

A Variational Approach to Superfluidity

R. H. Critchley¹ and A. I. Solomon¹

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A variational approach to problems in quantum statistical mechanics is described and it is shown how to determine the best quasi-free approximation to the equilibrium state. The relation between this approximation and the Bogoliubov approximation in superfluidity is discussed.

KEY WORDS: Superfluidity; variational approach; quantum statistical mechanics; Bogoliubov approximation.

1. INTRODUCTION

In the work reported here we discuss a variational approach to the determination of the thermodynamic equilibrium state of an infinitely extended system of bosons. Essentially, the problem consists in determining which state of an algebra corresponds to a given form of the energy density. By making the idealization of infinite volume we are able to exploit the translation invariance of the system, and to avoid the severe technical problems of demonstrating the convergence of various volume-dependent sequences. The definitions we make for infinite systems are, of course, motivated by consideration of the finite case.

Variational methods have been considered by several authors. Valatin and Butler⁽¹⁾ and Girardeau and Arnowitt,⁽²⁾ among others, have used a variation over a set of trial wave functions. Robinson⁽³⁾ and Ruelle⁽⁴⁾ have discussed the problem in a more algebraic setting. Švarc⁽⁵⁾ has formulated the

¹ Faculty of Mathematics, Open University, Milton Keynes, England, and Dublin Institute for Advanced Studies, Dublin, Ireland.

problem algebraically for a lattice system; we describe the boson problem in an analogous way. Robinson⁽⁶⁾ used a variational calculation to approximate the ground state (zero temperature) of a boson gas by a "quasi-free" state. We generalize his work to the excited states (nonzero temperature) and show how the quasi-free approximation is related to the Bogoliubov approximation.⁽⁷⁾ For Fermi lattice systems, Fannes and Verbeure⁽⁸⁾ have described a model in which the quasi-free approximation and the variational principle yield the Gibbs state.

In Section 2 we assemble the mathematical structures we require and formulate the variational principle. In Section 3 we discuss the quasi-free approximation and exhibit the equations resulting from a variation over the quasi-free states. In Section 4 we make a further approximation and show that the resulting state is identical to that derived from the Bogoliubov approximation. We conclude in Section 5 with a few brief remarks about the problem.

2. THE VARIATIONAL PRINCIPLE

A boson system may be described by means of a field $\psi(x)$ and its conjugate $\psi^*(x)$ assumed to satisfy the following commutation relations:

$$\begin{aligned} [\psi(x), \psi(y)] &= [\psi^*(x), \psi^*(y)] = 0 \\ [\psi(x), \psi^*(y)] &= \delta(x - y) \end{aligned} \quad (1)$$

Because of the singular nature of these relations, it is usual to introduce the smeared fields

$$\psi(h) = \int \bar{h}(x)\psi(x) dx, \quad \psi^*(h) = \int h(x)\psi^*(x) dx \quad (2)$$

where h is in some space M of test functions. We then have

$$[\psi(h_1), \psi^*(h_2)] = \langle h_1, h_2 \rangle \quad (3)$$

where $\langle h_1, h_2 \rangle = \int \bar{h}_1(x)h_2(x) dx$. Let

$$W(h) = \exp\{2^{-1/2}i[\psi(h) + \psi^*(h)]\} \quad (4)$$

Then the commutation relations (1) and (3) are formally equivalent to

$$W(h_1)W(h_2) = [\exp(-\frac{1}{2} \text{Im}\langle h_1, h_2 \rangle)]W(h_1 + h_2) \quad (5)$$

The product law (5) and certain technical conditions provide the starting point for mathematically rigorous discussions of the canonical commutation relations and boson systems. Equations (1)–(4) are regarded as heuristic justification for (5) since $\psi(h)$ and $\psi^*(h)$ cannot be realized as bounded operators for which (4) holds as a strict identity (see Refs. 9 and 22).

The algebra we require is the C^* -algebra $\mathcal{A}(M)$ generated by the set $\{W(h): h \in M\}$. We omit the details of its construction but remark that it is independent of the representation of (5) used to construct it.⁽¹⁰⁾

A state on $\mathcal{A}(M)$ is a continuous, positive, linear functional $\omega: \mathcal{A}(M) \rightarrow \mathbb{C}$ such that $\omega(\mathbf{1}) = 1$. It determines and is determined by a functional $\mu: M \rightarrow \mathbb{C}$ defined by

$$\mu(h) = \omega(W(h)) \tag{6}$$

μ is called the generating functional of the state. Araki⁽¹²⁾ and Segal⁽⁹⁾ have provided a characterization of generating functionals.

To discuss an infinitely extended boson system, we take M to be a dense subspace of $L^2(\mathbb{R}^3)$ (usually the space C_0^∞ of infinitely differentiable functions that vanish outside a finite region⁽¹³⁾). We restrict our attention to the Euclidean-invariant states on $\mathcal{A}(M)$ (i.e., those states whose generating functionals are invariant under the action of the Euclidean group) because we assume that the interaction between the particles is Euclidean-invariant. This means that the problem of the spontaneous breaking of Euclidean symmetry must be discussed separately. The other important physical restriction that we impose is that the states be locally normal.⁽³⁾ These states are such that a finite volume contains only a finite number of particles.⁽¹⁴⁾ Let

$$\xi = \{\text{Euclidean-invariant, locally normal states on } \mathcal{A}(M)\}$$

We assume that the interaction between the particles is mediated by a two-body (Euclidean-invariant) potential $V(x - y)$ so that the Hamiltonian H has the following formal expression:

$$H = \frac{1}{2} \int \psi^*(x)(-\nabla^2)\psi(x) dx + \frac{1}{2} \int \psi^*(x)\psi^*(y)V(x - y)\psi(y)\psi(x) dx dy \tag{7}$$

In the conventional approach to statistical mechanics the integrals in (7) are restricted to a finite volume Λ so that the resulting Hamiltonian H_Λ can be interpreted as an operator on Fock space. The generating functional of the grand canonical Gibbs state can, in theory, be computed and the thermodynamic limit taken. This program has had very limited success^(15,16) because of the severe technical difficulties involved.

The alternative approach that we adopt is to omit the finite-volume step and perform all calculations “in the thermodynamic limit,” thus obviating the need to take this limit. We use a variational principle which we now describe. It is based on the exploitation of the Euclidean invariance.

According to Švarc,⁽⁵⁾ Robinson,⁽³⁾ and Ruelle,⁽⁴⁾ we can define a particle density functional $\bar{N}: \xi \rightarrow \mathbb{R}$ and an entropy density functional $\bar{S}: \xi \rightarrow \mathbb{R}$ which are consistent with the local normality and with the usual (finite-volume)

definitions of particle number and entropy. Similarly, for each Euclidean-invariant formal Hamiltonian H we can define an energy density functional $\bar{H}: \xi \rightarrow \mathbb{R}$. (For a fuller discussion of this see Robinson.⁽³⁾) The variational principle states that the thermodynamic equilibrium state of the (infinite) system at temperature T and density ρ is the state $\omega \in \xi$ that minimizes the free energy density

$$\bar{F}(\omega) = \bar{H}(\omega) - T\bar{S}(\omega) \tag{8}$$

subject to $\bar{N}(\omega) = \rho$. We note that there is no reason to believe that the state so determined is unique. Indeed, the grand canonical state⁽¹⁵⁾ and the canonical state⁽¹³⁾ of the free boson gas are different at low temperatures but have the same (minimizing) free energy density.

It remains an open question whether this variational principle determines the same state, or even the same thermodynamics, as the usual approach (for a discussion of this see Ruelle⁽⁴⁾ and Robinson⁽³⁾).

In order to use the variational principle to discuss particular systems, it is necessary to have explicit expressions for the densities $\bar{F}(\omega)$ and $\bar{N}(\omega)$. For a particular class of states (the quasi-free states) these are obtainable and so, by minimizing the free energy density functional over these states, we determine the best quasi-free approximation to the equilibrium state.

3. THE QUASI-FREE APPROXIMATION

In principle, one can define the value of products of the smeared fields in the state ω by differentiating the generating functional; for example,

$$\omega(\psi^*(h_1)\psi(h_2)) = 2 \frac{\partial^2}{\partial z_1 \partial \bar{z}_2} \left[\exp\left(\frac{1}{4} \|z_1 h_1 + z_2 h_2\|^2\right) \mu(z_1 h_1 + z_2 h_2) \right]_{z_1 = z_2 = 0} \tag{9}$$

The truncation ω_T of ω is defined recursively by

$$\begin{aligned} \omega(\psi(h)) &= \omega_T(\psi(h)); & \omega(\psi^*(h)) &= \omega_T(\psi^*(h)) \\ \omega(\psi(h_1)\psi(h_2)) &= \omega_T(\psi(h_1)\psi(h_2)) + \omega_T(\psi(h_1))\omega_T(\psi(h_2)) \\ \omega(\psi^*(h_1)\dots\psi^*(h_n)\psi(h_{n+1})\dots\psi(h_{n+m})) &= \sum_P \omega_T(\psi^*(h_1)\dots)\dots\omega_T(\dots) \end{aligned} \tag{10}$$

where the sum \sum_P is taken over all partitions of

$$\{\psi^*(h_1) \dots \psi(h_{n+m})\}$$

and the order of the elements within each part of the partition is taken over from the left-hand side.

The state ω is said to be quasi-free⁽⁶⁾ if

$$\omega_T(\psi^*(h_1) \dots \psi(h_{n+m})) = 0 \tag{11}$$

for $n + m \geq 3$; that is, $\omega(\psi^*(h_1) \cdots \psi(h_{n+m}))$ is just a sum of products of the one- and two-point truncated functions. The quasi-free states are the only states having the property of being determined by a finite number of functions.⁽¹¹⁾

The generating functional of a quasi-free state can be obtained from the following formal identity:

$$\log \omega(W(h)) = -\frac{1}{4} \|h\|^2 + \sum_{m,n} \left(\frac{i}{\sqrt{2}}\right)^{m+n} \frac{1}{m!} \frac{1}{n!} \omega_T(\underbrace{\psi^*(h) \cdots \psi^*(h)}_m \underbrace{\psi(h) \cdots \psi(h)}_n)$$

If ω is quasi-free, there is no convergence problem and so this gives

$$\begin{aligned} \omega(W(h)) = \exp(-\frac{1}{4} \|h\|^2) \exp\{ & (i/\sqrt{2})[\omega_T(\psi^*(h) + \omega_T(\psi(h))] \\ & - \frac{1}{2} \omega_T(\psi^*(h)\psi(h)) \\ & - \frac{1}{4} [\omega_T(\psi(h)\psi(h)) + \omega_T(\psi^*(h)\psi^*(h))] \} \end{aligned} \tag{12}$$

Let

$$Q = \{\text{quasi-free states in } \xi\}$$

The physically important correlation functions or reduced density matrices are defined using (2). For example, $\langle \psi^*(x)\psi(y) \rangle$ is extracted from (9) as follows:

$$\omega(\psi^*(h_1)\psi(h_2)) = \int h_1(x) \langle \psi^*(x)\psi(y) \rangle \bar{h}_2(y) dx dy$$

If ω is Euclidean-invariant, then $\langle \psi^*(x)\psi(y) \rangle$ and $\langle \psi^*(x)\psi^*(y) \rangle$ are functions of $|x - y|$, and $\langle \psi(x) \rangle$ is independent of x . Thus the quasi-free state $\omega \in Q$ is completely determined by the following functions:

$$\langle \psi(x) \rangle = \alpha; \quad \langle \psi^*(x) \rangle = \bar{\alpha} \tag{13}$$

$$\begin{aligned} \langle \psi^*(x)\psi(y) \rangle &= \langle \psi^*(x)\psi(y) \rangle_T + \langle \psi^*(x) \rangle_T \langle \psi(y) \rangle_T \\ &= f(x - y) + |\alpha|^2 \end{aligned} \tag{14}$$

$$\langle \psi(x)\psi(y) \rangle = g(x - y) + \alpha^2; \quad \langle \psi^*(x)\psi^*(y) \rangle = \overline{g(x - y)} + \bar{\alpha}^2 \tag{15}$$

where α is a complex number, f is a real-valued function, and g is a complex-valued function, both depending only on $|x - y|$. The expression $\langle \psi^*(x)\psi(y) \rangle_T$ is the kernel of the corresponding truncation ω_T . Robinson⁽⁶⁾ showed that two functions f and g determine a quasi-free state as in (13)–(15) if and only if

$$\hat{f}(p) \geq \hat{a}(p) \geq 0 \tag{16}$$

where the caret denotes the Fourier transform and $\hat{a}(p)$ is defined by

$$[\hat{a}(p) + \frac{1}{2}]^2 = [\hat{f}(p) + \frac{1}{2}]^2 - |\hat{g}(p)|^2 \tag{17}$$

The thermodynamic functionals that we require for the variational principle are as follows. The particle density functional $\bar{N}: Q \rightarrow \mathbb{R}$ is

$$\bar{N}(\omega) = \langle \psi^*(x)\psi(x) \rangle = f(0) + |\alpha|^2 = \int \hat{f}(p) \frac{dp}{(2\pi)^3} + |\alpha|^2 \quad (18)$$

Similarly the kinetic energy density functional $\bar{K}: Q \rightarrow \mathbb{R}$ is

$$\bar{K}(\omega) = \int \frac{p^2}{2} \hat{f}(p) \frac{dp}{(2\pi)^3} \quad (19)$$

Generalizing a result of Critchley and Lewis,^(17,18) we show in the appendix that the entropy density functional $\bar{S}: Q \rightarrow \mathbb{R}$ is given by

$$\bar{S}(\omega) = \int \{ [1 + \hat{a}(p)] \log[1 + \hat{a}(p)] - \hat{a}(p) \log \hat{a}(p) \} \frac{dp}{(2\pi)^3} \quad (20)$$

The only thermodynamic quantity that depends on the interaction is the potential energy density functional $\bar{V}: Q \rightarrow \mathbb{R}$. It is given by

$$\bar{V}(\omega) = \frac{1}{2} \int \langle \psi^*(0)\psi^*(x)\psi(x)\psi(0) \rangle V(x) dx \quad (21)$$

Using the quasi-free nature of the state ω and Eqs. (13)–(15), we obtain for this

$$\begin{aligned} \bar{V}(\omega) &= \frac{\bar{N}(\omega)^2}{2} \hat{V}(0) + |\alpha|^2 \int \hat{f}(p) \hat{V}(p) \frac{dp}{(2\pi)^3} \\ &+ \frac{\alpha^2}{2} \int \bar{\hat{g}}(p) \hat{V}(p) \frac{dp}{(2\pi)^3} + \bar{\alpha}^2 \int \hat{g}(p) \hat{V}(p) \frac{dp}{(2\pi)^3} \\ &+ \frac{1}{2} \int \hat{f}(p) \hat{V}(p - q) \hat{f}(q) \frac{dp}{(2\pi)^3} \frac{dq}{(2\pi)^3} \\ &+ \frac{1}{2} \int \bar{\hat{g}}(p) \hat{V}(p - q) \hat{g}(q) \frac{dp}{(2\pi)^3} \frac{dq}{(2\pi)^3} \end{aligned} \quad (22)$$

The free energy density

$$\bar{F}(\omega) = \bar{K}(\omega) + \bar{V}(\omega) - T\bar{S}(\omega)$$

can now be minimized over Q and the best quasi-free approximation to the equilibrium state obtained. We take account of the condition $\bar{N}(\omega) = \rho$ by means of the Lagrange multiplier γ , and determine the equilibrium state by minimizing

$$\mathcal{F}(\omega) = \bar{F}(\omega) - \gamma(\bar{N}(\omega) - \rho) \quad (23)$$

with respect to the variables $|\alpha|$, $\phi = \arg \alpha^2$, $\phi(p) = \arg \hat{g}(p) - \phi$, $\hat{f}(p)$, $|\hat{g}(p)|$, and γ . With $\phi(p)$ defined in this way it is clear that $\bar{F}(\omega)$ is independent

of ϕ , and this quantity will be undetermined. For convenience we take it equal to zero. To take account of the positive-definiteness conditions (16) we minimize $\bar{F}(\omega)$ with respect to the alternative set α^2 , $\phi(p)$, $\hat{f}(p)$, $\hat{a}(p)$, and γ . The equations resulting from the variation $\delta\mathcal{F}(\omega)$ are

$$\frac{\partial\mathcal{F}}{\partial\alpha^2} = \langle f, V \rangle + \text{Re}\langle g, V \rangle + \bar{N}(\omega)\hat{V}(0) - \gamma = 0 \tag{24}$$

$$\frac{\partial\mathcal{F}}{\partial\phi(p)} = -\text{Im}\left\{ \hat{g}(p)\left[\alpha^2\hat{V}(p) + \int \hat{V}(p-q)\bar{\hat{g}}(q)\frac{dq}{(2\pi)^3}\right] \right\} = 0 \tag{25}$$

$$(2\pi)^3 \frac{\partial\mathcal{F}}{\partial f(p)} = \frac{p^2}{2} - \gamma + \bar{N}(\omega)\hat{V}(0) + \alpha^2\hat{V}(p) + \int \hat{f}(q)\hat{V}(p-q)\frac{dq}{(2\pi)^3} + \frac{\hat{f}(p) + \frac{1}{2}}{|\hat{g}(p)|^2} \text{Re}\left\{ \hat{g}(p)\left[\alpha^2\hat{V}(p) + \int \hat{V}(p-q)\bar{\hat{g}}(q)\frac{dq}{(2\pi)^3}\right] \right\} = 0 \tag{26}$$

$$(2\pi)^3 \frac{\partial\mathcal{F}}{\partial\hat{a}(p)} = -\frac{\hat{a}(p) + \frac{1}{2}}{|\hat{g}(p)|^2} \text{Re}\left\{ \hat{g}(p)\left[\alpha^2\hat{V}(p) + \int \hat{V}(p-q)\bar{\hat{g}}(q)\frac{dq}{(2\pi)^3}\right] \right\} - T \log\left(1 + \frac{1}{\hat{a}(p)}\right) = 0 \tag{27}$$

$$\frac{\partial\mathcal{F}}{\partial\gamma} = \rho - \bar{N}(\omega) = 0 \tag{28}$$

The solution to this set of equations, provided it exists and is a global minimum, determines the canonical equilibrium quasi-free state. However, it is possible that *no* solution to this set exists; for example, for the free boson gas ($V = 0$) Eq. (27) becomes

$$\frac{\partial\mathcal{F}}{\partial\hat{a}(p)} = -\frac{T}{(2\pi)^3} \log\left(1 + \frac{1}{\hat{a}(p)}\right)$$

This is negative since $0 \leq \hat{a}(p) \leq \hat{f}(p)$, and so the minimum of $\mathcal{F}(\omega)$ occurs on the hyperplane $\hat{a}(p) = \hat{f}(p)$. It is not determined by solving (24)–(28), since this set of equations has no solution, but by solving the analogous equations produced by a variation over the trial states with $g = 0$. This is an approximation considered by Critchley,⁽²³⁾ who shows that for the free boson gas this procedure gives the thermodynamic limit of the canonical Gibbs state.

Similar equations to (24)–(28) have also been derived by Robinson⁽⁶⁾ in his discussion of the quasi-free approximation to the ground state ($T = 0$) of a boson system.

In the next section we make a further approximation; we assume that the quantities $\hat{f}(p)$ and $\hat{g}(p)$ are “small,” so that we may drop second-order

terms in the potential energy density. This simplifies our variational equations to exactly soluble form. A comparison of the generating functional thus obtained with that resulting from the Bogoliubov approximation shows that the two approximations are equivalent.

4. THE BOGOLIUBOV APPROXIMATION

Retaining only those terms linear in $\hat{f}(p)$ and $\hat{g}(p)$ in the expression for the potential energy density (22), we obtain the following simplified forms of (24)–(28):

$$\langle f, V \rangle + \text{Re}\langle g, V \rangle + \bar{N}(\omega)\hat{V}(0) - \gamma = 0 \tag{29}$$

$$\text{Im}\{g(p)\alpha^2\hat{V}(p)\} = 0 \tag{30}$$

$$\frac{p^2}{2} - \gamma + \alpha^2\hat{V}(0) + \alpha^2\hat{V}(p) + \frac{\hat{f}(p) + \frac{1}{2}}{|\hat{g}(p)|^2} \text{Re}\{\hat{g}(p)\alpha^2\hat{V}(p)\} = 0 \tag{31}$$

$$-\frac{\hat{a}(p) + \frac{1}{2}}{|\hat{g}(p)|^2} \text{Re}\{\hat{g}(p)\alpha^2\hat{V}(p)\} = T \log\left(1 + \frac{1}{\hat{a}(p)}\right) \tag{32}$$

$$\rho = \alpha^2 + \int \hat{f}(p) \frac{dp}{(2\pi)^3} \tag{33}$$

From (32) and (30) we see that $\alpha \neq 0$ and

$$\hat{g}(p)\hat{V}(p) < 0 \tag{34}$$

Using (17), we introduce $\theta(p)$ defined by

$$[\hat{a}(p) + \frac{1}{2}] \cosh \theta(p) = \hat{f}(p) + \frac{1}{2}, \quad [\hat{a}(p) + \frac{1}{2}] \sinh \theta(p) = -\hat{g}(p) \tag{35}$$

(the conventional minus sign ensures positive θ for positive \hat{V}).

Equations (31) and (32) now become

$$\alpha^2\hat{V}(p) \coth \theta(p) = \varepsilon(p) \tag{36}$$

where

$$\varepsilon(p) = \frac{1}{2}p^2 - \gamma + \hat{V}(0)\alpha^2 + \hat{V}(p)\alpha^2 \tag{37}$$

and

$$\alpha^2\hat{V}(p) \text{cosech } \theta(p) = T \log[1 + (1/\hat{a}(p))] \tag{38}$$

Eliminating $\theta(p)$ between (36) and (38), we obtain

$$\hat{a}(p) = (e^{\beta E(p)} - 1)^{-1} \tag{39}$$

where

$$E(p) = [\varepsilon(p)^2 - \alpha^4\hat{V}(p)^2]^{1/2} \tag{40}$$

We may obtain $f(p)$ and $g(p)$ from (35), (36), and (39), and then γ and α are determined from (29) and (33).

From (36) we note that for a solution to exist we must have

$$|\varepsilon(p)| \geq \alpha^2 |\hat{V}(p)| \tag{41}$$

For a positive-type potential [$\hat{V}(p) \geq 0$], (41) holds if

$$-\gamma + \alpha^2 \hat{V}(0) \geq 0$$

Using (12), we can now write down the generating functional of the quasi-free state determined by this system of equations. It is

$$\begin{aligned} \mu(h) = & \exp\left(-\frac{1}{4} \|h\|^2\right) \exp\left\{\frac{i\alpha}{\sqrt{2}} [\hat{h}(0) + \bar{h}(0)]\right. \\ & - \frac{1}{2} \int |\hat{h}(p)|^2 \{\hat{a}(p) \cosh \theta(p) + \frac{1}{2} [\cosh \theta(p) - 1]\} \frac{dp}{(2\pi)^3} \\ & \left. + \frac{1}{4} \int [\hat{h}(-p)\hat{h}(p) + \bar{h}(-p)\bar{h}(p)] \left[\hat{a}(p) + \frac{1}{2}\right] \sinh \theta(p) \frac{dp}{(2\pi)^3}\right\} \tag{42} \end{aligned}$$

We do not investigate whether this state is the *best* quasi-free state. This requires a detailed investigation of the behavior of $\bar{F}(\omega)$, particularly on the boundary.

We now show how this is related to the Bogoliubov approximation by calculating the generating functional corresponding to the latter. Bogoliubov's prescription⁽⁷⁾ was that at low temperatures a weakly interacting Bose system could be described by a truncated Hamiltonian

$$\begin{aligned} H_B = & \frac{1}{2} |\alpha|^4 \hat{V}(0) + \sum_{k \neq 0} [\varepsilon_k + |\alpha|^2 \hat{V}(k) + |\alpha|^2 \hat{V}(0)] a_k^* a_k \\ & + \frac{1}{2} \sum_{k \neq 0} \hat{V}(k) (\alpha^2 a_k^* a_{-k}^* + \bar{\alpha}^2 a_k a_{-k}) \tag{43} \end{aligned}$$

where ε_k is the kinetic energy of the k th level and $|\alpha|^2$ is the density of particles in the ground state. H_B describes the excited particles; we follow Ginibre⁽¹⁹⁾ and assume that the ground-state particles are described by a coherent state. More precisely, if the system is in volume Λ , we define $h_0 \in L^2(\Lambda)$ by $h_0(x) = |\Lambda|^{-1/2}$ and let \mathcal{H}_0 be the Fock space constructed on the one-dimensional Hilbert space spanned by h_0 , and \mathcal{H}' be the Fock space constructed on the orthogonal complement h' of h_0 in the one-particle space $L^2(\Lambda)$. The equilibrium state of the system is described by the following density matrix on the Fock space $\mathcal{H} = \mathcal{H}_0 \otimes \mathcal{H}'$:

$$\rho_B = |\alpha\rangle\langle\alpha| \otimes \{\exp[-\beta(H_B - \gamma N')]\} \{\text{tr} \exp[-\beta(H_B - \gamma N')]\}^{-1} \tag{44}$$

where $|\alpha\rangle$ is the coherent state

$$|\alpha\rangle = \left[\exp\left(-\frac{1}{2} |\alpha|^2\right) \right] \sum_0^\infty \frac{\alpha^m}{m!} (a_0^*)^m \Omega$$

(Ω is the vacuum state in \mathcal{H}_0 and a_0^* is the operator that creates a ground-state particle). N' is the number operator on \mathcal{H}' and γ is a Lagrange multiplier determined by fixing the total particle density. $H_B - \gamma N'$ can be diagonalized by a transformation of the operators $a_k, a_k^* \mapsto b_k, b_k^*$ (for the details see, for example, Solomon⁽²⁰⁾); the elementary excitations have energy spectrum $\{E_k\}$, a discrete form of (40) with, in (37), $\frac{1}{2}p^2$ replaced by ϵ_k . The same transformation can be applied to $W(h)$; it is equivalent to a transformation $R: \hat{h}' \rightarrow \hat{h}'$. Thus we can calculate the generating functional using the usual Fock space methods^(21,18):

$$\begin{aligned} \mu_B(h) &= \langle \alpha | W(\hat{h}(0)) | \alpha \rangle \frac{\text{tr}'\{\exp[-\beta(H_B - \gamma N')]W(h')\}}{\text{tr}' \exp[-\beta(H_B - \gamma N')]} \\ &= \langle \alpha | W(\hat{h}(0)) | \alpha \rangle \frac{\text{tr}'[\exp(-\beta \sum E_k b_k^* b_k)W(Rh')]}{\text{tr}' \exp(-\beta \sum E_k b_k^* b_k)} \\ &= \exp\left(-\frac{1}{4} \|\hat{h}(0)\|^2\right) \exp\left(-\frac{1}{4} \|Rh'\|^2\right) \\ &\quad \times \exp\left\{\frac{i}{\sqrt{2}} [\widehat{\alpha\hat{h}(0)} + \overline{\alpha\hat{h}(0)}] - \frac{1}{2|\Lambda|} \sum |\widehat{Rh'(k)}|^2 \hat{a}_k\right\} \quad (45) \end{aligned}$$

where \hat{a}_k is a discrete form of (39), and $h = \hat{h}(0) \oplus h'$. But as can readily be checked

$$\widehat{Rh'(k)} = e^{-i\phi/2}\hat{h}(k) \cosh(\frac{1}{2}\theta_k) - e^{i\phi/2}\overline{\hat{h}(-k)} \sinh(\frac{1}{2}\theta_k) \quad (46)$$

where $\phi = \arg \alpha^2$ and θ_k is a discrete form of (36). Substituting (46) into (45), we see that $\mu_B(h)$ is a discrete (i.e., finite-volume) form of (42). This establishes the connection between the two approximations and justifies our calling the first “the Bogoliubov approximation.”

5. CONCLUSION

The generating functional (42) may be regarded as the exact solution of the Bogoliubov problem given the assumption that the ground-state particles are described by a coherent state. In this note we have shown that this generating functional results from a variational principle based on minimizing an appropriate free energy functional over the class of quasi-free states. This approach draws attention to some of the problems of the Bogoliubov approximation. For example, the approximations made in deriving (42) (e.g., quasi-free state, linearized potential energy density functional) seem considerable, but in this formulation it may be possible to estimate their effect. Furthermore, although (42) may be a local minimum of $\overline{F}(\omega)$ ($\omega \in Q$), it may not be a global minimum. There may be a point on the boundary [for example, the boundary

$\hat{a}(p) = \hat{f}(p)]$ which gives a lower value of the free energy density. We do not discuss this any further here, but a similar problem has been considered by Critchley⁽²³⁾ in an example.

Finally we note that it may be possible to achieve a better quasi-free approximation by substituting a perturbation of the Bogoliubov solution into Eqs. (24)–(28).

APPENDIX. ENTROPY DENSITY

In this appendix we discuss the definition (20) of the entropy density of the quasi-free state determined by (13)–(15). This state has generating functional

$$\begin{aligned} \mu(h) = \exp\left(-\frac{1}{4} \|h\|^2\right) \exp\left\{\left[\frac{i}{\sqrt{2}} (\bar{\alpha}\hat{h}(0) + \alpha\overline{\hat{h}(0)})\right] - \frac{1}{2} \int |\hat{h}(p)|^2 \hat{f}(p) \frac{dp}{(2\pi)^3}\right. \\ \left. - \frac{1}{4} \left[\int \hat{h}(p) \overline{\hat{g}(p)} \hat{h}(-p) \frac{dp}{(2\pi)^3} + \int \overline{\hat{h}(p)} \hat{g}(p) \overline{\hat{h}(-p)} \frac{dp}{(2\pi)^3} \right] \right\} \end{aligned} \tag{A.1}$$

For the case $\alpha = 0$, this can be diagonalized as $\mu_D(Rh)$, where

$$\widehat{R\hat{h}}(p) = [\cosh \frac{1}{2}\theta(p)]\hat{h}(p) + e^{i\phi(p)}[\sinh \frac{1}{2}\theta(p)]\overline{\hat{h}(-p)} \tag{A.2}$$

and

$$\mu_D(h) = \exp\left(-\frac{1}{4} \|h\|^2\right) \exp\left\{-\frac{1}{2} \int |\hat{h}(p)|^2 \hat{a}(p) \frac{dp}{(2\pi)^3}\right\} \tag{A.3}$$

where $\hat{a}(p)$ is as defined in (17), $\phi(p) = \arg \hat{g}(p)$, and $\theta(p) \geq 0$ is defined by

$$\begin{aligned} \hat{f}(p) + \frac{1}{2} &= [\hat{a}(p) + \frac{1}{2}] \cosh \theta(p) \\ |\hat{g}(p)| &= [\hat{a}(p) + \frac{1}{2}] \sinh \theta(p) \end{aligned}$$

We show that at the finite-volume level, the states determined by μ_D and μ (suitably restricted) are related by a unitary transformation. Since the entropy is invariant under such transformations, we will take $\bar{S}(\mu) = \bar{S}(\mu_D)$. But according to Critchley and Lewis⁽¹⁷⁾

$$\bar{S}(\mu_D) = \int \{[1 + \hat{a}(p)] \log[1 + \hat{a}(p)] - \hat{a}(p) \log \hat{a}(p)\} \frac{dp}{(2\pi)^3} \tag{A.4}$$

as required by (20). They justified this by constructing a sequence of density matrices $\{\rho_n\}$ and a corresponding sequence of finite volumes $\{\Lambda_n\}$ such that:

1. ρ_n is a density operator on the Fock space $F(L^2(\Lambda_n))$.
2. $\{\Lambda_n\}$ is an unbounded increasing sequence of volumes.

3. $\lim_{n \rightarrow \infty} \text{tr}^{(n)} W(h)\rho_n = \mu_D(h).$
4. $\lim_{n \rightarrow \infty} \{[-\text{tr}^{(n)} \rho_n \log \rho_n]/|\Lambda_n|\}$
 $= \int \{[1 + \hat{a}(p)] \log[1 + \hat{a}(p)] - \hat{a}(p) \log \hat{a}(p)\} [dp/(2\pi)^3].$

[Their proof requires technical assumptions to be made about $\hat{a}(p)$, but it is thought that the result (A.4) holds even when the assumptions do not. Because of the heuristic nature of the present work, we omit further discussion of these technical considerations.]

We now exhibit a unitary operator U_n on $F(L^2(\Lambda_n))$ such that $\rho_n' = U_n^* \rho_n U_n$ is a density operator on $F(L^2(\Lambda_n))$ for which (at least heuristically)

$$\mu(h) = \lim_{n \rightarrow \infty} \text{tr}^{(n)} W(h)\rho_n' \tag{A.5}$$

As in Section 4 we use subscripts to denote the restriction of the functions $\theta(p)$, $\phi(p)$, etc., to a finite-volume index set [corresponding to the eigenvalues of the Laplacian in $L^2(\Lambda_n)$ with periodic boundary conditions]. Let

$$V_n = \exp\left[i \sum \theta_k J_k^{(n)}\right] \tag{A.6}$$

where

$$J_k^{(n)} = \frac{1}{2}i(e^{i\phi_k} a_k^* a_{-k}^* - e^{-i\phi_k} a_k a_{-k})$$

then (compare with Solomon⁽²⁰⁾), for $h \in L^2(\Lambda_n)$

$$V_n W(h) V_n^* = W(Rh)$$

So that $\lim_{n \rightarrow \infty} \text{tr}\{W(h)V_n^* \rho_n V_n\} = \mu_D(Rh)$. Thus for the case $\alpha = 0$, we may take $U_n = V_n$.

Now when $\alpha \neq 0$ we define $\gamma_n \in L^2(\Lambda_n)$ by

$$\gamma_n(x) = i\sqrt{2} \alpha \chi_n(x)$$

where χ_n is the characteristic function of Λ_n ; then

$$W(\gamma_n)W(h)W(-\gamma_n) = \{\exp[(i/\sqrt{2})(\alpha\langle h, \chi_n \rangle + \bar{\alpha}\langle \chi_n, h \rangle)]\}W(h)$$

So take $U_n = V_n W(\gamma_n)$ and $\rho_n' = U_n^* \rho_n U_n$. Then (A.5) holds and

$$S(\rho_n') = -\text{tr}^{(n)}(\rho_n' \log \rho_n') = -\text{tr}^{(n)}(\rho_n \log \rho_n) = S(\rho_n)$$

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