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Vortices in infinite free Bose systems

by

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ABSTRACT. — We study a class of KMS states of the infinite free Bose gas in the condensation region. These states fail to be translationally invariant, exibit off-diagonal long range order, and give rise to a velocity field $v_s(x)$ which is stationary and irrotational everywhere in space except on vortex lines. Typical vortex lines are straight or circular. The circulation around any vortex line is quantized. We show that these states are limits of finite volume Gibbs states with appropriate boundary conditions.

1. KMS STATES OF THE FREE BOSE GAS

The generally accepted view regarding superfluid behavior, first advocated by London [*1*], is that superfluidity and Bose condensation have the same origin. Therefore, sustained effort has gone into working out the detailed properties of the infinitely extended free Bose gas as a model system. We start out by assuming that the equilibrium states of the infinite system satisfy the Kubo-Martin-Schwinger boundary condition, then discuss their hydrodynamic behavior (Section 2), and show how these states appear as infinite volume limits of Gibbs states (Section 3).

The general emphasis is in the appearance of a classical time-independent field $P(x)$ describing the condensate. This field is polynomially bounded and satisfies Laplace's equation $\Delta P(x) = 0$, hence is a harmonic polynomial. Recently, Haag and Trych-Pohlmeyer [*2*] employed a stability condition to discuss equilibrium states, thereby confirming the occurrence and structure of $P(x)$.

Earlier work of Bogoliubov [3] and Gross [4] attacked the similar but more difficult problem to determine the « condensate wave function » for a weakly interacting Bose gas which then played a fundamental role in the theory of quantized vortices. However, the developed formalism was non-rigorous in that a self-consistent field approximation was employed to obtain a classical wave equation and incomplete in that the boundary conditions for this wave equation have never been specified.

It would be desirable to persue this problem within the algebraic setting of field theory. Whereas very little is known in the interacting case, the free Bose gas has been extensively studied by various authors [5-9] using the Weyl formalism. Especially, Rocca, Sirugue, and Testard [9] obtained the most general KMS state at inverse temperature β. Specializing their result we take the Schwartz space $\mathcal{S} := \mathcal{S}(\mathbb{R}3)$ with scalar product

$$(f, g) = \int dx\, \overline{f(x)} g(x) \quad , \quad f, g \in \mathcal{S} \tag{1.1}$$

as the underlying vector space of a Weyl algebra determined by the relations

$$\mathrm{W}(f)\mathrm{W}(g) = \mathrm{W}(f+g)e^{i\,\mathrm{Im}\,(f,g)}, \tag{1.2}$$

$\mathrm{W}(f)^* = \mathrm{W}(-f)$, and $\mathrm{W}(0) = 1$. The Weyl relation (1.2) is a convenient transcription of the more familiar but difficult to handle canonical commutation relations. In a formal manner, the Bose field $a(x)$ is recovered from

$$\mathrm{W}(f) = \exp i \int dx [f(x)a^*(x) + \overline{f(x)}a(x)]. \tag{1.3}$$

The ideal gas is characterized by the time evolution

$$\alpha_t(\mathrm{W}(f)) = \mathrm{W}(e^{ith}f) \tag{1.4}$$

where we included the chemical potential $\mu \leq 0$ in the one-particle Hamiltonian

$$h = -\frac{1}{2}\Delta - \mu. \tag{1.5}$$

The choice of a particular μ at this stage could be avoided by restricting α_t to the gauge invariant part of the Weyl algebra. Concerning the role of the chemical potential see [10].

Since the emphasis is on states, it is worth pointing out that any state ω on the Weyl algebra is completely specified by its characteristic functional

$$\mathrm{E}(f) = \omega(\mathrm{W}(f)). \tag{1.6}$$

Given β and $\mu < 0$, the KMS state is unique with functional

$$\mathrm{E}_{\beta,\mu}(f) = \exp\left[-\frac{1}{2}\left(f, \coth\frac{\beta h}{2} f\right)\right]. \tag{1.7}$$

There are, however, many KMS states for fixed β and $\mu = 0$. The extremal KMS states are primary and are given by

$$E(f) = E_{\beta,0}(f)e^{iF(f)} \tag{1.8}$$

where F is an arbitrary time invariant real linear functional $F : \mathcal{S} \to \mathbb{R}$,

$$F(e^{ith} f) = F(f). \tag{1.9}$$

Here we shall concentrate on continuous functionals F. This will allow us to relate them to elements of the dual space $\mathcal{S}'$. If $\mu = 0$, time invariance (1.9) implies that the Fourier transform of F has point support at the origin of the momentum space, hence is a finite linear combination of the δ-functional and its derivatives. This then implies that there exists a complex polynomial $P(x)$ (of three variables) in position space such that

$$F(f) = 2\mathrm{Re}\int dx\overline{P(x)}f(x). \tag{1.10}$$

In order that F be invariant under the time evolution, the polynomial $P(x)$ must solve the three-dimensional Laplace equation

$$\Delta P(x) = 0 \tag{1.11}$$

interpreted as the Schroedinger equation for zero energy. However, unlike as in Schroedinger's theory we accept all polynomial solutions of (1.11) in field theory. The most general polynomial solution of (1.11) is a superposition of homogeneous harmonic polynomials [*11*]

$$P(x) = \sum_{l=0}^{L}\sum_{m=-l}^{l} c_{lm}y_{lm}(x) \tag{1.12}$$

with arbitrary complex coefficients c_{lm}.

Using polar coordinates we may write

$$y_{lm}(x) = r^l Y_{lm}(\vartheta, \varphi) \tag{1.13}$$

where the functions Y_{lm} are the spherical harmonics. Thus there are exactly $2l + 1$ harmonic polynomials of degree l.

Let us now consider an equilibrium state (1.8) with invariant functional F given by (1.10). It follows that for any $f \in \mathcal{S}$ the functional $E(sf)$ is C^∞ with respect to the real parameter s and hence all n-point functions of the unbounded Bose field exist. In particular, we have that

$$\omega(a(x)) = P(x) \tag{1.14}$$

$$\omega(a^*(x)a(y)) = \overline{P(x)}P(y) + w(x - y) \tag{1.15}$$

with correlation function of the non-condensed phase,

$$w(x) = (2\pi)^{-3} \int d^3p(e^{\beta p^2} - 1)^{-1} e^{ipx}. \tag{1.16}$$

We note that $w(x)$ is the Fourier transform of an L^1 function. By the Riemann-Lebesgue lemma, $w(x)$ vanishes at infinity proving the cluster property of the state ω:

$$\lim_{|x-y| \to \infty} \omega(a^*(x)a(y)) - \omega(a^*(x))\omega(a(y)) = 0 \tag{1.17}$$

This is clearly satisfied for the extremal KMS states only. Penrose and Onsager [*12*] suggested that the general form (1.15) of the two-point function, i. e. off-diagonal long range order, characterizes superfluidity also in interacting Bose systems.

2. SUPERFLOW CURRENT AND QUANTIZED VORTICES

We ascribe to the « normal » component of the fluid the short-range part $w(x - y)$ of the two-point function (1.15) and to the superfluid the long-range part $\overline{P(x)}P(y)$. For convenience, we continue to put $\hbar = m = 1$ where m is the mass of the Bose particle. Then the current operator is

$$j(x) = \frac{1}{2i}(a^*(x)\nabla a(x) - (\nabla a^*(x))a(x)) \tag{2.1}$$

and (1.15) assigns to the current the following expectation value

$$j_s(x) = \langle j(x) \rangle = \text{Im}\,(\overline{P(x)}\nabla P(x)) \tag{2.2}$$

which we interpret as the superflow (particle) current. From $j_s = v_s\rho_s$ and $\rho_s = |\,P\,|^2$ we obtain the velocity field

$$v_s(x) = \text{Im}\,\frac{\nabla P(x)}{P(x)} \tag{2.3}$$

well-defined everywhere in space except on the manifold

$$V = \{\, x \in \mathbb{R}^3 \mid P(x) = 0 \,\} \tag{2.4}$$

where we encounter a singular behavior. In general, the singular manifold will be one-dimensional, namely the intersection of the two surfaces $\text{Re}\,P(x) = 0$ and $\text{Im}\,P(x) = 0$. If this is the case, we speak of a *line vortex*. However, it will be seen later that the dimensionality of the manifold V may well be zero or two. If we exclude V from the fluid domain, we are left in general with a multi-connected region and equation (2.3) shows quite incidentally that the velocity field $v_s(x)$ is irrotational:

$$\nabla \times v_s(x) = 0, x \notin \mathrm{V}. \tag{2.5}$$

By Stokes theorem, the circulation

$$\mathrm{C}(\Gamma) = \int_\Gamma dx v_s(x) \tag{2.6}$$

is zero provided the closed loop Γ does not wind around the vortex line. If Γ winds around it, the line will contribute to the integral (2.6). To prove that the circulation $\mathrm{C}(\Gamma)$ is, in any event, a multiple of 2π (« quantized » vortex) we introduce the image $\tilde{\Gamma}$ of the path Γ with respect to the continous map $\mathrm{P} : \mathbb{R}^3 \to \mathbb{C}$, $x \mapsto z = \mathrm{P}(x)$. Whereas Γ is a closed path in the 3-dimensional euclidean space, $\tilde{\Gamma}$ is a closed path in the complex plane. Now, $\tilde{\Gamma}$ does not pass through the origin $z = 0$ if Γ does not intersect the singular manifold V which we assume. Then $dz = dx\nabla\mathrm{P}(x)$ and

$$\mathrm{C}(\Gamma) = \mathrm{Im} \int_{\tilde{\Gamma}} \frac{dz}{z} = 2\pi n(\tilde{\Gamma}) \tag{2.7}$$

$n(\tilde{\Gamma})$ being the number of times that $\tilde{\Gamma}$ winds around the point 0 of the complex plane, i. e. the index of 0 with respect to $\tilde{\Gamma}$ (sometimes called the « winding number »). The beauty of this result is that the circulation $\mathrm{C}(\Gamma)$ is entirely given by geometry and that the relation (2.7) is not restricted to cases where dim V = 1. As regards the geometric intuition, we warn the reader that if dim V = 1 and Γ winds around the vortex line once, its image $\tilde{\Gamma}$ may wind around zero $\pm n$ times where n is any natural number. This is readily seen from the example

$$\mathrm{P}(x) = (x_1 + ix_2)^n. \tag{2.8}$$

It is worth observing that (2.8) leads to what is called a *two-dimensional flow*. With regard to such flows the tools of complex analysis can be applied naturally. To illustrate, let us for a moment assume that $\mathrm{P}(x)$ does not depend on x_3 but is an analytic function of the complex variable $z = x_1 + ix_2$:

$$\mathrm{P}(x) = f(z). \tag{2.9}$$

As a consequence, $\nabla v_s = 0$ (except on V) stating that the flow is incompressible. Moreover, letting $u = v_{s2} + iv_{s1}$ we obtain

$$u(z) = f'(z)/f(z). \tag{2.10}$$

Thus the velocity field is found from the complex (possibly multi-valued) potential $w = \log f(z)$, i. e. $u = w'$.

For instance, let

$$f(z) = a(z - a_1)(z - a_2) \dots (z - a_n) \tag{2.11}$$

where $a, a_k \in \mathbb{C}$. Since $f(z)$ is analytic it is also harmonic. The manifold V consists of n straight lines parallel to the 3-axis meeting the (1,2)-plane in the points $z = a_k$. Each individual line contributes additively to the velocity field $u = v_{s2} + iv_{s1}$:

$$u = \sum_k (z - a_k)^{-1}. \tag{2.12}$$

The circulation is readily evaluated as

$$C(\Gamma) = \int_\Gamma dx v_s(x) = \sum_k \operatorname{Im} \int_{\tilde{\Gamma}} \frac{dz}{z - a_k} = 2\pi \sum_k n(\hat{\Gamma}, a_k) \tag{2.13}$$

where Γ is some closed path in $\mathbb{R}^3$, $\hat{\Gamma}$ is its projection onpoto the (1,2)-plane and $n(\hat{\Gamma}, a_k)$ is the index of a_k with respect to $\hat{\Gamma}$. By the *strength* of an individual line vortex we shall denote its contribution to the circulation each time Γ winds counterclockwise (as judged from the (1,2)-plane) around the line. Provided no two of the complex numbers a_k coincide, the strength of the individual line vortex is 2π. It will be observed that this value is positive. Consequently, all line vortices due to our Ansatz (2.11) are oriented the same way resulting in a counterclockwise motion of the fluid. Naturally, the common orientation of all vortices can be reversed if one simply replaces $x_1 + ix_2$ by $x_1 - ix_2$ in (2.11). What strikes us most is that oppositely oriented vortices do not seem to occur. Just how plausible is it, physically?

Next, let us assume that the polynomial $f(z)$ has a multiple zero of order m, i. e. that several of the numbers a_k coincide. Then the corresponding line vortex has strengh $2\pi m$. In some sense, such a vortex is no longer « elementary » but is made up of m identical vortices, each with strength 2π.

It remains to observe that the density $|f(z)|^2$ of the superfluid increases at the rate $|z|^{2n}$ as $z \to \infty$ where n is the strength of the vortex. Accordingly, each condensed particle spends most of its life near the walls of the vessel.

Another class of vortices arises if we let $P(x)$ depend on the two variables $\rho = \sqrt{x_1^2 + x_2^2}$ and $\zeta = x_3$. We may speak of *vortices with an axial symmetry*.

Now, let

$$P(x) = \sum a_n r^n P_n(\zeta/r) \tag{2.14}$$

where P_n is the Legendre polynomial of order n and $r^2 = \rho^2 + \zeta^2$. Let there be real constants α, β, $R_1, \ldots, R_n$ such that $\alpha \neq 0$, $\beta \neq 0$, $R_k > 0$, and

$$a_1 = i\beta \quad , \quad \sum a_n \rho^n P_n(0) = \alpha \sum_{k=1}^{N} (\rho^2 - R_k^2). \tag{2.15}$$

Then the singular manifold V is the union of N circles with radius R_k (vortex rings):

$$x_1^2 + x_2^2 = R_k^2 \quad , \quad x_3 = 0. \tag{2.16}$$

This establishes that the vorticity of equilibrium states may be confined to a bounded region of space. The simplest model where we deal with exactly one vortex ring is

$$P(x) = \alpha(x_1^2 + x_2^2 - 2x_3^2 - R^2) + i\beta x_3, \tag{2.17}$$

its strength is 2π, hence minimal.

3. LIMIT GIBBS STATES

We ask how states described in Section 1 may appear as infinite volume limits of Gibbs states. To this end we propose and investigate suitable limiting procedures.

One method uses attractive boundary conditions for the finite-volume Laplacian. As was found by Robinson [7], this kind of boundary condition tends to provoke a separation of phases. Indeed, certain one-particle states may be interpreted as « bound to the surface » and, in the limit, flow out of the bulk. However, with a slight modification, this method may also yield a finite but increasing density for the condensed states. This is done by introducing a volume dependent operator μ in place of a constant chemical potential in conjunction with attractive boundary conditions. Due to a matching condition (3.2-4) we obtain the desired states while μ tends to a constant and the Laplacian assumes the correct spectrum.

The boundary conditions in a compact volume $\Lambda \subset \mathbb{R}^3$, star-shaped (with respect to zero for convenience) and enclosed in a sufficiently smooth surface $\partial\Lambda$, are determined by some harmonic polynomial P, homogeneous with degree l and normalized in $L^2(\Lambda)$. On the surface $\partial\Lambda$, the function $\frac{\partial P}{P}$ is supposed to be real and bounded (∂P indicates the outer normal derivative of P) (1). For every $R > 0$ set $\Lambda_R := \{ x \mid R^{-1}x \in \Lambda \}$. Then the Laplacian with boundary conditions

$$P\partial\varphi = \varphi\partial P \quad \text{on} \quad \partial\Lambda_R \tag{3.1}$$

can be defined as a selfadjoint operator Δ on some dense domain in $L^2(\Lambda_R)$ and with a completely discrete spectrum, bounded from above. We write E for the projector of the subspace of $L^2(\Lambda_R)$ spanned by P and the positive eigenstates of $-\frac{1}{2}\Delta$. Trivially, E reduces $-\frac{1}{2}\Delta$. The subspace thus determined is physically understood as the subspace of all free one-particle states. The finite-dimensional orthogonal complement N then comprises all negative eigenstates of $-\frac{1}{2}\Delta$ and some, whose eigenvalues are zero, so N may be interpreted as the space of all one-particle states bound by an attractive surface potential. With regard to the zero-level states one may duely ask why some of these states are termed « free » and some of them « bound ». However, we may be content with noting that bound states disappear from the system when the confining walls are removed in a specified manner.

To state our main result we need a further detailed description of the system: For every $R > 0$, Δ with boundary conditions (3.1), E, N as indicated above and μ a function of E we define a positive one-particle Hamiltonian

$$h = -\frac{1}{2}\Delta - \mu.$$

For any $\beta \in \mathbb{R}_+$ let $z = e^{\beta\mu}$ be the fugacity operator for μ and

$$E^R_{\beta,\mu}(f) := \exp\left[-\frac{1}{2}\left(f, \coth\frac{\beta h}{2} f\right)\right] \quad , \quad f \in \mathscr{D}(\Lambda_R)$$

the characteristic functional of the grand canonical state, ω^R. Suppose

$$\mu \mid N \leq R^{-2}C \tag{3.2}$$

with any constant C smaller than the lowest eigenvalue of $-\frac{1}{2}\Delta$ for $R = 1$. Finally let

$$\lim_{R\to\infty} z = \zeta \in (0, 1] \tag{3.3}$$

uniformly,

$$\lim_{R\to\infty} z(1-z)^{-1}R^{-3-2l} = c \in [0, \infty) \tag{3.4}$$

weak convergence on $\mathscr{D}(\mathbb{R}^3) =: \mathscr{D}$ (clearly $\zeta = 1$ if $c > 0$).

Then we have the tollowing

(1) These conditions are trivially verified for every homogeneous harmonic polynomial in $\lambda = B^3$, in which case $\frac{\partial P}{P} \equiv l$ on $\partial\lambda = S^2$.

THEOREM. — Under the assumptions (3.2-4)

i) As $R \to \infty$, the functional $E^{R}_{\beta,\mu}$ converges simply on $\mathscr{D}$ and the limit two-point function is

$$\omega(a^*(x)a(y)) = c\overline{P(x)}P(y) + w_\zeta(x - y)$$

where

$$w_\zeta(x - y) := (2\pi\beta)^{-3/2} \sum_{n=1}^{\infty} n^{-3/2}\zeta^n \exp\left(\frac{-|x - y|^2}{2n\beta}\right)$$

ii) The state on the Weyl algebra over $\mathscr{D}$, determined by *i)* extends by continuity to a state on the Weyl algebra over $\mathscr{S}$, β-KMS with respect to the free evolution (cf. (1.4)),

iii) (critical density).

Let V be any fixed compact volume of $\mathbb{R}^3$ and let n_V be the mean total number of particles in the state $E^{R}_{\beta,\mu}$ reduced to V. Then

$$\lim_{R\to\infty} n^{R}_{V} = c\int_V dx\,|P(x)|^2 + |V|\, w_\zeta(0).$$

(The last statement is not a direct consequence of *i)*. Here we claim that the limit and the reduction to a finite volume density may be interchanged).

From *iii)* it follows at once that the density of the condensate $c\,|P(x)|^2$ is not identically zero ($c \neq 0$) iff in every fixed compact volume V the mean particle density exceeds the « critical density » $w_1(0)$ in the limit $R \to \infty$.

Proof. — We shall only sketch the proof following largely Lewis and Pulé [8] (The main idea of the proof seems to be due to Kac).

To *i)* : let

$$\{\varepsilon^{R}_{k}\}_{k\in\mathbb{N}} \quad \text{with} \quad \varepsilon^{R}_{k} \leq \varepsilon^{R}_{k+1} \quad ; \quad \varepsilon^{R}_{L} = 0 < \varepsilon^{R}_{L+1} \leq \dots$$

be the eigenvalues of $-\frac{1}{2}\Delta$ in $L^2(\Lambda_R)$. They satisfy

$$\varepsilon^{R}_{k} = R^{-2}\varepsilon_k$$

where $\{\varepsilon_k\}_{k\in\mathbb{N}}$ denotes the eigenvalues of $-\frac{1}{2}\Delta$ for $R = 1$. Chose a corresponding orthonormal set for $R = 1$: $\{e_k\}_{k\in\mathbb{N}}$ such that

$$e_L = P \qquad \text{and} \qquad E = \sum_{k=L}^{\infty} e_k \otimes \overline{e_k}.$$

The set $\{e^{R}_{k}\}_{k\in\mathbb{N}}$, defined by

$$e^{R}_{k}(x) := R^{-3/2}e_k(R^{-1}x)$$

obviously is an orthonormal set in $L^2(\Lambda_R)$ and

$$1 - E = \sum_{k<L} e_k^R \otimes \overline{e_k^R} \quad , \quad E = \sum_{k=L}^{\infty} e_k^R \otimes \overline{e_k^R}.$$

Write

$$\mu = \mu_0 E + \mu_1(1 - E) \qquad (\mu_\nu = \mu_\nu(R)).$$

Then (3.2) implies

$$R^2 \mu_1 \leq C < \varepsilon_0$$

where ε_0 is the eigenvalue of the ground state of $-\frac{1}{2}\Delta$ for $R = 1$. From this we deduce

$$\text{for} \quad k < L : \{ \exp [\beta(\varepsilon_k^R - \mu_1)] - 1 \}^{-1} \leq \left\{ \exp \left[\beta\left(\frac{\varepsilon_0 - C}{R^2} \right) \right] - 1 \right\}^{-1}.$$

Since

$$\lim_{R \to \infty} R^{-3} \left\{ \exp \left[\beta\left(\frac{\varepsilon_0 - C}{R^2} \right) \right] - 1 \right\}^{-1} = 0$$

the first sum of

$$\omega^R(a^*(f)a(f)) = \sum_{k<L} R^{-3} \{ \exp [\beta(\varepsilon_k^R - \mu_1)] - 1 \}^{-1} | (e_k(R^{-1}x), f) |^2$$
$$+ \sum_{k=L}^{\infty} R^{-3} \{ \exp [\beta(\varepsilon_k^R - \mu_0)] - 1 \}^{-1} | (e_k(R^{-1}x), f) |^2$$

vanishes in the limit $R \to \infty$.

Using (3.4) and the homogeneity of $P = e_L$ the first term ($k = L$) of the second sum becomes

$$c \int_{\mathbb{R}^3 \times \mathbb{R}^3} dx dy \overline{P(x)} P(y) \overline{f(x)} f(y) \qquad (R \to \infty)$$

while the rest tends to $(w_\zeta * f, f)$. This is rigorously proven in [*13*] and essentially the content of [*8*], Lemma 2.

The proof of *iii)* is similar with

$$n_V^R = \int_V dx \omega^R(a^*(x)a(x)) = \sum_{k=0}^{\infty} \int_V dx \, | e_k^R(x) |^2 \{ \exp [\beta(\varepsilon_k^R - \mu(k))] - 1 \}^{-1}$$

$$\mu(k) = \begin{cases} \mu_1 & k < L \\ \mu_0 & k \geq L. \end{cases}$$

To *ii)* : Again we refer to [*13*]. The proof is made in writing the limit functional as an integral over functionals (1.8).

Naturally, the equilibrium states thus obtained are gauge invariant. They are KMS states but not extremal stationary states. The decomposition of these states into extremal KMS states is easily obtained using standard techniques leaving the two-point function uneffected. This way we would obtain the extremal states discussed in Section 1. The extremal KMS states appear directly as limit Gibbs states of a modified finite-volume Hamiltonian [*13*] chap. 5.

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