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Bounds for a Bose Condensate in Dimensions $\nu \geqslant 3$

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A stronger version of the Bogoliubov inequality is used to derive an upper bound for the anomalous average $|\langle a(x)\rangle|$ of an interacting nonrelativistic Bose field $a(x)$ at a finite temperature. This bound is $|a(x)^2| < \rho R$, where R satisfies $1 - R = (RT/2T_c)^{\nu/2}$, with ν the dimensionality, and T_c the critical temperature in the absence of interactions. The formation of nonzero averages is closely related to the Bose–Einstein condensation and $|\langle a(x)\rangle|^2$ is often believed to coincide with the mean density ρ_0 of the condensate. We have found nonrigorous arguments supporting the inequality $\rho_0 \leqslant |\langle a(x)\rangle|^2$, which parallels the result of Griffiths in the case of spin systems.

KEY WORDS: Bose condensation; correlation inequalities; spontaneous symmetry-breaking; critical phenomena.

1. INTRODUCTION

Bose–Einstein condensation is mainly a theoretical phenomenon. Though it occurs in the exactly soluble model of the free Bose gas, provided the temperature is below a critical value, condensation is not likely to play a major role in the known interacting Bose systems. Even in favorable cases, like liquid ^{4}He, there is both experimental[(1)] and theoretical[(2)] evidence that only a few percent of the particles occupy the zero-momentum state near $T = 0$.

Nevertheless, there is fundamental interest in the condensation phenomenon for two reasons. First, it provides a clue to our understanding of phase transitions and spontaneous breakdown of symmetries in *continuous* systems. Second, it might become an indispensable facet of a future microscopic theory of superfluidity.

A typical goal of the theory is to calculate the condensate fraction for a given interaction (e.g., Lennard-Jones potentials). The intention of the present paper is different. We wish to establish bounds for the condensate that are

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uniform in the sense that they do not depend on the details of the interaction. In spirit, our investigation will follow the analysis of Hohenberg[3] and Chester *et al.*,[4] who aimed at the demonstration that condensation is absent from one- and two-dimensional systems.

The appropriate setting for our problem is provided by the quantum grand canonical ensemble for a nonrelativistic Bose field $a(x)$ interacting via a pair potential ϕ. To avoid catastrophic behavior,[5] we must restrict our attention to a class of "reasonable" ϕ's that satisfy the stability criterion. This is more than a technical condition and an uncritical extension to innocent looking potentials (e.g., $-\phi$) often results in nonthermodynamic behavior. Actually, we shall impose a stronger condition than classical stability: We let the potential be superstable.[6] This ensures the existence of an equilibrium state for any value of the chemical potential μ and thus excludes the free Bose system,[9] which seemingly is the only nonsuperstable system of interest.

We shall not repeat arguments to demonstrate the existence of the thermodynamic limit (in the sense of van Hove), which would require little more than is invoked here. For a concise account of the results we refer to Ruelle's book.[5]

We emphasize another feature common to all potential models: The potential energy U defined by

$$U = \tfrac{1}{2} \int dx \int dy\, \phi(x - y) a^+(x) a^+(y) a(x) a(y) \tag{1}$$

is invariant under local gauge transformations

$$a(x) \mapsto e^{if(x)} a(x), \qquad a^+(x) \mapsto e^{-if(x)} a^+(x) \tag{2}$$

even though the total Hamiltonian is not invariant [unless $f(x)$ is a constant]. To control condensation uniformly in ϕ, we use the fact that U commutes with the generators $\int dx\, f(x) a^+(x) a(x)$, thereby establishing an upper bound for the mean density ρ_0 of the condensate compared with the total mean density ρ at the inverse temperature β:

$$\rho_0/\rho \leqslant R(\beta) < 1 \tag{3}$$

The bound R solves the equation

$$1 - R = (R\beta_c/2\beta)^{\nu/2} \tag{4}$$

where ν is the dimension and β_c^{-1} is the critical temperature of the system without interaction:

$$\beta_c = (m/2\pi)[\rho^{-1}\zeta(\nu/2)]^{2/\nu}, \qquad \zeta(k) = \sum_{n \geqslant 1} n^{-k} \tag{5}$$

We put $\hbar = 1$ and have denoted the common mass of the particles by m. If $\nu = 1$ or 2, we have $\zeta(\nu/2) = \infty$ and thus $R(\beta) = 0$, confirming the result of Hohenberg.[3] Condensation is also absent from systems that are "two-dimensional" in the sense that their volume is $L \times L \times d$ with $L \to \infty$.[4] If $\nu \geqslant 3$, Eq. (4) compares with the known result for the free Bose gas,

$$1 - \rho_0/\rho = \min\{1, (\beta_c/\beta)^{\nu/2}\} \tag{6}$$

and [provided the bound $R(\beta)$ cannot be improved] suggests that there exist interactions that enhance condensation.

2. A HEURISTIC DISCUSSION

Hohenberg's argument[3] made use of an inequality[2] due to Bogoliubov[7]:

$$\beta\langle\{A, A^*\}\rangle\langle[C^*, [H, C]]\rangle \geqslant 2|\langle[A, C^*]\rangle|^2 \tag{7}$$

where H is the Hamiltonian and $\langle\cdot\rangle$ denotes the thermal average. The arbitrary operators A and C were suitably chosen within a finite-volume description of the system:

$$A = \int_\Lambda dx\, e^{ikx} a(x), \qquad C = \int_\Lambda dx\, e^{ikx} a^+(x) a(x) \tag{8}$$

Though (7) is sufficient to rule out condensation in two-dimensional systems, it gives poor results in three dimensions.

The first problem we thus encounter is to find a stronger version of the Bogoliubov inequality. The solution to this problem is contained in a previous work[8] concerning the Heisenberg ferromagnet.

The next question concerns the validity of both the inequality (7) and its stronger version when applied to unbounded operators. Ginibre[9] once formulated the condition that the operators should be bounded by some power of the number operator. Garrison and Wong[10] pointed out that the KMS property provides an elegant proof of (7), and finally Bouziane and Martin[11] gave a complete and satisfactory answer to this problem. Some of their ideas will be employed in our simplified argument.

Having overcome the first two difficulties, we are faced with another, more serious one. Following Bogoliubov's quasiaverage prescription,[12] a gauge-breaking term

$$VrK = \tfrac{1}{2}\int_\Lambda dx\, [\bar{z}a(x) + za^+(x)], \qquad z = re^{i\alpha} \tag{9}$$

is introduced into the Hamiltonian to stabilize the anomalous average

$$\eta e^{i\alpha} = \lim_{r\downarrow 0} \lim_{\Lambda\uparrow} V^{-1}\int_\Lambda dx\, \langle a(x)\rangle \tag{10}$$

[2] $\{A, B\} = AB + BA$, $[A, B] = AB - BA$.

Strictly speaking, Hohenberg's original proof merely gives the result $\eta = 0$ for $\nu \leqslant 2$, and extending his argument to $\nu \geqslant 3$, we get an upper bound for η. But unlike in the Heisenberg model, where the magnetic field replaces r and where the spontaneous magnetization replaces η, no direct physical significance can be attributed to the breaking term or to the anomalous average for a Bose system: These quantities merely test the spontaneous breakdown of gauge invariance. Instead, the quantity we really want to control is the mean density of the condensate

$$\rho_0 = \lim_{\Lambda\uparrow} V^{-2} \int_\Lambda dx \int_\Lambda dy \, \langle a^+(x)a(y)\rangle \tag{11}$$

where the breaking term is absent from the beginning. This then raises the question as to whether there is a relation between η and ρ_0.

As was previously argued by Haag,[13] in any primary (e.g., irreducible) representation, the space average of the field is represented by a constant. The way representations arise in our context is that one first obtains infinite-volume equilibrium states and then applies the Gel'fand–Segal construction.[5] For a Bose system different primary equilibrium states ω_α, the "pure phases," are expected to arise below the critical temperature and the assertion is that ω_α can be constructed following Bogoliubov's prescription:

$$\omega_\alpha(A) = \lim_{r\downarrow 0} \lim_{\Lambda\uparrow} \langle A\rangle, \qquad 0 \leqslant \alpha < 2\pi \tag{12}$$

Clearly, all states ω_α coincide on gauge-invariant elements of the field algebra. Notice also that the order of limits in (12) is essential and it is only above the critical temperature that these limits may be interchanged, yielding a unique equilibrium state.

Though the states ω_α reflect the translational invariance of the theory, they do not reflect its gauge invariance. Nevertheless, a standard gauge-invariant state ω may be constructed as an integral over the gauge group,

$$\omega(A) = (2\pi)^{-1} \int_0^{2\pi} d\alpha \, \omega_\alpha(A) \tag{13}$$

which is believed to coincide with the infinite-volume limit of Gibbs ensembles with respect to the gauge-invariant Hamiltonian:

$$\omega(A) = \lim_{\Lambda\uparrow} \langle A\rangle_{r=0} \tag{14}$$

Taking everything said for granted, we would obtain the desired, yet unproved, relation $\rho_0 = \eta^2$, the link between spontaneous symmetry-breaking and Bose–Einstein condensation.

In fact, all our assertions can be verified and the equality of ρ_0 and η^2 can be proved for the case of the free Bose gas. As for the general case, we would rather argue in favor of the inequality $\rho_0 \leqslant \eta^2$.

At this point we want to make contact with some work by Griffiths[14] concerning spontaneous magnetization in spin systems. Let $H_0 - hM$ be the Hamiltonian of a spin lattice if a magnetic field h is applied. Then spontaneous magnetization occurs if the average magnetic moment per lattice site has a nonzero limit:

$$m_0 = \lim_{h \uparrow 0} \lim_{N \to \infty} N^{-1} \langle M \rangle \tag{15}$$

There is, however, a second notion of phase transition, which deals with long-range correlation, hence with the quantity

$$m_2{}^2 = \lim_{N \to \infty} N^{-2} \langle M^2 \rangle_{h=0} \tag{16}$$

Griffiths proved that $m_2 \leqslant m_0$, while the equality $m_2 = m_0$ is expected on heuristic grounds. Subsequently, Hepp and Lieb[15] and Dyson *et al.*[16] found more abstract versions of this result. Unfortunately, the known proofs rely on the commutativity of M and H_0 and therefore do not apply to Bose systems with the obvious replacements (the breaking term K and the potential energy U do not commute). In Section 6 we take up certain ideas and techniques of Ref. 16 and indicate necessary changes.

3. THE BOSE SYSTEM IN A BOX

We first describe a system of identical bosons enclosed in a cubic box

$$\Lambda = \{x \in R^\nu \mid -L/2 \leqslant x^i \leqslant L/2\} \tag{17}$$

of volume $V = L^\nu$. We take $L^2(\Lambda)$ (with respect to the Lebesque measure dx) as the one-particle Hilbert space. The associated Fock space $\mathscr{H}$ is the completion of the symmetric tensor algebra constructed on $L^2(\Lambda)$ and may be decomposed into n-particle subspaces $\mathscr{H}_n$ such that each $\varphi \in \mathscr{H}$ is represented by a sequence $(\varphi_n)_{n \geqslant 0}$ of wave functions $\varphi_n \in \mathscr{H}_n$. We also consider the projectors E_n onto $\mathscr{H}_n$ and write the number operator as $N = \sum nE_n$.

As is well known, $\mathscr{H}$ serves as a representation space for the canonical commutation relations

$$[a(f), a^+(g)] = (f, g), \qquad f, g \in L^2(\Lambda) \tag{18}$$

uniquely determined by $a(f)E_0 = 0$. The polynomial algebra generated by these operators has $C^\infty(N)$ as common invariant dense domain.[3] In a formal manner, the Bose field is recovered by

$$a(f) = \int dx\, \overline{f(x)} a(x), \qquad a^+(f) = \int dx\, f(x) a^+(x) \tag{19}$$

[3] $C^\infty(N)$ consists of all vectors $\varphi \in \mathscr{H}$ that make $e^{itN}\varphi$ a C^∞ function of t.

We look upon Λ as a ν-dimensional torus, thereby maintaining translational symmetry given by Λ viewed as a group acting on the torus in the obvious way. The corresponding unitary action on $L^2(\Lambda)$ has the one-particle momentum as generator with the spectrum

$$\hat{\Lambda} = \{k | kL/2\pi \in Z^\nu\} \tag{20}$$

Let us consider one-particle states $f_k(x) = V^{-1/2}e^{ikx}$ with momentum $k \in \hat{\Lambda}$ and the associated creation and annihilation operators $a_k = a(f_k)$ and $a_k{}^+ = a^+(f_k)$. Then the kinetic energy T, corresponding to the νn-dimensional Laplacian in $\mathscr{H}_n$ with periodic boundary conditions, can also be characterized by $TE_0 = 0$ and

$$[T, a_k{}^+] = (k^2/2m)a_k{}^+ \tag{21}$$

whereas the potential energy U is a multiplication operator:

$$[U\varphi]_n(x_1,\dots, x_n) = \sum_{1 \leqslant i < j \leqslant n} \phi(x_i - x_j)\varphi_n(x_1,\dots, x_n) \tag{22}$$

The formal expression for the total Hamiltonian is

$$H = T + U - \mu N - VrK \tag{23}$$

where

$$K = \tfrac{1}{2}V^{-1/2}(e^{-i\alpha}a_0 + e^{i\alpha}a_0{}^+) \tag{24}$$

To give meaning to H as self-adjoint operator, we adhere to the Friedrichs extension method,[5] assuming that the restrictions of T and U to $\mathscr{H}_n$ have a common dense domain and that U is bounded below in $\mathscr{H}_n$. Moreover, if the superstability condition is satisfied,

$$\sum_{i=1}^{n} \sum_{j=1}^{n} \phi(x_i - x_j) \geqslant cV^{-1}n^2, \qquad c > 0 \tag{25}$$

then $N^j e^{-\beta H}$ is trace class for any $j \geqslant 0$, $\beta > 0$, and arbitrary chemical potential μ.[9]

The natural algebra associated with our finite system is the algebra $B(\mathscr{H})$ of all bounded operators. Obviously,

$$\langle A \rangle = \mathrm{Tr}\, e^{-\beta H}A/\mathrm{Tr}\, e^{-\beta H} \tag{26}$$

exists for $A \in B(\mathscr{H})$ and defines the finite-volume equilibrium state enjoying the KMS property[19] with respect to the time evolution $A_t = e^{-itH}Ae^{itH}$. The algebra $B(\mathscr{H})$ may be equipped with the Bogoliubov scalar product

$$(A, B) = \int_0^\beta ds\, \langle e^{sH}A^* e^{-sH}B \rangle \tag{27}$$

In Ref. 8 we proved the inequality

$$b \coth(b/c) \leqslant a \tag{28}$$

where

$$a = \tfrac{1}{2}\langle\{A^*, A\}\rangle \tag{29}$$

$$b = \tfrac{1}{2}\langle[A^*, A]\rangle \tag{30}$$

$$c = \beta^{-1}(A, A) \tag{31}$$

4. AN UPPER BOUND FOR THE ANOMALOUS AVERAGE

To apply (28) successfully to the problem of determining $\langle a(x)\rangle$, it will be necessary to incorporate unbounded operators. We wish to accomodate these operators within the completion $\mathscr{K}$ of $B(\mathscr{H})$ with respect to the norm

$$\|A\| = (A, A)^{1/2} \tag{32}$$

Notice that $\mathscr{K}$ is no longer an algebra but merely a Hilbert space with conjugation $A \to A^*$. The general inequality

$$\|A\|^2 \leqslant \tfrac{1}{2}\beta\langle\{A^*, A\}\rangle \tag{33}$$

following from (28) relates the norm $\|\cdot\|$ to the Gibbs state. An essential property of the Gibbs state at hand is the existence of

$$\langle N^j\rangle = \sum_{n=1}^{\infty} n^j\langle E_n\rangle, \qquad j > 0 \tag{34}$$

This suggests that we examine operators A that are *polynomially bounded* in the sense that A and A^* have a common dense domain larger than or equal to $C^\infty(N)$ on which

$$\|A\varphi\| + \|A^*\varphi\| \leqslant \|p(N)\varphi\| \tag{35}$$

for some polynomial $p(t)$.

Lemma. Any polynomially bounded operator A belongs to $\mathscr{K}$.

Proof. Let P_n be the projection $\sum_{r\leqslant n} E_r$ and assume (35). Then $A_n = P_nAP_n$ is in $B(\mathscr{H})$. We demonstrate that (A_n) is a Cauchy sequence with respect to $\|\cdot\|$. Due to the symmetry of the problem under the replacement $A \to A^*$, we need only show that the following quantity can be made small:

$$\begin{aligned}\langle(A_n - A_m)^*(A_n - A_m)\rangle\\ &= \langle P_nA^*(P_n - P_m)A\rangle + \langle(P_n - P_m)A^*P_mA(P_n - P_m)\rangle\\ &\leqslant \langle A^*(P_n - P_m)A\rangle + \langle(P_n - P_m)A^*A(P_n - P_m)\rangle \qquad (n > m)\end{aligned} \tag{36}$$

Since the eigenvectors of $e^{-\beta H}$ are in $C^\infty(N)$, (35) implies that $\langle A^*A\rangle \leqslant \langle p(N)^2\rangle$. Thus the second term in (36) can be made small for sufficiently large n and m. Moreover, the sequence $\langle A^*P_nA\rangle$, being monotone and bounded, converges; so the first term can be made small. ■

By the principle of extension of inequalities, we may apply (28) to any polynomially bounded operator A. Choosing $A = a_k$, we get

$$\langle a_k{}^+a_k\rangle \geqslant [\exp(\beta\|a_k\|^{-2}) - 1]^{-1} \tag{37}$$

For the grand canonical ensemble of the free Bose gas where $H = T - \mu N$, $\mu < 0$, we have that[8]

$$\|a_k\|^{-2} = \langle[a_k{}^+, [H, a_k]]\rangle = (k^2/2m) - \mu \tag{38}$$

and equality holds in (37). To find lower bounds for $\|a_k\|$ in the general case, we shall use the following variational principle:

$$\|A\|^2 = \sup_B \frac{|(A, B)|^2}{(B, B)} \tag{39}$$

Notice that the time evolution $A \to A_t$ extends to a strongly continuous one-parameter group of isomorphisms $\mathscr{K} \to \mathscr{K}$ with densely defined generator $\delta A = i[H, A]$ and the identity[17]

$$(A, \delta B) = i\langle[A^*, B]\rangle \tag{40}$$

holds. Now let B take the form δC in (39). Then by virtue of (40)

$$\|A\|^2 \geqslant \sup_C \frac{|\langle[A, C^*]\rangle|^2}{\langle[C^*, [H, C]]\rangle} \tag{41}$$

It remains for us to describe our option for the operator C. Let ρ_k with $k \in \hat{\Lambda}$ be the multiplication operator given by

$$(\rho_k\varphi)_n(x_1,\ldots, x_n) = \sum_{r=1}^{n} e^{ikx_r}\varphi_n(x_1,\ldots, x_n) \tag{42}$$

with same domain as N. Formally, ρ_k may be viewed as the Fourier transform of the density operator $a^+(x)a(x)$ and is, in fact, an important device in the theory of quantum fluids.[20]

The following commutators are obtained by an elementary calculation:

$$[a_k, \rho_k{}^*] = a_0 \tag{43}$$

$$[\rho_k{}^*, [H, \rho_k]] = (k^2/m)N + VrK \tag{44}$$

Notice that the potential ϕ drops out of (44), for we have that $[U, \rho_k] = 0$ as a consequence of local gauge invariance of the interaction. If $k = 0$, ρ_k

coincides with the number operator and the expectation of (44) in the Gibbs state leads to

$$Vr\langle K\rangle = \|\delta N\|^2 \geqslant 0 \tag{45}$$

Hence $\langle K\rangle \geqslant 0$ as $r > 0$. Within the finite-volume description, the order parameter η may be defined by

$$\eta = \langle K\rangle \tag{46}$$

Then

$$\eta e^{i\alpha} = V^{-1/2}\langle a_0\rangle = V^{-1}\int_\Lambda dx\,\langle a(x)\rangle = \langle a(x)\rangle \tag{47}$$

by the translational invariance of the Gibbs state.

We take a_k and ρ_k as the operators A and C in (41) and get the inequality

$$\|a_k\|^2 \geqslant \eta^2(\rho k^2/m + r\eta)^{-1} \tag{48}$$

where $\rho = V^{-1}\langle N\rangle$. It is now apparent that $\|a_k\|$ develops an infrared singularity in the thermodynamic limit (followed by $r \downarrow 0$) provided

$$\lim_{r\downarrow 0}\lim_{\Lambda\uparrow}\eta > 0 \tag{49}$$

Our estimate (37) shows that the same is true for the momentum distribution function:

$$\langle a_k^+a_k\rangle \geqslant \{\exp[\beta(r\eta + \rho k^2/m)\eta^{-2}] - 1\}^{-1} \tag{50}$$

Previous results[3,4] may be reproduced from (50) with the aid of the inequality $(e^x - 1)^{-1} > x^{-1} - 1/2$ valid for $x > 0$.

The formula (50) states that certain general features of a free Bose system persist regardless of the interaction. From $|\langle a_0\rangle|^2 \leqslant \langle a_0^+a_0\rangle$ it follows that

$$\begin{aligned}\rho - \eta^2 &\geqslant V^{-1}\sum_{k\neq 0}\langle a_k^+a_k\rangle\\ &\geqslant V^{-1}\sum_{k\neq 0}\{\exp[\beta(r\eta + \rho k^2/m)\eta^{-2}] - 1\}^{-1}\end{aligned} \tag{51}$$

In the thermodynamic limit ($L \to \infty$), the sum approaches a well-known integral:

$$\begin{aligned}\rho - \eta^2 &\geqslant (2\pi)^{-\nu}\int_{R^\nu} dk\,\{\exp[\beta(r\eta + \rho k^2/m)\eta^{-2}] - 1\}^{-1}\\ &= \left(\frac{m\eta^2}{4\pi\rho\beta}\right)^{\nu/2} g_{\nu/2}(e^{-\beta r/\eta})\end{aligned} \tag{52}$$

where

$$g_s(x) = \sum_{n=1}^{\infty} x^n/n^s \tag{53}$$

As $r \to 0$, $\eta(r)$ decreases and is bounded from below, assuring the existence of $\lim \eta(r)$ subject to the following relation of constraint:

$$\rho - \eta^2 \geqslant (m\eta^2/4\pi\rho\beta)^{\nu/2}\zeta(\nu/2) = \rho(\eta^2\beta_c/2\rho\beta)^{\nu/2} \tag{54}$$

This relation may be stated as $\eta^2 \leqslant R\rho$, where R solves the equation

$$1 - R = (R\beta_c/2\beta)^{\nu/2} \tag{55}$$

5. ENTROPY AND FINITE-VOLUME ESTIMATES

In this section we describe some operator-theoretic results which will be useful for our program.

Suppose that ω is a normal state on $B(\mathscr{H})$. Then

$$\omega(A) = \mathrm{Tr}\, \rho A \tag{56}$$

for some density operator ρ, and ω is assigned the entropy

$$S(\omega) = -\mathrm{Tr}\, \rho \log \rho \geqslant 0 \tag{57}$$

Given two normal states ω and ω_0, one writes

$$S(\omega|\omega_0) = \mathrm{Tr}(\rho \log \rho - \rho \log \rho_0) \geqslant 0 \tag{58}$$

for their relative entropy.[18] In particular, if ω_0 is a Gibbs state,

$$\rho_0 = e^{-\beta H}/\mathrm{Tr}\, e^{-\beta H} \tag{59}$$

[assuming $e^{-\beta H}$ is trace class and $\omega(H)$ exists], then

$$S(\omega|\omega_0) = \log \mathrm{Tr}\, e^{-\beta H} + \beta\omega(H) - S(\omega) \tag{60}$$

We shall now consider perturbations described by the Hamiltonian $H - VA$ and let A vary suitably. With no further assumptions on H, it will be safe to restrict A to the algebra $B(\mathscr{H})$. By the Golden–Thompson inequality

$$\mathrm{Tr}\, e^{\beta(VA - H)} \leqslant \mathrm{Tr}(e^{\beta VA}e^{-\beta H}) \tag{61}$$

the operator $e^{\beta(VA-H)}$ is trace class. A noteworthy consequence of (60) is the variational principle

$$S(\omega) = \inf_A [\log \mathrm{Tr}\, e^{\beta(VA-H)} + \beta\omega(H - VA)] \tag{62}$$

Then (60) may be restated as

$$V^{-1}S(\omega|\omega_0) = \beta \sup_A [\omega(A) - p(A)] \tag{63}$$

where $p(A)$ is the relative pressure:

$$p(A) = (\beta V)^{-1} \log[\mathrm{Tr}\, e^{\beta(VA-H)}/\mathrm{Tr}\, e^{-\beta H}] \tag{64}$$

The formula (63) characterizes the relative entropy per volume as the Legendre transform of the relative pressure, modulo a factor β.

In certain situations one may be able to derive estimates for the entropy. For instance, let ω be given by the density operator

$$\rho = Q/\mathrm{Tr}\, Q \tag{65}$$

and let

$$Q = \rho_0^{1/2} E \rho_0^{1/2} \tag{66}$$

where E is a projector. Since $Q \leqslant \rho_0$ and the log function is monotone on the self-adjoint operators (see Ref. 5, Prop. 2.5.8), we infer that

$$\begin{aligned} S(\omega|\omega_0) &= \mathrm{Tr}(\rho \log Q - \rho \log \rho_0) - \log \omega_0(E) \\ &\leqslant -\log \omega_0(E) \end{aligned} \tag{67}$$

The significance of (67) is as follows. Suppose the projector E refers to a macroscopic measurement, i.e., to a question with two possible answers: yes or no. Then $\omega_0(E)$ gives us the probability for the event "yes" to occur if the state was ω_0. Suppose we let the volume of the system increase. By (67), the probability $\omega_0(E)$ will generally decrease at least at $\exp(-sV)$, where

$$s = \lim_{\Lambda \uparrow} V^{-1} S(\omega|\omega_0) \geqslant 0 \tag{68}$$

Hence $\omega_0(E)$ goes to zero unless ω has zero macroscopic entropy relative to the Gibbs state. What can we say about ω?

In general, ω is not a Gibbs state, nor does it have any simple physical interpretation. However, if H and E commute, then $\omega(A) = \omega_0(EAE)/\omega_0(E)$ and equality holds in (67). Here, ω stands for the state after the property E has been confirmed in a measurement. With regard to the infinite system, we are thus faced with the following appealing situation:

(i) There may be a nonvanishing probability that the thermodynamic system exhibits the property E. In this case, the measurement does not alter the state on a macroscopic level (zero relative entropy per volume).

Conversely:

(ii) Suppose a measurement of E would give rise to a macroscopic change of the state (nonzero relative entropy per volume). In this case, the result of the experiment is predicted to be "no" for E.

To prove $s > 0$ for certain projections E, our strategy is to relate the entropy per volume to the pressure functional $p(A)$ via (63).

6. THE RELATION $\rho_0 \leqslant \eta^2$

In the preceding section we have developed the general theory. Our next task is to investigate how this theory may be applied to the Bose system in a box Λ. To start with, let us consider its pressure relative to a system without a gauge-breaking term:

$$p_\Lambda(r) = (\beta V)^{-1} \log[\mathrm{Tr}\, e^{-\beta(H_\Lambda - VrK_\Lambda)}/\mathrm{Tr}\, e^{-\beta H_\Lambda}] \tag{69}$$

where the dependence on Λ is now indicated explicitly ($H_\Lambda = T_\Lambda + U_\Lambda - \mu N_\Lambda$). By a comparison with (64), $A = rK_\Lambda$. Though A is not a bounded operator, the pressure is well defined and even tends to a limit,[9]

$$p(r) = \lim_{\Lambda\uparrow} p_\Lambda(r) \tag{70}$$

which is a convex, hence continuous, function of the real parameter r. Note also that $p(0) = 0$ and $p(-r) = p(r)$ [from the symmetry of the trace (69) under the unitary map $\exp(i\pi N)$].

If condensation occurs, we do not expect $p(r)$ to be differentiable at the point $r = 0$ (first-order phase transition with respect to r). Since the left and right derivatives of $p(r)$ always exist and are opposite in sign, the last assertion precisely states that

$$\eta \equiv \lim_{r\downarrow 0} r^{-1}p(r) > 0 \tag{71}$$

Another formulation uses the Legendre transform:

$$p^*(t) = \sup_{r\in R} [rt - p(r)], \qquad t \in R \tag{72}$$

Then $p^*(t) = 0$ iff $t \in [-\eta, \eta]$ and the interval

$$\partial p(0) = [-\eta, \eta] \tag{73}$$

is called the *subdifferential* of p at $r = 0$.[21]

In a suitable realization of the Fock space, K_Λ may be identified with q, where q and p constitute a canonical pair of oscillator variables satisfying $[q, p] = i$. In this way it is seen that the spectrum of the self-adjoint operator K_Λ is purely continuous, not degenerate, and covers the entire real axis. Let $\int t\, E_\Lambda(dt)$ be the spectral decomposition of K_Λ and let $I \subset R$ be a closed interval such that

$$I \cap [-\eta, \eta] = \varnothing \tag{74}$$

What do we predict for

$$m_\Lambda(I) \equiv \omega_\Lambda{}^0(E_\Lambda(I)) = \mathrm{Tr}\, e^{-\beta H_\Lambda} E_\Lambda(I)/\mathrm{Tr}\, e^{-\beta H_\Lambda} \tag{75}$$

in the thermodynamic limit? The results of the last section suggest that we introduce an auxiliary state ω_Λ and the expectation value

$$\omega_\Lambda(K_\Lambda) = \mathrm{Tr}[e^{-(\beta/2)H_\Lambda} E_\Lambda(I) e^{-(\beta/2)H_\Lambda} K_\Lambda]/[\mathrm{Tr}\, e^{-\beta H_\Lambda} E_\Lambda(I)] \tag{76}$$

From (63) and (67),

$$\beta[\omega_\Lambda(rK_\Lambda) - p_\Lambda(r)] \leqslant V^{-1}S(\omega_\Lambda|\omega_\Lambda{}^0) \leqslant -V^{-1}\log m_\Lambda(I) \tag{77}$$

We first take the lower limit with respect to Λ, then take the supremum with respect to r, and thus get

$$\beta p^*(t) \leqslant -\overline{\lim_{\Lambda}}\, V^{-1}\log m_\Lambda(I) \tag{78}$$

where

$$t = \underline{\lim}\, \omega_\Lambda(K_\Lambda) \tag{79}$$

We assert that $t \in I$; this would be at once clear if the operators $\exp[-(\beta/2)H_\Lambda]$ and K_Λ commute in (76). Recall that, for large Λ, K_Λ tends to an element in the center of the field algebra. We therefore expect that commutativity is restored in the thermodynamic limit and hence

$$\omega_\Lambda(K_\Lambda) = \int_I t\, dm_\Lambda(t)/m_\Lambda(I) + o(1) \tag{80}$$

where $o(1) \to 0$ as $V \to \infty$. Our argument is incomplete in that no precise estimate of $o(1)$ has been found.

Taking (80) for granted, we infer that $t \equiv \underline{\lim}\, \omega_\Lambda(K_\Lambda) \in I$ and $p^*(t) > 0$ by assumption (74). This in turn implies that $\overline{m_\Lambda(I)}$ tends to zero at least at the rate $\exp[-V\beta p^*(t)]$. Thus for any bounded continuous function f: $R \to R$,

$$\begin{aligned} \inf_{t\in[-\eta,\eta]} f(t) &\leqslant \underline{\lim} \int f\, dm_\Lambda \\ &\leqslant \overline{\lim} \int f\, dm_\Lambda \leqslant \sup_{t\in[-\eta,\eta]} f(t) \end{aligned} \tag{81}$$

The result may be extended to unbounded functions. For this we need some elementary facts and estimates. (We shall drop the index Λ for conciseness.)

(A) K is bounded by the number operator:

$$K^2 \leqslant V^{-1}(a_0{}^+a_0 + \tfrac{1}{2}) \leqslant V^{-1}(N + \tfrac{1}{2}) \tag{82}$$

(B) Remember that $H = T + U - \mu N$. The pressure

$$P(\mu) = \lim(\beta V)^{-1}\,\mathrm{Tr}\, e^{-\beta H} \tag{83}$$

considered as a function of the chemical potential μ, is analytic in a neighborhood of the real axis.[9] In particular, $\rho = dP/d\mu = \lim V^{-1}\omega^0(N)$.

(C) For any real s,

$$\lim \omega^0(\exp(sV^{-1}N)) = \exp(s\rho) \tag{84}$$

To prove this, we choose $V \geqslant V_0 = s(\beta\epsilon)^{-1} > 0$. Then

$$\exp[sV^{-1}\omega^0(N)] \leqslant \omega^0(\exp(sV^{-1}N)) \leqslant [\omega^0(\exp(sV_0^{-1}N))]^{V_0/V}$$

where we used the convexity of e^{sx} and the concavity of $x^{V_0/V}$ for $x \geqslant 0$. As Λ increases, the lower bound tends to $e^{s\rho}$, whereas the upper bound tends to

$$\exp\{s\epsilon^{-1}[P(\mu + \epsilon) - P(\mu)]\} \tag{85}$$

Taking $\epsilon \to 0$, we get (84).

Proposition. Under the hypothesis (80), the inequalities (81) hold for any continuous function f: $R \to R$ obeying

$$|f(t)| \leqslant a \exp(st^2) \tag{86}$$

with positive constants a and s.

Proof. For $n \geqslant 1$ and $x \geqslant 0$ we define

$$g_n(x) = \min(x/n, x^{1/2}) \tag{87}$$

Then g_n is a sequence of concave, increasing functions tending pointwise to zero. Put $h_n(x) = 1 - x^{-1}g_n(x^2)$. Obviously, g_n has bounded support and so has

$$f_n(t) = f(t)h_n(\exp(st^2)) \tag{88}$$

Thus,

$$\overline{\lim_{\Lambda}} \int f_n \, dm \leqslant \sup_{t\in[-n,n]} f_n(t) \xrightarrow[n\to\infty]{} \sup_{t\in[-n,n]} f(t) \tag{89}$$

Consider the error:

$$\begin{aligned}\int |f - f_n| \, dm &\leqslant a \int g_n(\exp(2st^2)) \, dm(t) \\ &\leqslant ag_n\left(\int \exp(2st^2) \, dm(t)\right) \\ &\leqslant ag_n(\omega^0(\exp[sV^{-1}(2N + 1)]))\end{aligned} \tag{90}$$

The first step follows from (86), the second step uses the concavity of g_n, and the third step is a consequence of (A) and the monotonicity of g_n. Next, we take the upper limit with respect to Λ and use (C):

$$\overline{\lim} \int |f - f_n| \, dm \leqslant ag_n(e^{2s\rho}) \xrightarrow[n\to\infty]{} 0 \tag{91}$$

This establishes

$$\overline{\lim} \int f \, dm \leqslant \sup_{t\in[-n,n]} f(t) \tag{92}$$

Replacing f by $-f$, we get (81). ∎

We are now ready to state the main result of this section.

Theorem. Under the hypothesis (80),

$$\overline{\lim_{\Lambda}}\ V^{-1}\omega^0(a_0{}^+a_0) \leqslant \eta^2 \tag{93}$$

Proof. By the gauge invariance of ω^0,

$$\omega^0(K^{2n}) = V^{-n}\omega^0(F_n(a_0{}^+a_0)) \tag{94}$$

where $F_n(x) = c_n x^n + \cdots + xc_1 + c_0$ is a certain polynomial with volume-independent coefficients. As $V \to \infty$, only the highest power survives, the coefficient of which is

$$c_n = 2^{-2n}\binom{2n}{n} \tag{95}$$

We may write

$$\begin{aligned} c_n[\overline{\lim}\ V^{-1}\omega^0(a_0{}^+a_0)]^n &\leqslant c_n\ \overline{\lim}\ V^{-n}\omega^0((a_0{}^+a_0)^n) \\ &= \overline{\lim}\ \omega^0(K^{2n}) \\ &= \overline{\lim} \int t^{2n}\, dm(t) \leqslant \eta^{2n} \end{aligned} \tag{96}$$

Now, $c_n^{1/n} \to 1$ as $n \to \infty$, yielding (93). ■

Suppose the ordinary limit exists:

$$\rho_0 = \lim_{\Lambda\uparrow} V^{-1}\omega^0(a_0{}^+a_0) \tag{97}$$

Then ρ_0 is interpreted as the mean density of the condensate. By (93), $\rho_0 \leqslant \eta^2 \leqslant R\rho$.

REFERENCES

1. L. J. Rodriguez and H. A. Gersch, *Phys. Rev. A* **9**:2085 (1974).
2. D. Schiff and L. Verlet, *Phys. Rev.* **160**:208 (1967); M. H. Kalos, D. Levesque, and L. Verlet, *Phys. Rev. A* **9**:2178 (1974).
3. P. C. Hohenberg, *Phys. Rev.* **158**:383 (1967).
4. G. V. Chester, M. E. Fisher, and N. D. Mermin, *Phys. Rev.* **185**:760 (1969).
5. D. Ruelle, *Statistical Mechanics* (Benjamin, New York, 1969).
6. D. Ruelle, *Comm. Math. Phys.* **18**:127 (1970).
7. N. N. Bogoliubov, *Phys. Abh. S.U.* **6**(1):229 (1962).
8. G. Roepstorff, *Comm. Math. Phys.* **53**:143 (1977).
9. J. Ginibre, *Comm. Math. Phys.* **8**:26 (1968).
10. J. C. Garrison and J. Wong, *Comm. Math. Phys.* **26**:1 (1972).
11. M. Bouziane and Ph. A. Martin, *J. Math. Phys.* **17**:1848 (1976).

12. N. N. Bogoliubov, *Lectures on Quantum Statistics*, Vol. 2 (Gordon and Breach, New York, 1970).
13. R. Haag, *Nuovo Cimento* **25**:287 (1962).
14. R. Griffiths, *Phys. Rev.* **152**:240 (1966).
15. K. Hepp and E. H. Lieb, *Phys. Rev. A* **8**:2517 (1973).
16. F. J. Dyson, E. H. Lieb, and B. Simon, Phase transitions in quantum spin systems with isotropic and non-isotropic interactions, to appear.
17. G. Roepstorff, *Comm. Math. Phys.* **46**:253 (1976).
18. G. Lindblad, *Comm. Math. Phys.* **39**:111 (1974).
19. R. Haag, N. M. Hugenholtz, and M. Winnink, *Comm. Math. Phys.* **5**:215 (1967).
20. E. Feenberg, *Theory of Quantum Fluids* (Academic Press, New York, 1969).
21. R. T. Rockafellar, *Convex Analysis* (Princeton Univ. Press, 1972).