Commun. math. Phys. 1, 159—174 (1965)

# The Ground State of the Bose Gas

By

DEREK W. ROBINSON

Max Planck-Institut für Physik und Astrophysik, München

**Abstract.** The mathematical formalism describing the Bose gas at zero temperature is analysed with the aid of methods that have recently been successful in relativistic quantum field theory. First the spectrum conditions for an infinitely extended system are given and the algebra of observables and the algebra of field operators are defined. General properties of states over these algebras are discussed and theorems are given which connect the linked cluster property, translation invariance and the purity of the states. It is proved that pure states over the algebra of observables have the property of 'factorisable off-diagonal long range order'. The class of 'quasi free states' is defined and of these states those which are translation invariant and possess the linked cluster property are analysed. It is shown that this class of states contains a subclass of pure states of the Bogoliubov type and a subclass of states which are mixtures of non-translationally invariant pure states. The applications of these 'quasi free states' to the interacting Bose gas are summarized.

## 1. Introduction

The problem of finding the ground state and excitation spectrum of the interacting Bose gas at zero temperature may be considered to be the question of choosing an appropriate representation of the canonical commutation relations corresponding to a given form of the energy and particle density operators. If the problem is phrased in this manner the most convenient method of procedure appears to be with the aid of Wightman functions rather than the more usual Green's functions. This approach is aided if one makes at the outset the idealization that the system is infinitely extended; this idealization will be made throughout the present paper. Consideration of an infinite system can of course lead to mathematical difficulties due to the non-existence of certain operators which would be well defined in the case of a finite system but we will avoid such difficulties.

The aim of this paper is twofold. Firstly we wish to discuss possible properties of the states of a Bose system and present a number of general results which describe the connections between translational invariance, the linked cluster property and the purity of the states. In this connection a careful distinction is made between states over the algebra of observables and states over the field algebra. A proof is given that all pure states over the algebra of observables have the property of "factorisable off-diagonal long range order". Secondly we wish to illustrate some of these general results by consideration of "quasi free states". It is shown that this class of states contains BOGOLIUBOV [1] states along with other states which are mixtures of non-translationally invariant states of the type considered by GROSS [2]. We also give a summary of the applications that these states have found for the interacting Bose system. A number of the results stated in this paper are already known in other contexts but they are collected here to show their possible relevance to investigations of the Bose gas.

In Sec. 2 we collect the definitions and formalism necessary for the further sections. Sec. 3 contains a discussion of theorems concerning the properties of states of a Bose system. In Sec. 4 the "quasi free states" are defined and the representations corresponding to these states are constructed. In Sec. 5 a discussion of the applications of the "quasi free states" is given. Sec. 6 comprises a summary and conclusion.

## 2. General formulation

The Bose system is defined in terms of a field operator $\varphi(x)$ and its Hermitian conjugate $\varphi^+(x)$ which satisfy the canonical commutation relations

$$[\varphi(x), \varphi^+(y)] = \delta(x-y)$$

and

$$[\varphi(x), \varphi(y)] = 0\,. \tag{1}$$

The variables $x$ and $y$ refer to points in three dimensional space. The two mathematical quantities which are of interest are the algebra of field operators $\mathfrak{A}_{\mathscr{F}}$ and the sub-algebra of observables $\mathfrak{A}_{\mathscr{O}}$; $\mathfrak{A}_{\mathscr{F}}$ is the algebra generated from the field operators by the processes of addition, multiplication, multiplication with complex numbers and conjugation; $\mathfrak{A}_{\mathscr{O}}$ is the algebra of elements chosen from $\mathfrak{A}_{\mathscr{F}}$ with the property that they are invariant under the transformation

$$\begin{aligned}\varphi(x) &\to \varphi'(x) = \varphi(x)e^{i\alpha}\\ \varphi^+(y) &\to \varphi^{+\prime}(y) = \varphi^+(y)e^{-i\alpha}\end{aligned} \tag{2}$$

where $\alpha$ is a real constant. We omit the details involved in giving a precise mathematical definition of the algebras $\mathfrak{A}_{\mathscr{F}}$ and $\mathfrak{A}_{\mathscr{O}}$. There are essentially two difficulties to be avoided; the first is due to the distribution character of the operators $\varphi(x)$ and $\varphi^+(x)$ and this may be circumvented by appropriate smearing of the operators; the second is due to the unboundedness of the operators and may be avoided by working with the algebra of associated bounded operators (see for instance [3]).

We now wish to formulate the mathematical description of the infinite Bose gas in the following manner. Assuming that interaction of the

Bose particles is mediated by a two-body potential $V(x)$, we take the energy density operator to have the form

$$\mathscr{H}(x) = \nabla\varphi^+(x) \cdot \nabla\varphi(x) + \frac{1}{2}\int d^3y\, \varphi^+(x)\varphi^+(y)\, V(x-y)\varphi(x)\varphi(y) \tag{3}$$

and the particle number density operator to have the form

$$\mathscr{N}(x) = \varphi^+(x)\varphi(x)\,. \tag{4}$$

The infinite Bose gas is then described in terms of a representation of the algebra $\mathfrak{A}_{\mathcal{O}}$, in a Hilbert space $H$, chosen such that the operator $K$, defined by

$$K = \int d^3x\, \{\mathscr{H}(x) - \mu\mathscr{N}(x) - c\} \tag{5}$$

is a positive semi-definite operator i.e. such that

$$(\psi, K\psi) \geqq 0 \qquad \text{for all} \qquad \psi \in H\,. \tag{6}$$

The constant $\mu$ is the chemical potential and the constant $c$ is chosen so that the lowest eigenvalue of $K$ is equal to zero; the corresponding eigenstate is then interpreted as the ground state of the system. Condition (6) is a reflection of the fact that for a finite system the spectrum of the Hamiltonian should be bounded from below; the introduction of the second term in (6) ensures that the particle density in the ground state may assume a finite value whilst the third term is necessary to make the eigenvalues of $K$ finite. It would also be possible to consider an alternative formulation whereby the second term in (6) is omitted and the mean particle density is prescribed by an auxiliary condition but we prefer the above.

It will, of course, only be possible to satisfy condition (6) for certain values of $\mu$ and a certain class of potentials $V(x)$ and then only in particular representations of $\mathfrak{A}_{\mathcal{O}}$. It would indeed be hoped that for reasonable values of $\mu$ and $V(x)$ at most one representation of $\mathfrak{A}_{\mathcal{O}}$ would be compatible with (6). In this representation the mean density operator

$$\varrho = \lim_{V\to\infty} \frac{1}{V}\int_V d^3x\, \mathscr{N}(x)$$

would then be a multiple of the identity. (The volume $V$ is considered here to be a sub-volume of the system.) This last remark is a consequence of the assumed uniqueness, or irreducibility, of the representation and the Lemma due to HAAG [4]. Although no proof is a yet available that the energy and particle number densities determine uniquely a representation of $\mathfrak{A}_{\mathcal{O}}$, in the manner described above, it does appear to be reasonable from experience of quantum field theory. In an analogous problem in field theory one finds that each representation of the appropriate algebra determines a particular form for the interaction Hamiltonian, and conversely [5, 6]. That a similar property is true for the many body problem is made unclear however by the counterexample of the free Bose gas. In this case $V(x)$ is identically zero and $K$ is positive semi-definite if, and only if, $\mu \leqq 0$. Further, for each value of $\mu < 0$ there is just one representation of $\mathfrak{A}_{\mathcal{O}}$ compatible with (6), namely the vacuum representation with mean particle density zero, and for $\mu = 0$ there are an infinite number of representations, each corresponding to a different finite mean density. The general belief is that an interaction between the particles has the effect of making the chemical potential a one-to-one function of the mean density and although this would not yet imply the irreducibility of any representation of $\mathfrak{A}_{\mathcal{O}}$ compatible with (6) for fixed $\mu$ and $V(x)$ it would imply that the operator $\varrho$ is a multiple of the identity in all such representations.

It now appears appropriate to consider the representations of the algebra $\mathfrak{A}_{\mathcal{O}}$. The standard mathematical procedure used in studying the representations of an algebra $\mathfrak{A}$ is to consider all positive linear functionals $W(Q)$ over $\mathfrak{A}$ i.e. functionals $W(Q)$ defined for all $Q \in \mathfrak{A}$ having the two properties

a) $$W(\lambda_1 Q_1 + \lambda_2 Q_2) = \lambda_1 W(Q_1) + \lambda_2 W(Q_2)\,,$$

where $\lambda_1$, $\lambda_2$ are constants and $Q_1$, $Q_2 \in \mathfrak{A}$, and

b) $$W(Q^+ Q) \geqq 0 \quad \text{for all} \quad Q \in \mathfrak{A}\,. \tag{7}$$

This procedure is used because of a well known theorem (see for instance [7]) that concludes that corresponding to every such functional there exists a cyclic representation of $\mathfrak{A}$ in a Hilbert space $H$. This theorem is the basis of the Wightman approach to relativistic field theory where the identification

$$W(Q) = \langle 0\,|Q|\,0\rangle$$

is made and $|\,0\rangle$ is understood to be the vacuum state. We will make a similar identification in studying the representations of $\mathfrak{A}_{\mathcal{O}}$ but interpret $|\,0\rangle$ as the ground state of the Bose gas. Mathematically functionals $W(Q)$ satisfying the above conditions are termed "states" and this terminology will be adopted in the following. No confusion should arise with the use of the word state to describe a vector in Hilbert space. Corresponding to the normalization of the cyclic state in Hilbert space it is possible to normalize the states $W(Q)$ by requiring

$$W(1) = 1$$

where 1 is the unit element in $\mathfrak{A}$. In the following we consider only normalized states. The reducibility of the representation constructed from knowledge of $W(Q)$ can be characterized by the following property of the state. If $W(Q)$ may be decomposed into a convex sum of two other states $W_1(Q)$ and $W_2(Q)$, i.e. if we have the decomposition

$$W(Q) = \lambda\, W_1(Q) + (1-\lambda)\, W_2(Q) \quad \text{where} \quad 0 < \lambda < 1$$

for all $Q \in \mathfrak{A}$, then the corresponding representation is reducible and if such a decomposition is not possible the representation is irreducible; in the former case $W(Q)$ is called a mixed state and in the latter a pure state, a terminology corresponding to that used in statistical mechanics. The most general decomposition of a mixed state $W(Q)$ in terms of pure states $W_k(Q)$ is given by

$$W(Q) = \int d\mu(k)\, W_k(Q) \tag{8}$$

where $\mu(k)$ is a positive measure. If all states involved are normalized we must then require that

$$\int d\mu(k) = 1\,. \tag{9}$$

In the next section we use the above formalism to discuss the restraints placed upon the states of $\mathfrak{A}_{\mathcal{O}}$ and $\mathfrak{A}_{\mathcal{F}}$ by various general physical requirements and the interconnection of these restraints.

## 3. Possible properties of the states

The first property we wish to consider concerns behaviour at large distances and to aid the discussion we first recall the usual definition of the linked cluster property. Consider an algebra $\mathfrak{A}$ generated by certain elements $Q_i(x) \in \mathfrak{A}$, e.g. $\mathfrak{A}_{\mathcal{F}}$ is generated by $\varphi(x)$ and $\varphi^+(x)$, $\mathfrak{A}_{\mathcal{O}}$ is generated by $\varphi^+(x)\,\varphi(x+y)$, and consider also a state $W(Q)$ over $\mathfrak{A}$. From $W(Q)$ we construct a "truncated" state $W^T(Q)$ with the aid of the recursive definition

$$W(Q_1(x_1)\ldots Q_n(x_n)) = \sum W^T(Q_{i_1}(x_{i_1})\ldots)\ldots W^T(\ldots Q_{i_l}(x_{i_l}))\,; \tag{10}$$

the sum is over all possible partitions of the $Q_i(x_i)$ and the order in each partition is taken over from the left hand side. The linked cluster property is then expressed by the statement that

$$\lim_{|x_i - x_j| \to \infty} |W^T(Q_1(x_1)\ldots Q_m(x_m))| = 0\,. \tag{11}$$

Let us now restrict the algebra $\mathfrak{A}$ to be an algebra of quasilocal elements, i.e. we require that for each pair $Q, Q' \in \mathfrak{A}$ that

$$\lim_{|x| \to \infty} [Q(x), Q'] = 0$$

where $Q(x)$ is understood to be $Q$ translated to the point $x$. We note that both the algebra $\mathfrak{A}_{\mathcal{O}}$ and the algebra $\mathfrak{A}_{\mathcal{F}}$ have this property of quasilocality as a result of the commutation relations (1) and the fact that general elements of these algebras are constructed from fields smeared out with test functions which decrease for large distances. We next have the result of BORCHERS, HAAG and SCHROER [8];

**Theorem 1.** *All pure states $W(Q)$ over an algebra $\mathfrak{A}$ of quasilocal elements have the linked cluster property.*

The above authors deduce this result by proving what is in essence a generalization of SCHUR's lemma. They prove, if a sequence of operators

$Q_n \in \mathfrak{A}$ has the property that

$$\lim_{n\to\infty} [Q_n, A] = 0 \quad \text{for all} \quad A \in \mathfrak{A}$$

then for every vector $\psi$ in an irreducible representation of $\mathfrak{A}$.

$$\lim_{n\to\infty} \left| (\psi, Q_n A\psi) - \frac{(\psi, Q_n\psi)(\psi, A\psi)}{(\psi, \psi)} \right| = 0 .$$

Details of the proof are given in the reference quoted [8].

Thus it is possible to conclude from Theorem 1 that pure states over $\mathfrak{A}_{\mathcal{O}}$ and $\mathfrak{A}_{\mathcal{F}}$ have the linked cluster property. Let us consider in more detail the consequences of the linked cluster property for a state $W_{\mathcal{O}}(Q)$ over $\mathfrak{A}_{\mathcal{O}}$. For this purpose we consider the value of $W_{\mathcal{O}}(Q)$ for a particular $Q_1 \in \mathfrak{A}_{\mathcal{O}}$;

$$Q_1 = \varphi^+(x_1)\,\varphi^+(x_2)\,\varphi(x_3)\,\varphi(x_4) .$$

If the sets of points $(x_1, x_3)$ and $(x_2, x_4)$ are moved far apart the observable $Q_1$ factors into the product of two observables, i.e. elements of $\mathfrak{A}_{\mathcal{O}}$, and if $W_{\mathcal{O}}(Q)$ has the linked cluster property we then find that

$$\lim_{|x|\to\infty} |W_{\mathcal{O}}(\varphi^+(x_1)\varphi^+(x_2+x)\varphi(x_3)\varphi(x_4+x)) - \\ - W_{\mathcal{O}}(\varphi^+(x_1)\varphi(x_3))\, W_{\mathcal{O}}(\varphi^+(x_2+x)\varphi(x_4+x))| = 0 .$$

Similarly we may conclude that

$$\lim_{|x|\to\infty} |W_{\mathcal{O}}(\varphi^+(x_1)\,\varphi^+(x_2+x)\,\varphi(x_3+x)\,\varphi(x_4)) - \\ - W_{\mathcal{O}}(\varphi^+(x_1)\,\varphi(x_4))\, W_{\mathcal{O}}(\varphi^+(x_2+x)\,\varphi(x_3+x))| = 0 .$$

However in the case that the sets of points $(x_1, x_2)$ and $(x_3, x_4)$ are moved far apart it is not possible to conclude, that

$$\lim_{|x|\to\infty} |W_{\mathcal{O}}(\varphi^+(x_1)\,\varphi^+(x_2)\,\varphi(x_3+x)\,\varphi(x_4+x)) - \\ - W_{\mathcal{O}}(\varphi^+(x_1)\,\varphi^+(x_2))\, W_{\mathcal{O}}(\varphi(x_3+x)\,\varphi(x_4+x))| = 0$$

because $W_{\mathcal{O}}(Q)$ is only defined for $Q \in \mathfrak{A}_{\mathcal{O}}$ and neither $\varphi^+(x_1)\varphi^+(x_2)$ nor $\varphi(x_3)\varphi(x_4)$ is an element of this algebra. There is also no reason, in general, to believe that

$$\lim_{|x|\to\infty} |W_{\mathcal{O}}(\varphi^+(x_1)\,\varphi^+(x_2)\,\varphi(x_3+x)\,\varphi(x_4+x))| = 0$$

and YANG [9] has called states for which this latter limit is non-zero states with 'off-diagonal long range order'. We now wish to prove that pure states $W_{\mathcal{O}}(Q)$ over $\mathfrak{A}_{\mathcal{O}}$ have in general this property of off-diagonal long range order and an additional factorization property. This latter property ensures that a function $f(x_1, x_2)$, which is in general non-zero, exists such that

$$\lim_{|x|\to\infty} |W_{\mathcal{O}}(\varphi^+(x_1)\,\varphi^+(x_2)\,\varphi(x_3+x)\,\varphi(x_4+x)) - \\ - f^+(x_1, x_2)\, f(x_3+x, x_4+x)| = 0 \tag{12}$$

and we call states with this property, states with 'factorisable off-diagonal long range order'. A general characterization of such states is as follows. Consider sets of points $\{x_{i_r}\}$ and elements $Q_r(\{x_{i_r}\})$ of the algebra $\mathfrak{A}_{\mathscr{F}}$ constructed algebraically from field operators having the points of the sets as arguments and such that

$$Q = \prod_{r=1}^{n} Q_r(\{x_{i_r}\}) \in \mathfrak{A}_{\mathscr{O}} .$$

Then a state $W_{\mathscr{O}}(Q)$ over $\mathfrak{A}_{\mathscr{O}}$ is defined to have 'factorisable off-diagonal long range order' if functions $f_r(\{x_{i_r}\})$ exist such that

$$\lim |W_{\mathscr{O}}(Q_1(\{x_{i_1}\}) \ldots Q_n(\{x_{i_n}\})) - f_1(\{x_{i_1}\}) \ldots f_n(\{x_{i_n}\})| = 0 \tag{13}$$

and such that

$$f_j(\{x_{i_j}\}) = W_{\mathscr{O}}(Q_j(\{x_{i_j}\})) \quad \text{if} \quad Q_j(\{x_{i_j}\}) \in \mathfrak{A}_{\mathscr{O}} . \tag{14}$$

The limit is understood to be the product of any series of translations which move the clusters infinitely far apart. With this definition we have

**Theorem 2.** *Pure states $W_{\mathscr{O}}(Q)$ over $\mathfrak{A}_{\mathscr{O}}$ have the property of 'factorisable off-diagonal long range order'.*

The proof of this theorem may be constructed in the following manner. Because the algebra $\mathfrak{A}_{\mathscr{O}}$ is a sub-algebra of the algebra $\mathfrak{A}_{\mathscr{F}}$ a state $W_{\mathscr{O}}(Q)$ over $\mathfrak{A}_{\mathscr{O}}$ may be extended to a state $W_{\mathscr{F}}(Q)$ over $\mathfrak{A}_{\mathscr{F}}$ and generally this extension may be made in an infinite number of ways. However the extension theorem [10] tells us that a pure state over $\mathfrak{A}_{\mathscr{O}}$ may be extended to a pure state over $\mathfrak{A}_{\mathscr{F}}$ i.e. if $W_{\mathscr{O}}(Q)$ is a pure state over $\mathfrak{A}_{\mathscr{O}}$ then there exists at least one pure state $W_{\mathscr{F}}(Q)$ over $\mathfrak{A}_{\mathscr{F}}$, defined for all $Q \in \mathfrak{A}_{\mathscr{F}}$, such that

$$W_{\mathscr{O}}(Q) = W_{\mathscr{F}}(Q) \quad \text{if} \quad Q \in \mathfrak{A}_{\mathscr{O}} . \tag{15}$$

Now applying Theorem 1 we may conclude that $W_{\mathscr{F}}(Q)$ has the linked cluster property. Thus as an example

$$\lim_{|x| \to \infty} |W_{\mathscr{F}}(\varphi^+(x_1)\,\varphi^+(x_2)\,\varphi(x_3+x)\,\varphi(x_4+x)) - \\ - W_{\mathscr{F}}(\varphi^+(x_1)\,\varphi^+(x_2))\,W_{\mathscr{F}}(\varphi(x_3+x)\,\varphi(x_4+x))| = 0$$

from which we may, with the help of (15), conclude the validity of (12) and further make the identification

$$f(x_1, x_2) = W_{\mathscr{F}}(\varphi(x_1)\,\varphi(x_2)) .$$

The general property (13) follows, in a similar manner, from the fact that $W_{\mathscr{F}}(Q)$ has the linked cluster property and we have the identification

$$f_j(\{x_{i_j}\}) = W_{\mathscr{F}}(Q_j(\{x_{i_j}\}))$$

of which (14) is a special case.

It is to be noted that the extension of the pure state $W_{\mathscr{O}}(Q)$ to the pure state $W_{\mathscr{F}}(Q)$ is not unique; there is a one-parameter family of pure states $W_{\mathscr{F}_\alpha}(Q)$ over $\mathfrak{A}_{\mathscr{F}}$ which are extensions of $W_{\mathscr{O}}(Q)$. This non-uniqueness is due to the invariance of $\mathfrak{A}_{\mathscr{O}}$ under the gauge transformation (2) which ensures that the functions $f_j(\{x_j\})$ defined by (13) are determined only up to a phase. Thus if $Q \in \mathfrak{A}_{\mathscr{F}}$ and if under the gauge transformation (2)

$$Q \to Q' = Q_\alpha$$

then from one extension $W_{\mathscr{F}}(Q)$ we may define another extension $W_{\mathscr{F}_\alpha}(Q)$ by the identification

$$W_{\mathscr{F}_\alpha}(Q) = W_{\mathscr{F}}(Q_\alpha)\,.$$

These states are, in general, inequivalent [3, 4]. If we construct from the $W_{\mathscr{F}_\alpha}(Q)$ a mixed state $\overline{W}_{\mathscr{F}}(Q)$ over $\mathfrak{A}_{\mathscr{F}}$ through the prescription

$$\overline{W}_{\mathscr{F}}(Q) = \frac{1}{2\pi}\int_0^{2\pi} d\alpha\, W_{\mathscr{F}_\alpha}(Q)$$

it is in some ways possible to identify this state with $W_{\mathscr{O}}(Q)$. In fact

$$\begin{aligned} \overline{W}_{\mathscr{F}}(Q) &= W_{\mathscr{O}}(Q) \quad &&\text{if} \quad Q \in \mathfrak{A}_{\mathscr{O}} \\ &= 0 &&\text{if} \quad Q \notin \mathfrak{A}_{\mathscr{O}}\,. \end{aligned}$$

Although Theorem 1 tells us that all pure states over an algebra $\mathfrak{A}$ of quasilocal elements have the linked cluster property the converse statement is not true. A state with the linked cluster property is not necessarily pure. However the class of mixed states with this property is restricted by a number of conditions [11]. If we consider a mixed state, given generally by (8), with the normalization condition (9), we find

$$\begin{aligned} W(Q_1 Q_2(x)) &- W(Q_1)\,W(Q_2(x)) \\ &= \int d\mu(k)\,\{W_k(Q_1 Q_2(x)) - W_k(Q_1)\,W_k(Q_2(x))\} + \\ &+ \frac{1}{2}\int d\mu(k)\,d\mu(l)\,\{W_k(Q_1) - W_l(Q_1)\} \times \\ &\times \{W_k(Q_2(x)) - W_l(Q_2(x))\}\,. \end{aligned}$$

Now by definition the states $W_k(Q)$ are pure and therefore have the linked cluster property. Thus in order that $W(Q)$ may also have this property it is necessary that

$$\lim_{|x|\to\infty} \left|\int d\mu(k)\,d\mu(l)\,\{W_k(Q_1) - W_l(Q_1)\}\{W_k(Q_2(x)) - W_l(Q_2(x))\}\right| = 0\,. \quad (16)$$

This condition immediately rules out the possibility that all the states $W_k(Q)$ are translationally invariant, because translational invariance requires that

$$W_k(Q(x)) = W_k(Q)$$

and then choosing $Q_1 = Q_2$ in (16) we would get the contradiction

$$\int d\mu(k)\, d\mu(l)\, \{W_k(Q_1) - W_l(Q_1)\}^2 = 0\ .$$

Thus we have, for instance,

**Theorem 3.** *A mixed state over $\mathfrak{A}_{\mathcal{F}}$ possessing the linked cluster property must be a mixture of pure states some of which are not translationally invariant.*

It should be noted that the mixed state may be translationally invariant even if the component pure states are not. Analysis of condition (16) appears, in general, to be difficult and not much progress has been made toward the exact characterization of the class of mixed states with the linked cluster property.

The discussion contained in this section has been quite general but we now turn our attention to a class of states which concretely demonstrates most of the properties and features mentioned above.

## 4. Quasi free states

Quasi free states are examples of states $W_\alpha(Q)$ over $\mathfrak{A}_{\mathcal{F}}$ and are defined in terms of the truncated states $W^T_\alpha(Q)$ given by (10).

If

$$Q_{nm} = \varphi^+(x_1) \ldots \varphi^+(x_n)\, \varphi(x_{n+1}) \ldots \varphi(x_{n+m})$$

then the states are defined by setting

$$W^T_\alpha(Q_{nm}) = 0 \qquad \text{for} \qquad n + m \geqq 3\ . \tag{17}$$

We restrict our attention to translationally invariant states and introduce the parametrization

$$W^T_\alpha(\varphi(x)) = \varrho_0^{\frac{1}{2}}\, e^{i\alpha} \qquad\qquad W^T_\alpha(\varphi^+(x)) = \varrho_0^{\frac{1}{2}}\, e^{-i\alpha}$$

$$W^T_\alpha(\varphi^+(x_1)\, \varphi(x_2)) = \varrho(x_1 - x_2)\ W^T_\alpha(\varphi(x_1)\, \varphi(x_2)) = \sigma(x_1 - x_2)\ .$$

The linked cluster property follows if we assume that

$$\lim_{|x| \to \infty} \varrho(x)\ , \qquad \sigma(x) = 0\ .$$

For simplicity we consider the case $\alpha = 0$ only which corresponds to chosing a particular gauge for the field $\varphi(x)$; by a suitable gauge transformation the general case $\alpha \neq 0$ may be obtained from this special case. The simplicity of the quasi free states is that they are completely described in terms of $\varrho_0$, $\varrho(x)$ and $\sigma(x)$. In a recent paper [12] it was shown that this class of states is the only possible class having the simple property of being determined by a finite number of functions. To proceed further we must now analyse the restrictions placed upon $\varrho_0$, $\varrho(x)$ and $\sigma(x)$ by the condition of positive definiteness.

If we define

$$Q_L = \int d^3x \{\varphi^+(x) f(x) + \varphi(x) g(x)\}$$

it is clearly necessary that

$$W_\alpha(Q_L Q_L^+) \geqq 0 \,. \tag{18}$$

What is not quite so evident is that this condition alone is enough to ensure positive definiteness of the state. This statement is independent of such assumptions as translational invariance and the linked cluster property. However, as the proof is not very enlightening we do not include it here. The advantage of assuming translational invariance and the linked cluster property is that under these circumstances condition (18) can be easily analysed. In fact we find that (18) is equivalent to

$$\int d^3p \{|\tilde{f}(p)|^2 \tilde{\varrho}(p) + |\tilde{g}(p)|^2 (1 + \tilde{\varrho}(-p)) + \\ + \tilde{g}(p) \tilde{f}^+(p) \tilde{\sigma}(p) + \tilde{g}^+(p) \tilde{f}(p) \tilde{\sigma}^+(p)\} \geqq 0$$

where the tilde denotes the Fourier transform. The necessary and sufficient conditions ensuring the validity of this latter inequality are

$$\tilde{\varrho}(p) \geqq 0 \tag{19}$$

and

$$\tilde{\tau}(p)^2 = \tilde{\varrho}(p)\,(1 + \tilde{\varrho}(-p)) - |\tilde{\sigma}(p)|^2 \geqq 0 \,. \tag{20}$$

We next turn our attention to the construction of the representations of $\mathfrak{A}_{\mathscr{F}}$ corresponding to the above ansatz. The functions $\tilde{\varrho}(p)$ and $\tilde{\sigma}(p)$ must of course satisfy inequalities (19) and (20) and it is found that the nature of the representations depends critically upon the value of $\tilde{\tau}(p)$. We consider two classes; class I corresponds to $\tilde{\tau}(p) = 0$ and class II contains representations for which $\tilde{\tau}(p) \neq 0$.

*Class I representations*

These representations are constructed in terms of the Fock representation of operators $a_F(p)$ and $a_F^+(p)$, which satisfy the canonical commutation relations

$$[a_F(p), a_F^+(q)] = \delta(p - q) \qquad \text{etc.,}$$

in a Hilbert space $\mathfrak{H}_F$. We denote by $|\,0\rangle_F$ the vacuum state, defined by

$$a_F(p)\,|\,0\rangle_F = 0 \qquad \text{for all } p\,.$$

If $a(p)$ is the Fourier transform of $\varphi(x)$ i.e. if

$$a(p) = \int d^3x\, e^{-ipx} \varphi(x)$$

we then construct the representations by the identification

$$a(p) = e^{i\alpha(p)} \left(\sqrt{1 + \tilde{\varrho}(p)}\, a_F(p) + \sqrt{\tilde{\varrho}(p)}\, a_F^+(-p)\right) + \varrho_0^{\frac{1}{2}}\, \delta(p)$$

and

$$a^+(p) = e^{-i\alpha(p)}\left(\sqrt{1+\tilde{\varrho}(p)}\, a_F^+(p) + \sqrt{\tilde{\varrho}(p)}\, a_F(-p)\right) + \varrho_0^{\frac{1}{2}}\, \delta(p)$$

where

$$\alpha(p) = \frac{1}{2} \arg \tilde{\sigma}(p) .$$

We have used the fact that $\tilde{\tau}(p) = 0$ by setting

$$|\tilde{\sigma}(p)| = \sqrt{\tilde{\varrho}(p)\,(1+\tilde{\varrho}(-p))} .$$

From the above identification we see immediately that $|\,0\rangle_F$ is cyclic, with respect to the algebra $\mathfrak{A}_{\mathscr{F}}$, in $\mathfrak{H}_F$. It also follows directly from the irreducibility of the Fock representation that this class of representations of $\mathfrak{A}_{\mathscr{F}}$ is also irreducible.

Representations of the above type were first used by Bogoliubov [1] in his early work on the Bose gas. Since then they have been applied extensively by many authors. We now consider the second class of representations given by the quasi free states.

*Class II representations*

These representations are slightly more complicated than the previous ones and in order to construct them we need the Fock representations of two sets of operators $a_{F_1}(p)$, $a_{F_1}^+(p)$ and $a_{F_2}(p)$, $a_{F_2}^+(p)$ each satisfying the canonical commutation relations. If $\mathfrak{H}_{F_1}$ and $\mathfrak{H}_{F_2}$ are the Hilbert spaces in which these operators are represented then the class II representations are defined in the direct product Hilbert space $\mathfrak{H}$, given by

$$\mathfrak{H} = \mathfrak{H}_{F_1} \otimes \mathfrak{H}_{F_2} .$$

The field operator is represented as

$$a(p) = e^{i\alpha(p)}\left(\sqrt{1+\tilde{\varrho}_{\mathrm{II}}(p)}\, a_{F_1}(p) + \sqrt{\tilde{\varrho}_{\mathrm{II}}(p)}\, a_{F_1}^+(-p)\right) \otimes 1 + 1 \otimes$$

$$\otimes\, e^{i\alpha(p)}\,\nu(p)\,(a_{F_2}(p) + a_{F_2}^+(-p)) + \varrho_0^{\frac{1}{2}}\, 1 \otimes 1$$

and $a^+(p)$ is given by Hermitian conjugation. The functions $\tilde{\varrho}_{\mathrm{II}}(p)$ and $\nu(p)$ appearing in this formula are defined by

$$\tilde{\varrho}_{\mathrm{II}}(p) = \frac{(|\tilde{\sigma}(p)| - \tilde{\varrho}))^2}{(1 + 2\,\tilde{\varrho}(p) - 2\,|\tilde{\sigma}(p)|)}$$

and

$$\nu(p) = \frac{\tilde{\tau}(p)}{\sqrt{(1+2\tilde{\varrho}(p) - 2\,|\tilde{\sigma}(p)|)}}$$

respectively. Now if $|\,0\rangle_{F_1}$ and $|\,0\rangle_{F_2}$ are the vacuum states of the two Fock representations it is found that the state $|\,0\rangle$ defined by

$$|\,0\rangle = |\,0\rangle_{F_1} \otimes |\,0\rangle_{F_2}$$

is cyclic, with respect to the algebra $\mathfrak{A}_{\mathscr{F}}$, in the space $\mathfrak{H}$.

Class II representations are, in contrast to those of class I, reducible. This is clearly demonstrated by remarking that $b(p)$, defined by

$$b(p) = \nu(p)\,(a_{F_1}(p) + a^+_{F_1}(-p)) \otimes 1 + 1 \otimes \otimes \left(\sqrt{1 + \tilde{\varrho}_{\mathrm{II}}(p)}\; a_{F_2}(p) + \sqrt{\tilde{\varrho}_{\mathrm{II}}(p)}\; a^+_{F_2}(-p)\right)$$

along with its Hermitian conjugate $b^+(p)$ commute with all operators of the algebra $\mathfrak{A}_{\mathscr{F}}$ but, nevertheless, are not multiples of the identity. (It might be remarked that $b(p)$ and $b^+(p)$ also provide a representation of the canonical commutation relations but the significance of this is unclear).

As the above representations have the linked cluster property but nevertheless are reducible we may deduce from Theorem 3 that they contain irreducible representations which are not translationally invariant. This feature is now borne out by explicit calculation. In order to reduce out the representations it suffices to note that the components of $a(p)$, $a^+(p)$ in $\mathfrak{H}_{F_2}$ are, up to a phase, both equal to $\chi(p)$ where

$$\chi(p) = \nu(p)\,(a_{F_2}(p) + a^+_{F_2}(-p))\,.$$

If we chose a representation of $a_{F_2}(p)$, $a^+_{F_2}(p)$ such that $\chi(p)$ is diagonal the representation of $\mathfrak{A}_{\mathscr{F}}$ is then given as a direct integral of irreducible representations. In each of these representations we have

$$a(p) = e^{i\alpha(p)}\left(\sqrt{1 + \tilde{\varrho}_{\mathrm{II}}(p)}\; a_{F_\varkappa}(p) + \sqrt{\tilde{\varrho}_{\mathrm{II}}(p)}\; a^+_{F_\varkappa}(-p)\right) + \varrho_\varkappa(p)\,.$$

The states $|\,0_\varkappa\rangle$ defined by

$$a_{F_\varkappa}(p)\,|\,0_\varkappa\rangle = 0 \qquad \text{for all } p$$

are cyclic, with respect to $\mathfrak{A}_{\mathscr{F}}$, in Fock spaces $\mathfrak{H}_{F_\varkappa}$. It is to be noted that the breaking of translational invariance is contained solely in the term

$$\varrho_\varkappa(x) = \langle 0_\varkappa|\varphi(x)|\,0_\varkappa\rangle\,;$$

the truncated two point functions are still functions of the difference variable e.g.

$$\varrho_{\mathrm{II}}(x_1 - x_2) = \langle 0_\varkappa|\varphi^+(x_1)\,\varphi(x_2)|\,0_\varkappa\rangle\,.$$

This completes our discussion of Class II representations. ARAKI and WOODS [3], in considering the infinite free Bose gas with fixed density distribution, gave an example of such a representation, corresponding to the case $\sigma(x) = 0$. Their discussion is mathematically more refined than the above and they consider a number of interesting mathematical properties of the representation, which are also valid for $\sigma(x) \neq 0$, and which we have not mentioned.

To conclude our discussion of the quasi free states we mention one point of interest which arises from the positive definiteness conditions (19). These conditions were derived under the assumption (17) that the higher truncated functions vanished and in this case they were necessary and sufficient to ensure positive definiteness of the representation. In the general case, where (17) is not assumed, these conditions are still necessary and we note that if $\tilde{\tau}(p) = 0$ this has the consequence that (17) must also hold. This follows from the existence of destruction operators linear in $\varphi(x)$ and $\varphi^+(y)$. This feature might be useful in the discussion of more general representations because one could use $\tilde{\tau}(p)$ as a small parameter.

We now turn our attention to the applications of the quasi free states.

## 5. Applications of the quasi free states

We now consider the states $W_\alpha(Q)$, over $\mathfrak{A}_{\mathscr{F}}$, as a set of trial states and apply a variational principle to select the most suitable state for the approximate description of the ground state of the Bose system. Corresponding to the minimization of the ground state energy density we must, in the present formalism, minimize the value of $c$, defined by (6). From the condition

$$W_\alpha(K) = 0$$

we calculate $c$ to be given by

$$\begin{aligned} c = \int d^3p \Big\{ &(p^2 - \mu + \varrho_0 \tilde{V}(p))\, \tilde{\varrho}(p) + \varrho_0 \tilde{V}(p) \operatorname{Re} \tilde{\sigma}(p) + \\ &+ \frac{1}{2} \int d^3q\, \tilde{V}(p-q)\, [\tilde{\varrho}(p)\tilde{\varrho}(q) + \tilde{\sigma}(p)\tilde{\sigma}^+(q)] \Big\} + \frac{1}{2} \varrho^2 \tilde{V}(0) - \mu \varrho_0 . \end{aligned} \tag{21}$$

We have introduced the mean density $\varrho$ as

$$\varrho = \varrho_0 + \int d^3p\, \tilde{\varrho}(p) \, .$$

The value of $c$ must now be minimized with respect to $\tilde{\varrho}(p)$, $|\tilde{\sigma}(p)|$, $\alpha(p)$ and $\varrho_0$, taking into account the positive definiteness conditions. The most practical method of ensuring the validity of these inequalities is to minimize with respect to the alternative real variables $\sqrt{\tilde{\varrho}(p)}$, $\tilde{\tau}(p)$, $\alpha(p)$ and $\varrho_0$. Using these variables we find as conditions for a minimum

$$\begin{aligned} \frac{\delta c}{\delta \sqrt{\tilde{\varrho}(p)}} &= 2 \sqrt{\tilde{\varrho}(p)} \Big\{ \Big( p^2 - \mu + \varrho_0 \tilde{V}(p) + \varrho \tilde{V}(0) + \int d^3q\, \tilde{V}(p-q)\, \tilde{\varrho}(q) \Big) + \\ &+ \frac{(\frac{1}{2} + \tilde{\varrho}(p))}{|\tilde{\sigma}(p)|^2} \operatorname{Re} \Big( \tilde{\sigma}(p) \Big( \varrho_0 \tilde{V}(p) + \int d^3q\, \tilde{V}(p-q) \tilde{\sigma}^+(q) \Big) \Big) \Big\} = 0 \\ \frac{\delta c}{\delta \tilde{\tau}(p)} &= -\frac{\tilde{\tau}(p)}{|\tilde{\sigma}(p)|^2} \operatorname{Re} \Big( \tilde{\sigma}(p) \Big( \varrho_0 \tilde{V}(p) + \int d^3q\, \tilde{V}(p-q)\, \tilde{\sigma}^+(q) \Big) \Big) = 0 \\ \frac{\delta c}{\delta \alpha(p)} &= -2 \operatorname{Im} \Big( \tilde{\sigma}(p) \Big( \varrho_0 \tilde{V}(p) + \int d^3q\, \tilde{V}(p-q) \tilde{\sigma}^+(q) \Big) \Big) = 0 \end{aligned} \tag{22}$$

and

$$\frac{\delta c}{\delta \varrho_0} = -\mu + \varrho\, \tilde{V}(0) + \int d^3p\, \tilde{V}(p)\, (\tilde{\varrho}(p) + \operatorname{Re} \tilde{\sigma}(p)) = 0 \, .$$

From these conditions we may deduce that the absolute minimum of $c$ is reached when

$$\tilde{\tau}(p) = 0\,, \qquad \mathrm{Im}\,\tilde{\sigma}(p) = 0 \qquad \text{and} \qquad \tilde{\sigma}(p) = -\sqrt{\tilde{\varrho}(p)\,(1 + \tilde{\varrho}(p))}\,. \tag{23}$$

Thus we conclude that of the translationally invariant states contained in the quasi free states a pure state of Class I yields the minimal value of $c$. GIRARDEAU and ARNOWITT [13] have earlier performed a variational calculation to find the ground state of the Bose system and they used as trial states those states contained in Class I. Although our ansatz is more general the above calculation leads us immediately to the Class I states and further consideration of conditions (22) leads us to the specific state given by GIRARDEAU and ARNOWITT. We omit further details of this calculation.

It is unfortunate that the above minimization procedure leads to Class I states for it is well known that certain physical properties of the interacting Bose system are not reflected by these states. This may be demonstrated by considering the liquid structure factor $\tilde{S}(p)$ (see for instance [14]). This form factor is defined as the Fourier transform of $S(x)$ where

$$S(x-y) = W(\varphi^+(x)\,\varphi(x)\,\varphi^+(y)\,\varphi(y)) - W(\varphi^+(x)\,\varphi(x))\;W(\varphi^+(y)\,\varphi(y))\,.$$

If we evaluate $\tilde{S}(p)$ for the state $W_\alpha(Q)$ and use conditions (23) we find that

$$\tilde{S}(p) = \tilde{S}_1(p) + \tilde{S}_2(p)$$

where

$$\tilde{S}_1(p) = \varrho_0\big(\sqrt{\tilde{\varrho}(p)} - \sqrt{1 + \tilde{\varrho}(p)}\big)^2 + \varrho(0)$$

and

$$\tilde{S}_2(p) = \int d^3q\,\{\tilde{\varrho}(q)\,\tilde{\varrho}(q-p) + \sqrt{\tilde{\varrho}(q)\,(1+\tilde{\varrho}(q))}\,\sqrt{\tilde{\varrho}(q-p)\,(1+\tilde{\varrho}(q-p))}\}\,.$$

Now $\tilde{S}_1(p)$ and $\tilde{S}_2(p)$ are both positive and we must therefore conclude that

$$\tilde{S}(p) > 0 \qquad \text{for all } p\,.$$

There are however good reasons to believe that in the general problem

$$\lim_{|p|\to 0} \tilde{S}(p) = 0\,. \tag{24}$$

This condition, which is related to the phonon structure of the ground state of the Bose system, can therefore never be fulfilled in the states under consideration.

It might be added for completeness that the early work of BOGOLIUBOV does not suffer from this unfortunate feature, although BOGOLIUBOV only considers states of Class I. This is due to further approximations based upon the assumptions of low density and weak interaction. Under such assumptions it may be argued that it is consistent to approximate $c$, as given by (21), to first order in $\tilde{\varrho}(p)$ and $\tilde{\sigma}(p)$. These arguments which are well known lead eventually to an expression for the ground state energy density $\varepsilon_B$, where

$$\varepsilon_B = \int d^3p \, \{(p^2 + \varrho \tilde{V}(p)) \, \tilde{\varrho}(p) + \varrho \tilde{V}(p) \, \mathrm{Re}\, \tilde{\sigma}(p)\} + \frac{1}{2} \varrho^2 \tilde{V}(0) \, .$$

Minimization of $\varepsilon_B$, with respect to $\tilde{\varrho}(p)$ and $\tilde{\sigma}(p)$, taking into account the positive definiteness conditions leads to the choice

$$\tilde{\sigma}(p) = -\sqrt{\tilde{\varrho}(p)\,(1 + \tilde{\varrho}(p))} = -\frac{1}{2} \frac{\varrho \tilde{V}(p)}{\sqrt{p^2(p^2 + 2\varrho \tilde{V}(p))}} \, . \qquad (25)$$

To the same degree of approximation $\tilde{S}(p)$ is replaced by $S_B(p)$, where

$$\tilde{S}_B(p) = \varrho(\sqrt{\tilde{\varrho}(p)} - \sqrt{1 + \tilde{\varrho}(p)})^2 \, .$$

Substituting the value of $\tilde{\varrho}(p)$ given by (25) we find

$$\tilde{S}_B(p) = \varrho \frac{|p|}{\sqrt{p^2 + 2\varrho \tilde{V}(p)}}$$

a form which is in agreement with (24). Although this model is very useful it does give a higher value for the ground state energy density than that obtained by the minimization procedure described at the beginning of this section.

Finally we note that although the conditions of minimization ruled out the Class II states it is still possible that the non-translationally invariant pure states contained in these mixed states might lead to lower values of $c$ than that obtained with the Class I states. Non-translationally invariant states of the above type have been considered by Gross [2].

## 6. Summary and conclusion

In this paper we have discussed the problem of the many body Boson system with the aid of mathematical methods which have found great use in relativistic field theory. The successes in the analysis of asymptotic behaviour in field theory follow essentially from the use of the locality condition in configuration space and the spectrum conditions in momentum space. In the many body problem an analogue of the locality condition is provided by the canonical commutation relations which are explicitly given. The spectrum conditions are however only given implicitly and it therefore appears at the moment to be more difficult to analyse long distance behaviour in the many body problem.

The information which one might hope to derive for the asymptotic behaviour is firstly the validity of the linked cluster property and secondly the rate in which the limits (11) defined by this property go to zero. The question of the validity of the linked cluster property for observables is closely related to the nature of the ground state of the system. We have pointed out that this property would hold if the representation of $\mathfrak{A}_{\mathcal{O}}$ selected by the spectrum condition (6) were irreducible, but we also have mentioned that irreducibility is not necessary to obtain this result. The rate in which the limits (11) go to zero is related to the properties of the low lying energy spectrum of the system and is less accessible to analysis. One interesting feature which results for irreducible representations of is the property of "factorisable off-diagonal long range order". This latter property has previously found use [15] in approximate calculations of superfluid and superconducting properties.

The only states characterisable by a finite number of functions which are available for analysis of the many body problem are the quasi free states. We have given the general definition of these states, summarized their applications to the Bose system, and mentioned the difficulties encountered in such applications. In contrast to the Fermi system, it appears to be impossible to find a quasi free state which satisfactorily reproduces the low lying spectrum of the interacting Bose system except in the low density limit.

The author is indebted to Prof. R. HAAG for much helpful advice and many critical discussions concerning the subject matter of this paper and to Prof. N. HUGENHOLTZ for a number of informative discussions.

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*(Received March 29, 1965)*