integrated density of states $F(\lambda)$ as $\lambda \downarrow 0$.

3. The equation of state of the imperfect gas follows directly from the theorem: the pressure $\pi^a(\rho)$ as a function of the density ρ is given by

$$\pi^a(\rho) = a\rho^2/2 + (p \circ \mu)(\rho) \tag{2.21}$$

where $\mu(\rho)$ is zero for $\rho \geqslant \rho_c$ and is the unique root in $(-\infty, 0)$ of $p'(\mu - a\rho) = \rho$ for $\rho < \rho_c$. The pressure-density isotherm, is not flat for $\rho > \rho_c$, as it is in the case of the free boson gas. Nevertheless there is a singularity in $\pi^a(\rho)$ at $\rho = \rho_c$ (its precise order being determined by the behavior of the integrated density of states $F(\lambda)$ as $\lambda \downarrow 0$) so that the critical density for the imperfect boson gas is the same as for the free gas.

3. GENERALIZED CONDENSATION

The persistence of condensation in the mean-field model is a direct consequence of the theorem stated in Section 2. We show that

$$\lim_{\delta \downarrow 0} \lim_{l \uparrow \infty} \mathbb{E}_l^{a,\mu}[N_l(\delta)/V_l] = (\rho - \rho_c)^+ \tag{3.1}$$

where $\rho = (p^a)'(\mu)$ and $\mathbb{E}_l^{a,\mu}[X]$ is the expectation of a random variable X in the grand canonical ensemble of the mean-field model. Now $\mathbb{E}_l^{a,\mu}[X]$ is given in terms of the free gas expectations by

$$\mathbb{E}_l^{a,\mu}[X] = \mathbb{E}_l^{\mu}[Xe^{-\beta a N^2/2V_l}]/\mathbb{E}_l^{\mu}[e^{-\beta a N^2/2V_l}] \tag{3.2}$$

A straightfoward computation using (2.13) and (2.14) yields

$$\mathbb{E}_l^{a,\mu}[\exp\{\beta\sigma N_l(\delta)\}] = \exp[\beta V_l\{\tilde{p}_l^a(\mu + \delta) - \tilde{p}_l^a(\mu)\}] \tag{3.3}$$

where $\tilde{p}_l^a(\mu)$ is the grand canonical pressure in a mean-field model with single-particle Hamiltonian $\tilde{h}_l$ having eigenvalues $\{\tilde{\lambda}_l(k)\colon k = 1, 2,...\}$ related to those of h_l by

$$\tilde{\lambda}_l(k) = \begin{cases} \lambda_l(k), & \text{if } \lambda_l(k) < \delta \\ \lambda_l(k) + \sigma, & \text{otherwise} \end{cases} \tag{3.4}$$

It follows from (3.2) that

$$\mathbb{E}_l^{a,\mu}[N_l(\delta)/V_l] = \frac{\partial}{\partial\sigma} \tilde{p}_l^a(\mu + \sigma)\bigg|_{\sigma=0} \tag{3.5}$$

Now $\{(\tilde{h}_l, V_l)\colon l = 1, 2,...\}$ satisfies condition (A) whenever $\{(h_l, V_l)\colon l = 1, 2,...\}$ does, so that it follows from the theorem that

$$\tilde{p}^a(\mu) = \lim_{l \uparrow \infty} \tilde{p}_l^a(\mu) \tag{3.6}$$

exists and is given by

$$\tilde{p}^a(\mu) = [\mu - \tilde{\alpha}(\mu)]^2/2a + (\tilde{p} \circ \tilde{\alpha})(\mu) \tag{3.7}$$

where

$$\tilde{p}(\mu) = \int_{[0,\delta)} p(\mu \mid \lambda)\, dF(\lambda) + \int_{[\delta,\infty)} p(\mu \mid \lambda + \sigma)\, dF(\lambda) \tag{3.8}$$

and $\tilde{\alpha}(\mu)$ is zero for $\mu \geqslant a\tilde{\rho}_c(\sigma)$ and is the unique root in $(-\infty, 0)$ of $\alpha + a\tilde{p}'(\alpha) = \mu$ for $\mu < a\tilde{\rho}_c(\sigma)$. Thus $(\partial/\partial\sigma)\, \tilde{p}^a(\mu + \sigma)|_{\sigma=0}$ exists and is continuous and given by

$$\frac{\partial}{\partial\sigma} \tilde{p}^a(\mu + \sigma)\bigg|_{\sigma=0} = (\mu - \alpha(\mu))/a + \int_{[\delta,\infty)} p(\alpha(\mu) \mid \lambda)\, dF(\lambda) \tag{3.9}$$

But $\sigma \to \tilde{p}_l^a(\mu + \sigma)$ is convex and so, by Griffith's lemma in the version proved by Hepp and Lieb,[8]

$$\lim_{l \uparrow \infty} \frac{\partial}{\partial\sigma} \tilde{p}_l^a(\mu + \sigma)\bigg|_{\sigma=0} = \frac{\partial}{\partial\sigma} \tilde{p}^a(\mu + \sigma)\bigg|_{\sigma=0} \tag{3.10}$$

It then follows from (3.5), (3.9), and (3.10) that

$$\lim_{\delta \downarrow 0} \lim_{l \uparrow \infty} \mathbb{E}_l^{a,\mu}[N_l(\delta)/V_l] = (\rho - \rho_c)^+ \tag{3.11}$$

where $\rho = (p^a)'(\mu)$.

4. THE PROOF OF THE THEOREM

The proof is straightforward in the case in which $\mu < a\rho_c$, so we give that first. We can rewrite (2.18) as

$$\begin{aligned} \exp[\beta V_l p_l^a(\mu) = {} & \exp[\beta V_l\{(\mu - \alpha)^2/2a + p_l(\alpha)\}] \\ & \times \mathbb{E}_l^\alpha\{\exp(-\beta a[N - (\mu - \alpha) V_l/a]^2/2V_l)\} \end{aligned} \tag{4.1}$$

for arbitrary $\alpha < 0$. But

$$e^{-\mathbb{E}_l^\alpha[X^2]} \leqslant \mathbb{E}_l^\alpha[e^{-X^2}] \leqslant 1 \tag{4.2}$$

where the lower bound follows from Jensen's inequality, so that

$$\begin{aligned} & (\mu - \alpha)^2/2a + p_l(\alpha) - \frac{a}{2} \mathbb{E}_l^\alpha\left[\left(\frac{N}{V_l} - \frac{\mu - \alpha}{a}\right)^2\right] \\ & \quad \leqslant p_l^a(\mu) \leqslant (\mu - \alpha)^2/2a + p_l(\alpha) \end{aligned} \tag{4.3}$$

for $\alpha < 0$. The upper bound gives

$$\limsup_{l \uparrow \infty} p_l^a(\mu) \leqslant \inf_{\alpha < 0} \{(\mu - \alpha)^2/2a + p(\alpha)\} \tag{4.4}$$

since, by Lemma 1 of Ref. 6, the limit $p(\alpha) = \lim_{l \uparrow \infty} p_l(\alpha)$ exists for $\alpha < 0$ when condition (A) holds. For $\mu < ap_c$ the infimum is attained at $\alpha(\mu)$, the unique root in $(-\infty, 0)$ of $\alpha + ap'(\alpha) = \mu$, so that

$$\limsup_{l \uparrow \infty} p_l^a(\mu) \leqslant [\mu - \alpha(\mu)]^2/2a + (p \circ \alpha)(\mu) \tag{4.5}$$

Now let $\alpha_l(\mu)$ be the unique root in $(-\infty, 0)$ of $\alpha + ap_l'(\alpha) = \mu$. By an argument based on that used to prove Lemma 3 of Ref. 6 we can show that $\lim_{l \uparrow \infty} \alpha_l(\mu) = \alpha(\mu) < 0$. But

$$\mathbb{E}_l^{\alpha_l(\mu)} \left\{ \left[\frac{N}{V_l} - \frac{\mu - \alpha_l(\mu)}{a} \right]^2 \right\} = \frac{\beta}{V_l} p_l''(\alpha_l(\mu)) \tag{4.6}$$

and by Lemma 1 of Ref. 6,

$$\lim_{l \uparrow \infty} p_l''(\alpha_l(\mu)) = p''(\alpha(\mu)) \tag{4.7}$$

which is finite since $\alpha(\mu)$ is strictly negative, and

$$\lim_{l \uparrow \infty} p_l(\alpha_l(\mu)) = p(\alpha(\mu)) \tag{4.8}$$

Thus we have

$$(\mu - \alpha(\mu))^2/2a + (p \circ \alpha)(\mu) \leqslant \liminf_{l \uparrow \infty} p_l^a(\mu) \tag{4.9}$$

Combining (4.4) and (4.9), the claim is proved for $\mu < ap_c$.

In the case $\mu \geqslant ap_c$ the lower bound provided by Jensen's inequality is too crude; if there is macroscopic occupation of the ground state then there are anomalous fluctuations so that the variance (4.6) of the number density does not go to zero as l increases to infinity. However, it turns out that the bound (4.9) still holds, but the estimation required to prove it is more delicate. We have to prove that

$$\liminf_{l \uparrow \infty} V_l^{-1} \log \mathbb{E}_l^{\alpha_l(\mu)}[\exp(-\beta a \{N - [\mu - \alpha_l(\mu)]\}^2/2V_l)] = 0 \tag{4.10}$$

in the case $\mu \geqslant ap_c$; in this case we can show, as in Lemma 3 of Ref. 6, that

$$\lim_{l \uparrow \infty} \alpha_l(\mu) = 0, \qquad \lim_{l \uparrow \infty} p_l(\alpha_l(\mu)) = p(0) \tag{4.11}$$

To prove (4.10), we split-off $\lambda_l(1)$ from the rest of the spectrum and write

$$\mathbb{E}_l^\alpha[\exp\{-\beta a V_l[N/V_l-(\mu-\alpha)/a]^2/2\}]$$
$$= \iint_{[0,\infty)\times[0,\infty)} \exp\{-\beta a V_l[x+y-(\mu-\alpha)/a]^2/2\}\, dH_l^\alpha(x)\, d\check{K}_l^\alpha(y) \quad (4.12)$$

where

$$H_l^\alpha(x)=\mathbb{P}_l^\alpha[n_l(1)/V_l\leqslant x] \quad (4.13)$$

$$\check{K}_l^\alpha(y)=\mathbb{P}_l^\alpha\left[\sum_{k\geqslant 2} n_l(k)/V_l\leqslant y\right] \quad (4.14)$$

But $H_l^\alpha(x)$ is determined by its Laplace transform

$$\int_{[0,\infty)} e^{-tx}\, dH_l^\alpha(x)=(1-e^{\beta\alpha})/(1-e^{\beta(\alpha-t/\beta V_l)})$$
$$=(1-e^{\beta\alpha})\sum_{n=0}^{\infty} e^{n\beta\alpha}\, e^{-tn/V_l} \quad (4.15)$$

It follows that (4.12) can be rewritten

$$\mathbb{E}_l^\alpha[\exp\{-\beta a V_l[N/V_l-(\mu-\alpha)/a]^2/2\}]$$
$$=\sum_{n=0}^{\infty}[1-\exp(\beta\alpha)]\exp(n\beta\alpha)$$
$$\times\int_{[0,\infty)} \exp\{-\beta a V_l[n/V_l+y-(\mu-\alpha)/a]^2/2\}\, d\check{K}_l^\alpha(y)$$
$$\geqslant\sum_{n=0}^{\infty}[1-\exp(\beta\alpha)]\exp(n\beta\alpha)$$
$$\times\int_{[0,(\mu-\alpha)/a)} \exp\{-\beta a V_l[n/V_l+y-(\mu-\alpha)/a]^2/2\}\, d\check{K}_l^\alpha(y)$$
$$\geqslant[1-\exp(\beta\alpha)]\exp(\beta V_l\alpha^2/2a)$$
$$\times\int_{[0,(\mu-\alpha)/a)} \exp\{-\beta V_l\alpha[y-(\mu-\alpha)/a]\}\, d\check{K}_l^\alpha(y) \quad (4.16)$$

where we have replaced the infinite series by its largest term.

But

$$\int_{[0,(\mu-\alpha)/a)} \exp\{-\beta V_l \alpha[y-(\mu-\alpha)/a]\}\, d\check{K}_l^\alpha(y)$$

$$\geqslant \exp[\beta V_l \alpha(\mu-\alpha)/a] \int_{[0,(\mu-\alpha)/a)} d\check{K}_l^\alpha(y)$$

$$\geqslant \exp[\beta V_l \alpha(\mu-\alpha)/a] \int_{[0,\infty)} [1-ay/(\mu-\alpha)]\, d\check{K}_l^\alpha(y) \tag{4.17}$$

Since we have

$$\int_{[0,\infty)} x\, dH_l^\alpha(x) = \frac{e^{\beta\alpha}}{V_l(1-e^{\beta\alpha})} \tag{4.18}$$

$$\int_{[0,\infty)} z\, dK_l^\alpha(z) = p_l'(\alpha) \tag{4.19}$$

it follows that

$$\int_{[0,\infty)} \left(1-\frac{ay}{\mu-\alpha}\right) d\check{K}_l^\alpha(y) = 1 - \frac{a}{\mu-\alpha}\left[p_l'(\alpha) - \frac{e^{\beta\alpha}}{V_l(1-e^{\beta\alpha})}\right]$$

$$= \frac{a}{\mu-\alpha}\cdot\frac{e^{\beta\alpha}}{V_l(1-e^{\beta\alpha})} \tag{4.20}$$

when $\alpha = \alpha_l(\mu)$. Thus we have

$$(\beta V_l)^{-1} \log \mathbb{E}_l^{\alpha_l(\mu)} \left\{\exp\left[-\frac{\beta a V_l}{2}\left(\frac{N}{V_l} - \frac{\mu-\alpha_l(\mu)}{a}\right)^2\right]\right\}$$

$$\geqslant \frac{\alpha_l(\mu)^2}{2a} + \alpha_l(\mu)\frac{(\mu-\alpha_l(\mu))}{a} + \frac{\alpha_l(\mu)}{V_l} - \frac{\log V_l(\mu-\alpha_l(\mu))}{V_l} \tag{4.21}$$

For $\mu \geqslant ap_c$ the right-hand side of (4.21) converges to zero as $l \uparrow \infty$ so that (4.10) is proved. It follows that $\lim_{l\uparrow\infty} \inf p_l^\alpha(\mu) \geqslant \mu^2/2a + p(0)$.

But by (4.4)

$$\limsup_{l\uparrow\infty} p_l^\alpha(\mu) \leqslant \mu^2/2a + p(0)$$

and the proof of the theorem is concluded.

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