

# THE BOSE FLUID\*†

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## I. Introduction

Many years ago helium was liquified and it became apparent that its weird properties were a manifestation of quantum mechanics in bulk. These macroscopic quantum effects were far more profound and much more baffling than something comparatively simple like the depressed specific heats of solids at low temperatures. Early attempts at understanding such a quantum liquid were largely unsuccessful. On the one hand, not enough mathematical experience and sophistication were available to know what really to look for and try to calculate. On the other hand, even such a relatively simple calculation as the ground state energy was beset with enormous computational difficulties, for this energy is the difference between a large, positive kinetic energy and a large, negative potential energy – both of which resist a simple classical approximation. This latter difficulty still plagues calculations on solid helium, but we are learning to overcome it for not too dense systems, possibly including liquid helium at low pressure.

Faced with this failure, theorists retreated into the corner of low density gases with weak interactions. The systematic and more or less correct treatment of this problem was given by Bogoliubov [1] in 1947. Since that time we have been working our way out of the corner and today the understanding of the liquid is hoving into view. To be sure, there have been attempts in the past to calculate the thermodynamic properties of liquid and solid helium, but in view of the fact that we are still not overconfident about even the low-lying states of the system such calculations can hardly be the final word on the subject.

Humility, therefore, requires that we acknowledge that our mathematics is still some distance behind physical reality and hasty calculations and surmises cannot make it otherwise. Accordingly, these lectures will view the Bose gas for what it is – a chapter in applied mathematics. As such it has its own intrinsic mathematical interest and it is not without its share of elegance. In the near future, hopefully, it will be an introduction to a proper theory of the quantum liquid, but until then we must be cautious in inferring properties of the liquid from what we learn about the gas. Moreover, so much has been written about the Bose gas that it would be presumptuous to try to review everything. The presentation here must therefore of necessity be very much an individual point of view requiring no apology for its omissions.

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## II. The Bogoliubov Theory

Almost all work in the field has its genesis in Bogoliubov's 1947 paper and we shall begin with a brief summary of its main features. His theory is important because it set us on the right track. But of equal importance is understanding, with a little hindsight, the failures of the theory, for its success led to a regrettable tendency to take its predictions as gospel. Moreover, like many great approximation schemes in mathematical physics, the first order approximation is qualitatively correct in a certain regime (weak coupling). Attempts to push out of this regime through higher approximations have led to great difficulties. Having learned the predictions of the theory, therefore, we should be prepared to have to seek a new method in order to understand intermediate and strong coupling.

The basic Hamiltonian  $H$  of the problem is

$$H = -(\hbar^2/2m) \sum_{i=1}^N \nabla_i^2 + \frac{1}{2} \sum_{i \neq j} v(\underline{\mathbf{r}}_i - \underline{\mathbf{r}}_j) \quad (\text{II.1})$$

wherein  $v$  is the two-body potential (no one has yet considered systems with more-body forces),  $\underline{\mathbf{r}}_i$  is the coordinate of the  $i^{\text{th}}$  particle, and  $N$  is the number of bosons. The potential  $v$  is necessarily symmetric (i.e.,  $v(\underline{\mathbf{x}}) = v(-\underline{\mathbf{x}})$ ), but it is not necessary that it be spherically symmetric, although this assumption is generally made. The scene of action is a box of volume  $V = L \times L \times L$  and  $\rho = N/V$  is the density of particles. We are interested in the bulk limit:  $N \rightarrow \infty$  with  $\rho = \text{constant}$ .

The first question that arises is that of boundary conditions, and this is intimately connected with the question of extensivity (or saturation in the terminology of nuclear physics). The ground state energy,  $E_0$ , is said to be extensive if it is of the form  $E_0 = N \times \text{function}(\rho)$ . Similarly, extensivity is defined for the free energy,  $F$ , at some non-zero temperature. The system is said to be extensive if both  $E_0$  and  $F$  are. Unfortunately, necessary and sufficient conditions on  $v$  that the system be extensive are far from known, but one can prove extensivity for a wide class of potentials. For some of these, in turn, one can further show that  $E_0$  and  $F$  are independent of boundary conditions (to leading order in  $N$ ), provided they are fixed homogeneous conditions. We shall assume that our  $v$  is of this kind and shall use periodic boundary conditions which, while they may be somewhat unphysical, are mathematically most convenient. They state that if  $\psi(\underline{\mathbf{r}}_1, \dots, \underline{\mathbf{r}}_N)$  be an eigenfunction of  $H$  and if  $\underline{\mathbf{r}}_j$  (for all  $j$ ) be on the wall of the box (so that  $\underline{\mathbf{r}}_j = (x, y, 0)$  for example), then the value of  $\psi$  on the opposite wall ( $\underline{\mathbf{r}}_j = (x, y, L)$ ) must be the same as on the first wall. This is to be true for all values of  $\underline{\mathbf{r}}_k$  ( $k \neq j$ ), and a similar condition is imposed on the normal derivative of  $\psi$ .

Periodic conditions can *always* be imposed, but they become *useful* only if  $H$  can be periodically extended to all of space. This in turn requires that  $v(\underline{\mathbf{r}}_1 - \underline{\mathbf{r}}_2)$  be periodic in  $\underline{\mathbf{r}}_1$  and  $\underline{\mathbf{r}}_2$ , which means, in effect, that  $v$  must depend upon  $L$ . Thus, the one-dimensional potential  $v(x_2 - x_1) = \exp(-\gamma|x_2 - x_1|)$  is not periodic for  $x_1$  and  $x_2$  in  $(0, L)$ , but it can be replaced by  $\exp(-\gamma|x_2 - x_1|) + \exp(-\gamma L + \gamma|x_2 - x_1|)$  which is periodic in this

region. It can then be periodically extended to all of space and one can show that the addition to  $v$  will not affect  $E_0$  or  $F$  in the bulk limit.

The virtue of having  $H$  periodic is that one can trivially show that  $\psi(\underline{\mathbf{r}} + \underline{\mathbf{a}})$  is an eigenfunction with the same energy as  $\psi$  (by this we mean that any constant vector  $\underline{\mathbf{a}}$  is added to all coordinates). Since all irreducible representations of the translation group are one-dimensional, every eigenfunction *can be* chosen to have a constant total momentum, i.e.,

$$P\psi = -i\hbar \left( \sum_{i=1}^N \nabla_i \right) \psi = \underline{\mathbf{p}}\psi \quad (\text{II.2})$$

where  $\underline{\mathbf{p}}$  is a real vector. Another advantage is that for  $\underline{\mathbf{r}}_1$  and  $\underline{\mathbf{r}}_2$  in  $V$ , the potential can be written as

$$v(\underline{\mathbf{r}}_2 - \underline{\mathbf{r}}_1) = V^{-1} \sum_{\underline{\mathbf{k}}} \nu(\underline{\mathbf{k}}) e^{i\underline{\mathbf{k}} \cdot (\underline{\mathbf{r}}_2 - \underline{\mathbf{r}}_1)} \quad (\text{II.3})$$

where the  $\underline{\mathbf{k}}$  are vectors of the form  $(2\pi/L)(n_1, n_2, n_3)$ , (the  $n_j$  are integers). The point here is that any potential can always be written as a double Fourier series, but the series is diagonal as in (II.3) only when  $v$  is periodic. The Fourier transform is given by

$$\nu(\underline{\mathbf{k}}) = \int_V v(\underline{\mathbf{x}}) e^{-i\underline{\mathbf{k}} \cdot \underline{\mathbf{x}}} d\underline{\mathbf{x}}. \quad (\text{II.4})$$

Now the essence of the Bogoliubov method is that we go into momentum space. To do this we define

$$\varphi(\underline{\mathbf{k}}_1, \dots, \underline{\mathbf{k}}_N) = \int_V d\underline{\mathbf{r}}_N \cdots \int_V d\underline{\mathbf{r}}_1 \phi(\underline{\mathbf{r}}_1, \dots, \underline{\mathbf{r}}_N) \exp\left(i \sum_{i=1}^N \underline{\mathbf{k}}_i \cdot \underline{\mathbf{r}}_i\right) \quad (\text{II.5a})$$

$$\psi(\underline{\mathbf{r}}_1, \dots, \underline{\mathbf{r}}_N) = V^{-N} \sum_{\underline{\mathbf{k}}_1} \cdots \sum_{\underline{\mathbf{k}}_N} \varphi(\underline{\mathbf{k}}_1, \dots, \underline{\mathbf{k}}_N) \exp\left(-i \sum_{i=1}^N \underline{\mathbf{k}}_i \cdot \underline{\mathbf{r}}_i\right) \quad (\text{II.5b})$$

and the equation  $H\psi = E\psi$  becomes

$$\left[ \sum_{i=1}^N \epsilon(\underline{\mathbf{k}}_i) \right] \varphi(\underline{\mathbf{k}}_1, \dots, \underline{\mathbf{k}}_N) + (1/2V) \sum_{\underline{\mathbf{p}}} \sum_{i \neq j} \varphi(\underline{\mathbf{k}}_1, \dots, \underline{\mathbf{k}}_i + \underline{\mathbf{p}}, \dots, \underline{\mathbf{k}}_j - \underline{\mathbf{p}}, \dots, \underline{\mathbf{k}}_N) \nu(\underline{\mathbf{p}}) = E\varphi(\underline{\mathbf{k}}_1, \dots, \underline{\mathbf{k}}_N) \quad (\text{II.6})$$

where  $\epsilon(\underline{\mathbf{k}}) = (\hbar^2/2m)\mathbf{k}^2$ .

Since we are interested in bosons we require solutions,  $\varphi$ , to (II.6) which are symmetric in  $\underline{\mathbf{k}}_1, \dots, \underline{\mathbf{k}}_N$ . Since  $\varphi$  is symmetric, the sums on  $i$  and  $i \neq j$  in (II.6) are to some extent repetitive and it is convenient to introduce a device to handle automatically the factors of  $N$ ,  $\binom{N}{2}$ , etc. that will continually appear on the left hand side of (II.6).

The device used is to introduce boson creation and annihilation operators. But we wish to emphasize strongly that they are not essential to the theory. They are merely a convenient bookkeeping device. For every  $\underline{k}$  one introduces a creation operator  $a_{\underline{k}}^+$  and its Hermitian conjugate (the annihilation operator)  $a_{\underline{k}}$  which satisfy the following commutation rules:

$$\begin{aligned} \left[ a_{\underline{k}}, a_{\underline{k}'} \right] &= 0 = \left[ a_{\underline{k}}^+, a_{\underline{k}'}^+ \right] \\ \left[ a_{\underline{k}}, a_{\underline{k}'}^+ \right] &= \delta_{\underline{k}, \underline{k}'} \end{aligned} \quad (\text{II.7})$$

The  $\delta$  is a Kroenecker delta since the  $\underline{k}$ 's are discrete. A vacuum state  $|0\rangle$  in a Hilbert space is also introduced such that

$$a_{\underline{k}}|0\rangle = 0 \quad (\text{for all } \underline{k}). \quad (\text{II.8})$$

One can show that the state  $|0\rangle$  is essentially unique and that any state in the Hilbert space is a sum of products of various  $a^+$ 's acting on the vacuum. Next one defines an isomorphism between the functions  $\varphi$  and states  $\Psi$  in the Hilbert space as follows:

$$\Psi = \sum_{\underline{k}_N} \cdots \sum_{\underline{k}_1} \varphi(\underline{k}_1, \dots, \underline{k}_N) a_{\underline{k}_1}^+ \cdots a_{\underline{k}_N}^+ |0\rangle. \quad (\text{II.9})$$

Using (II.7) it is easy to see that knowing  $\Psi$  one can find  $\varphi$ , so that the correspondence is indeed one to one. It is then slightly tedious, but simple, to show that if  $\varphi$  satisfied (II.6) then  $\Psi$  satisfies

$$\mathcal{H}\Psi = \left\{ \sum_{\underline{k}} \in (\underline{k}) a_{\underline{k}}^+ a_{\underline{k}} + (1/2V) \sum_{\underline{k}, \underline{q}, \underline{p}} a_{\underline{k}+\underline{p}}^+ a_{\underline{q}-\underline{p}}^+ a_{\underline{k}} a_{\underline{q}} \nu(\underline{p}) \right\} \Psi = E\Psi. \quad (\text{II.10})$$

Equation (II.10) is the starting point for Bogoliubov's approximation.

Before proceeding it is well to keep in mind certain properties of the  $a_{\underline{k}}$ 's. We define the total number operator

$$\eta = \sum_{\underline{k}} a_{\underline{k}}^+ a_{\underline{k}} \quad (\text{II.11})$$

and the total momentum operator

$$\underline{P} = \hbar \sum_{\underline{k}} \underline{k} a_{\underline{k}}^+ a_{\underline{k}}. \quad (\text{II.12})$$

These commute with  $\mathcal{H}$  and when acting on  $\Psi$  yield  $N$  and  $\underline{p}$  respectively.

Now, consider the state  $a_{\underline{k}}\Psi$ . This state has particle number  $N - 1$  and momentum  $\underline{p} - \hbar\underline{k}$ . We can go back through (II.9) and (II.5) and ask what function this corresponds to in configuration space. The result is

$$a_{\underline{k}}\Psi \iff N \int_V \Psi(\underline{r}_1, \dots, \underline{r}_N) e^{-i\underline{k} \cdot \underline{r}_N} d^3 r_N. \quad (\text{II.13})$$

Likewise, the state  $a_{\underline{k}}^+ \Psi$  has  $N + 1$  particles and momentum  $\underline{p} + \hbar \underline{k}$ . It corresponds to

$$a_{\underline{k}}^+ \Psi \iff (N + 1)V \sum e^{i\underline{k} \cdot \underline{r}_N} \Psi(\underline{r}_1, \dots, \underline{r}_N) \quad (\text{II.14})$$

where the sum is on  $N + 1$  similar terms.

It is also convenient to define density operators which are generalizations of (II.11), namely

$$\rho(\underline{k}) = \sum_{\underline{q}} a_{\underline{k}+\underline{q}}^+ a_{\underline{q}}; \quad (\text{II.15})$$

it conserves particle number and increases the momentum by an amount  $\hbar \underline{k}$ . Its effect in configuration space is given by using (II.13) and (II.14) and is

$$\rho(\underline{k}) \Psi \iff \left( \sum_{j=1}^N e^{i\underline{k} \cdot \underline{r}_j} \right) \Psi(\underline{r}_1, \dots, \underline{r}_N). \quad (\text{II.16})$$

We shall have occasion to use the relations (II.13) to (II.16) later.

Returning to (II.10), the reason for going into momentum space is the following: If there were no interaction then  $\Psi_0 = (N!)^{1/2} (a_0^+)^N |0\rangle$  would be the normalized ground state with energy zero. The interaction  $v$  has the property that it converts a pair of particles with momenta  $\underline{p}$  and  $\underline{q}$  into a pair with momenta  $\underline{p} + \underline{k}$  and  $\underline{q} - \underline{k}$ . The matrix element is  $(1/2V)\nu(\underline{k})$ . Starting with all  $N$  particles having momentum zero (so-called condensed state), we would first get  $(N - 2)$  with momentum zero, together with one pair having momenta  $\underline{k}$  and  $-\underline{k}$ . When the potential is applied again we could get two possibilities: one would be two pairs  $\underline{k}, -\underline{k}$  and  $\underline{q}, -\underline{q}$ ; the other would be a genuine triplet  $\underline{k}, \underline{q}, \underline{r}$ , such that  $\underline{k} + \underline{q} + \underline{r} = 0$ . But the probability of the former relative to the latter would be  $(N - 2)(N - 3)/4$  because there are  $(N - 1)$  particles with zero momentum and only 2 with non-zero momentum. Applying  $v$  over and over again we will ultimately get a finite fraction of triplets, quartets, etc. as well as pairs, but hopefully if the interaction is weak enough we need consider explicitly only pairs in the ground state wave function. Stating this more precisely, we suppose that to a good approximation  $\Psi_0$  is a sum of terms each of which contains several factors like  $a_{\underline{k}}^+ a_{-\underline{k}}^+$ , as well as  $a_0^+$ , acting on  $|0\rangle$ .

Another way of motivating this *ansatz* is to note that in the non-interacting ground state  $n_{\underline{k}} = \langle a_{\underline{k}}^+ a_{\underline{k}} \rangle = N \delta_{\underline{k}, 0}$ , that is to say all the particles are condensed. With a weak interaction we suppose that  $n_0/N$  is still a number of order unity and that the remaining fractions are largely grouped into pairs, for it is only pairs that can give rise to triplets. The idea that  $n_0/N$  is of order unity is called the condensation hypothesis. It need not be true for sufficiently strong interaction and we remark that Girardeau [2] has generalized this concept somewhat.

If  $\Psi$  as given by (II.7) has only pairs (more precisely, for every  $a_{\underline{k}}^+$  with  $\underline{k} \neq 0$ , there is an  $a_{-\underline{k}}^+$ ) then only certain parts of  $H$  result in pair functions when applied to  $\Psi$ . There are three possibilities as far as the interaction is concerned: The first is when all indices

are zero, giving  $(a_0^+)^2(a_0)^2$ ; the second is when two indices are zero, giving  $(a_0^+)^2 a_{\underline{k}} a_{-\underline{k}}$  or  $a_{\underline{k}}^+ a_{-\underline{k}}^+ (a_0)^2$  or  $a_{\underline{k}}^+ a_0^+ a_{-\underline{k}} a_0$ ; the third is when no indices are zero, giving  $a_{-\underline{q}}^+ a_{\underline{q}}^+ a_{\underline{k}} a_{-\underline{k}}$  or  $a_{\underline{k}}^+ a_{\underline{q}}^+ a_{\underline{k}} a_{\underline{q}}$ . Collecting together all such parts of  $H$  we derive the pair Hamiltonian,

$$\begin{aligned}
H_{\text{pair}} = & \frac{1}{2}(n-1)\rho v(0) + \sum_{\underline{k}}' [\epsilon(\underline{k}) + (1/V)N_0\nu(\underline{k})] N_{\underline{k}} \\
& + (1/2V) \sum_{\underline{k}}' \nu(\underline{k}) \left[ \alpha_{\underline{k}}^+ \alpha_0 + \alpha_0^+ \alpha_{\underline{k}} \right] \\
& + (1/2V) \sum_{\underline{k}, \underline{q}}' \nu(\underline{k}) \left[ \alpha_{\underline{q}}^+ \alpha_{\underline{q}-\underline{k}} + N_{\underline{q}-\underline{k}} N_{\underline{q}} \right]
\end{aligned} \tag{II.17}$$

where  $\alpha_{\underline{k}} = a_{\underline{k}} a_{-\underline{k}}$ ,  $N_{\underline{k}} = a_{\underline{k}}^+ a_{\underline{k}}$  and the prime on the summation means we delete the terms  $\underline{k} = 0$  and/or  $\underline{q} = 0$  as well as the term  $\underline{q} = \underline{k}$  in the double summation (note that  $N_0$  and  $\alpha_0$  are operators). In deriving (II.17) we used the fact that  $\eta\Psi = N\Psi$ .

It is important to note that  $H_{\text{pair}}$  has a *double* significance. On the one hand if we can diagonalize it we should have a good approximation to the ground state and low lying states of the system for the reasons mentioned above. On the other hand we have seen that if we take the expectation value of the total  $H$  with respect to *any* state having *only* pairs then  $H_{\text{pair}}$  is the only part of  $H$  that contributes to the final result. Hence, from the variational theorem, the exact ground state energy,  $E_{0,\text{pair}}$ , of  $H_{\text{pair}}$  is a true upper bound to the ground state energy,  $E_0$ , of  $H$ . Moreover, any variational upper bound to  $E_{0,\text{pair}}$  is thus an upper bound to  $E_0$ . It turns out that  $E_{0,\text{pair}}$  can indeed be found if one is prepared to solve a finite set of non-linear integral equations. This can be done in certain limiting cases and has been exploited by Girardeau and Arnowitt, [3, 4, 5, 6].

Basically, what permits us to find the ground state energy of (II.17) in the bulk limit, as well as the free energy for non-zero temperature, is the following observation. What we have in (II.17) are bilinear forms in operators whose expectation values we believe to be extensive. Consider, for instance

$$\sum_{\underline{q} \neq \underline{k}}' N_{\underline{q}} \left( \sum_{\underline{k}}' \nu(\underline{k}) N_{\underline{q}-\underline{k}} \right).$$

The operator in parenthesis (call it  $F_{\underline{q}}$ ) we believe has an expectation value of order  $N$  (call it  $Nf_{\underline{q}}$ ). The root-mean-square fluctuation of  $F_{\underline{q}}$  in the ground state ought to be of order  $\sqrt{N}$ , and if so, replacing  $F$  by  $Nf$  in (II.17) should make no difference to the energy to order  $N$ . It is possible to make this argument more precise [6, 7, 8] by formally expanding the operators about their mean values in a power series in  $N^{-1}$ . The difficulty is that no one has shown that these series converge and they might well not. Nevertheless, the energy (or free energy) obtained under the assumption can be shown to be a genuine variational energy and so is a true upper bound.

Having replaced  $F_{\underline{q}}$  by  $Nf_{\underline{q}}$  we do the same thing with the term corresponding to  $\alpha_{\underline{q}-\underline{k}}$ ,  $N_0$ ,  $\alpha_0$  and  $\alpha_0^+$ . We are then left with a Hamiltonian involving only quadratic expressions in the  $a$ 's and  $a^+$ 's. This can be diagonalized in the standard way. The ground state wave function will then depend upon the  $c$ -numbers  $f_{\underline{q}}$ , etc. as parameters. We then adjust these parameters so that the expectation value of  $F_{\underline{q}}$  is indeed  $Nf_{\underline{q}}$ , etc. This leads to integral equations and it is clear that what we have really done is a self-consistent field calculation that we hope is rigorously correct in the bulk limit.

There is, however, still one difficulty which we have glossed over. If we replace  $\alpha_0$  by a  $c$ -number then the expression  $\alpha_{\underline{k}}^+\alpha_0$  will no longer conserve particles because  $\alpha_{\underline{k}}^+$  always creates two particles. Another way of saying this is that the expectation value of  $\alpha_0$  in the true ground state is, strictly speaking, zero. There are two ways around this difficulty. The first is the method used by Bogoliubov, namely to introduce a chemical potential. We write

$$\begin{aligned} H'_{\text{pair}} &= H_{\text{pair}} - \mu\eta, \\ (\text{or } H' &= H - \mu\eta). \end{aligned} \tag{II.18}$$

We then diagonalize  $H'_{\text{pair}}$  by replacing  $\alpha_0$ , etc. by  $c$ -numbers and in addition to the above consistency conditions we choose  $\mu$  by requiring that  $\langle N \rangle = N$  in the ground state. To calculate the free energy we must use a grand canonical ensemble. This method can be justified to the same extent as in the above discussion. In the second method [6, 9] we redefine operators so that particles are conserved even after the  $c$ -number substitution. Following Kromminga and Bolsterli we introduce operators  $b_{\underline{k}} = a_0^+(N_0 + 1)^{-1/2}a_{\underline{k}}$  and their conjugates. It is then easy to show that  $b_{\underline{k}}^+b_{\underline{q}} = a_{\underline{k}}^+a_{\underline{q}}$  (all  $\underline{k}, \underline{q}$ ) and that  $b_{\underline{k}}b_{\underline{q}}^+ = a_{\underline{k}}a_{\underline{q}}^+$  (if  $\underline{k} \neq 0$  and  $\underline{q} \neq 0$  and if this operator does not act on a state with  $N_0 = 0$ ). An annoying operator such as  $\alpha_{\underline{k}}^+\alpha_0$  is then equal to  $b_{\underline{k}}^+b_{-\underline{k}}^+(N_0(N_0 - 1))^{1/2}$  on any state. Also  $\alpha_{\underline{k}}\alpha_0^+ = (N_0(N_0 - 1))^{1/2}b_{\underline{k}}b_{-\underline{k}}$  and  $\alpha_{\underline{q}}^+\alpha_{\underline{k}} = b_{\underline{q}}^+b_{-\underline{q}}^+b_{\underline{k}}b_{-\underline{k}}$ . In addition one easily proves that the  $b$ 's satisfy the same commutation relations (II.7) as the  $a$ 's (provided  $\underline{k} \neq 0$  and also the  $b$ 's conserve particle number (i.e., they commute with  $N$ ). Thus either  $H_{\text{pair}}$  or  $H$  may be rewritten in terms of the  $b$ 's which behave just like the  $a$ 's except that now any  $c$ -number substitution will automatically preserve particle number. All the sums explicitly exclude  $\underline{k} = 0$ , so the only way in which  $a_0$  and  $a_0^+$  appear in the new Hamiltonian is through  $N_0$ . But  $N_0$  may be eliminated in favor of  $b$ 's by the relation

$$N_0 = N - \sum' a_{\underline{k}}^+a_{\underline{k}} = N - \sum' b_{\underline{k}}^+b_{\underline{k}}.$$

Now the particle number appears explicitly in  $H$ , which it did not before (although it did appear in  $H_{\text{pair}}$ ), and a term such as  $N_0N_{\underline{k}}$  becomes now a quartic form in the  $b$ 's.

This is a neat trick to overcome the problem of particle conservation that plagued previous authors (such as Bogoliubov). It obviates the need for lengthy (and unrigorous) arguments that method (II.18) gives the correct answer in the bulk limit. Needless to say, however, in every calculation anyone has ever done, the more cumbersome method 2 does indeed give the same result as method 1 and we shall therefore use the latter.

Bogoliubov did not actually use  $H_{\text{pair}}$ . He made a further simplification which consisted in deleting the last sum in (II.17) on the grounds that these terms are quadratic pair operators and so may be expected to be small in comparison with the first two sums. This omission unfortunately destroys the bounding property of the Hamiltonian, but it does turn out that for sufficiently weak interaction Bogoliubov's ground state energy is indeed an upper bound to  $E_0$  as was to be expected. To that extent his simplification is justified.

We begin by replacing  $N_0, \alpha_0$  and  $\alpha_0^+$  by a (common)  $c$ -number,  $N_0$ . For weak interaction we expect this number to be close to  $N$ , and indeed it turns out to be so. The correction,  $N - N_0$ , (the so-called ground state depletion) gives a higher order contribution to  $E_0$  — a correction which is of the same order as that caused by the neglected quartic terms. Since the qualitative results do not depend upon the ground state depletion effect, we shall simply take  $N_0$  to be  $N$ . We thus have Bogoliubov's Hamiltonian (replacing  $N - 1$  by  $N$  in the bulk limit):

$$H_B = \frac{1}{2}N\rho\nu(0) + \sum_{\underline{k}}' f(\underline{k})a_{\underline{k}}^+a_{\underline{k}} + \frac{1}{2}g(\underline{k})(a_{\underline{k}}a_{-\underline{k}} + a_{-\underline{k}}^+a_{\underline{k}}^+), \quad (\text{II.19})$$

where

$$\begin{aligned} f(\underline{k}) &= \epsilon(\underline{k}) + \rho\nu(\underline{k}) \\ g(\underline{k}) &= \rho\nu(\underline{k}). \end{aligned} \quad (\text{II.20})$$

This Hamiltonian is a quadratic form in the  $a$ 's and may be diagonalized in the usual way. The transformation that accomplishes this is  $\exp(iS)$ , where

$$iS = \frac{1}{2} \sum_{\underline{k}}' (a_{\underline{k}}^+a_{-\underline{k}}^+ - a_{\underline{k}}a_{-\underline{k}}) \psi(\underline{k}), \quad (\text{II.21})$$

so that

$$a_{\underline{k}} \rightarrow b_{\underline{k}} = e^{iS}a_{\underline{k}}e^{-iS} = a_{\underline{k}} \cosh \psi(\underline{k}) - a_{\underline{k}}^+ \sinh \psi(\underline{k}). \quad (\text{II.22})$$

If we now choose

$$\tanh 2\psi(\underline{k}) = g(\underline{k})/f(\underline{k}), \quad (\text{II.23})$$

then

$$\begin{aligned} H_B \rightarrow H'_B &= \frac{1}{2}N\rho\nu(0) - \frac{1}{2} \sum_{\underline{k}}' f(\underline{k}) - (f(\underline{k})^2 - g(\underline{k})^2)^{1/2} \\ &+ \sum_{\underline{k}}' b_{\underline{k}}^+b_{\underline{k}}\epsilon'(\underline{k}), \end{aligned} \quad (\text{II.24a})$$

where

$$\epsilon'(\underline{k}) = [\epsilon(\underline{k})^2 + 2\epsilon(\underline{k})\rho\nu(\underline{k})]^{1/2}. \quad (\text{II.24b})$$

Notice that this transformation is impossible unless  $|g| < |f|$ . It is also necessary that  $f(\underline{k}) > 0$  for all  $\underline{k}$ . Unless these two conditions are fulfilled the Hamiltonian has no ground state and it would then be unphysical. This means that  $\nu(\underline{k})$  cannot be too negative (attractive), but it can be as repulsive as we please.



Now let us consider the implications of (II.24). Since the  $b$ 's are bosons, the ground state wave function is given by  $\Psi'_0$ , the vacuum of the  $b$ 's, i.e.,

$$b_{\underline{k}}\Psi'_0 = 0 \quad \text{all } \underline{k} \neq 0. \quad (\text{II.25})$$

The ground state energy is then simply

$$E_0 = \frac{1}{2}N\rho\nu(0) - N(4\pi^2\rho)^{-1} \int_0^\infty k^2 dk \{ \epsilon(k) + \rho\nu(k) - (\epsilon(k)^2 + 2\epsilon(k)\rho\nu(k))^{1/2} \}, \quad (\text{II.26})$$

where we have gone to the bulk limit by replacing

$$\sum_{\underline{k}} \quad \text{by} \quad (L/2\pi)^3 \int d^3k,$$

and have further assumed that the problem is spherically symmetric. At first sight it appears that the second term in (II.26) is order  $\rho^{-1}$ , thereby violating our intuition that it should be small for low density. This is not so because as  $\rho \rightarrow 0$  the integrand itself vanishes. To see what happens let us assume that  $\nu(\underline{k})$  goes to zero for large  $\underline{k}$  faster than  $k^{-1}$ . Let us rewrite the integral in (II.26) as follows:  $I = I_1 + I_2$  where

$$I_1 = \int_0^\infty k^2 dk \{ \alpha^2 k^2 + \rho\nu(k) - (\alpha^4 k^4 + 2\alpha^2 k^2 \rho\nu(k))^{1/2} - \nu(k)^2 / 2\alpha^2 k^2 \}$$

and

$$I_2 = \rho^2 / 2\alpha^2 \int_0^\infty \nu(k)^2 dk \quad (\text{II.27})$$

where  $\alpha^2 = \hbar^2/2m$ . The integral  $I_2$  certainly converges. In  $I_1$  the integrand goes to zero faster than  $k^{-3}$  and is absolutely convergent. We see that as  $\rho \rightarrow 0$  only very small  $k$  will play a role. Let us assume that  $\nu(k)$  is smooth for small  $k$  and that  $\nu(0) \neq 0$ . We may then replace  $\nu(k)$  by  $\nu(0)$  everywhere and the integral is then elementary.

Let us define

$$a_0 = (8\pi\alpha^2)^{-1}\nu(0),$$

and

$$a_1 = -(2\pi^2)^{-1}(8\pi\alpha^2)^{-2} \int d^3k \nu(k)/k^2. \quad (\text{II.28})$$

The result for  $E_0$  is then

$$E_0 = 4\pi N\rho(\hbar^2/2m)(a_0 + a_1) + 4\pi N\rho(\hbar^2/2m)a_0(128/15\sqrt{\pi})(\rho a_0^3)^{1/2}. \quad (\text{II.29})$$

What is the significance of this result? If we had neglected the integral in (II.26) we would have gotten  $E_0 = \frac{1}{2}N\rho\nu(0) = 4\pi N\rho\hbar^2(2m)^{-1}a_0$ . We may call this the zeroth order Bogoliubov approximation. But notice that it really does not depend upon Planck's constant and the mass – a conclusion that is certainly meaningless because if the mass were infinite  $E_0$  would be equal to the minimum potential energy which is not necessarily  $N\rho\nu(0)$ . The integral term comes to the rescue, however. We had naively expected it to

contribute a higher power of the density than  $\rho$ , but it in fact contributed a term of the same order as the zeroth approximation – namely  $\rho a_1$ . This term now truly depends on  $\alpha^2$ . If we look a little closer we notice that  $a_0 + a_1$  are just the first two terms in the Born series for the scattering length. That is to say, if we consider the zero-energy scattering equation

$$\left[ -\alpha^2(\nabla_1^2 + \nabla_2^2) + v(\mathbf{r}_1 - \mathbf{r}_2) \right] \psi(\mathbf{r}_1 - \mathbf{r}_2) = 0, \quad (\text{II.30})$$

the asymptotic behavior of  $\psi$  is  $\psi \sim 1 - a/|r_1 - r_2|$ . The quantity  $a$  is defined to be the scattering length. (From (II.30), it is also given by  $a = (8\pi\alpha^2)^{-1} \int v(r)\psi(r)d^3r$ ). We therefore suspect, despite what we had originally thought, that Bogoliubov's method is really an expansion in the density *and* in the potential  $v$ . It is not truly a low density expansion unless the potential is very weak. This idea has been confirmed by doing perturbation theory on the parts of  $H$  not included in (II.19), using our wave function previously found as the starting point. It is indeed true that higher order corrections give contributions proportional to  $\rho$ . They can be recognized as constituting the full Born series for the scattering length. Likewise, the second term in (II.19) (which came from  $I_1$ ) looks like it is the beginning of a similar series. Hence we are tempted to write

$$E_0 = (\hbar^2/2m)4\pi N\rho a \left\{ 1 + (128/15\sqrt{\pi})(\rho a^3)^{1/2} + \dots \right\} \quad (\text{II.31})$$

and presumably we now have the beginning of a genuine series in the density *alone*.

Nevertheless, it is important to note that what started out to be a very reasonable hypothesis – the pair approximation – is invalid as a density expansion. Even the full pair Hamiltonian (II.17) will not give (II.31)<sup>4</sup>. The trouble was that we had thought we were making some sort of cluster expansion as one does in classical statistical mechanics. This may be a reasonable thing to do, but it is essential that we treat the two-body interaction fully and completely, and this cannot be done very easily by perturbation theory. We shall discuss this matter more fully later but for the present let us make some attempt to justify (II.31).

The expression (II.31) for  $E_0$  has not yet been proved to be correct. But it is very reasonable. For one thing the first term is simply the number of pairs of particles,  $\frac{1}{2}N(N-1)$ , times the ground state energy of two particles in a large box,  $\alpha^2 8\pi a/V$ . (We shall show this later.) The second term is harder to understand. There is no analogue of it for two particles and it is clearly some sort of quantum-mechanical correlation effect (we shall also return to this later). Nevertheless, if the true second order term in the density is of the form  $\rho^{3/2}$  given by (II.31) it must, for dimensional reasons, be proportional to a (length)<sup>5/2</sup>. But the only relevant length at low energy is the scattering length.

Having considered the ground state energy let us return to the second term in (II.24). Apart from the fact that  $\epsilon'$  is different from  $\epsilon$ , this spectrum of  $H_B$  is the same as for the original Hamiltonian without interaction. Any number,  $n$ , of Bosons (or phonons) of any momentum  $\mathbf{k}$  can be excited independently of each other with energy  $n\epsilon'(\mathbf{k})$ .

The important difference is that for low momentum  $\epsilon(\underline{k})$  is proportional to  $k^2$ , whereas  $\epsilon'(k) = [2\alpha^2\rho\nu(0)]^{1/2}k$ . This new spectrum is definitely phonon-like (without an energy gap) and we expect that it is associated with sound propagation. If so, the velocity of sound would be

$$v_s = \lim_{k \rightarrow 0} (1/\hbar k)\epsilon'(k) = (\rho\nu(0)/m)^{1/2} = (\hbar/m)(4\pi\rho a_0)^{1/2}. \quad (\text{II.32})$$

We can check this result by using the fundamental definition of the velocity of sound in terms of the compressibility,

$$v_s = \left[ m^{-1}(\partial/\partial\rho)\rho^2\partial/\partial\rho(E_0/N) \right]^{1/2}.$$

Using (II.29) this gives

$$v_s = \hbar/m \left[ 4\pi\rho(a_0 + a_1) + 64\rho a_0(\pi\rho a_0^3)^{1/2} \right]^{1/2}. \quad (\text{II.33})$$

There is agreement between (II.33) and (II.32) and we are led to surmise as before that the correct expression to the first two orders in the density is

$$v_s = \hbar/m \left[ 4\pi\rho a(1 + (16/\pi)(\pi\rho a^3))^{1/2} \right]^{1/2}. \quad (\text{II.34})$$

It is interesting to note that the expression (II.33), obtained from  $E_0$ , is more accurate than (II.32) obtained from the phonon spectrum. This is curious since we would have expected that whatever accuracy was inherent in  $H_B$ , it should be the same for  $\epsilon'(k)$  as for  $E_0$ .

Another important feature of the boson type spectrum that we have obtained is that while there may be something qualitatively correct about it, it is much too simple to be taken literally. It is hardly to be expected that the spectroscopy of the true spectrum will fall into a pattern associated with independent normal modes. It must be more complicated and indeed higher order perturbation theory indicates that the phonons interact with one another. There are two ways to describe this state of affairs. The usual way is to say that the interaction causes the phonons to decay with a finite lifetime. The second way is to say that the unitary transformation leading to the  $b_{\underline{k}}$ 's was only a partial diagonalization of the full Hamiltonian which must always have real eigenvalues since it is Hermitian. In other words the true energy spectrum and eigenfunctions are simply more complicated than we have so far envisaged. Still, the independent phonon idea may be justified provided we do not excite too many of them – this would be true at low temperature.

We might, however, anticipate a difficulty of another sort. The Bogoliubov approximation is essentially perturbation theory, albeit of a sophisticated sort, because it assumes that the system does not change drastically when we switch on the interaction. Were it otherwise  $H_B$  could not be justified. It is generally held that if we imagine  $v(\underline{r})$  to be proportional to a coupling constant  $\lambda$ , then after passing to the bulk limit there will

be an analytic singularity in  $\lambda$  (in  $E_0(\lambda)$  for example) at  $\lambda = 0$ . A Bose gas with an interaction, however weak, may be qualitatively different from the non-interacting gas. If this is so then we might expect new types of normal modes (or phonons) that have no counterpart for free Bosons. Indeed, when we examine a one-dimensional model later we shall see that to the extent that the spectrum is phonon like, it can best be described by two separate  $\epsilon(k)$  curves, not one.

Where might this second phonon spectrum come from? In the Bogoliubov ground state most of the particles are still condensed at  $\underline{k} = 0$  and there is a small (but non-zero) background of particles with  $\underline{k} \neq 0$ . The Bogoliubov phonons are qualitatively the same as the free “phonons”; particles are excited out of  $\underline{k} = 0$  sea. The renormalized energy  $\epsilon'$  comes about because the  $\underline{k} = 0$  background now has to readjust itself. It is quite possible that there is another type of excitation which would be associated directly with excitation of the  $\underline{k} \neq 0$  background. Similar suggestions have been made before (see [10]).

A physical reason for the possibility of another spectrum is the critical velocity failure of current theory. Some time ago Landau gave an argument to account for superfluidity based on the phonon hypothesis. Suppose one has a mass,  $M$ , of fluid moving with velocity  $v$  and momentum  $P = Mv$ . Let us suppose that in the rest system of the fluid it is in its ground state and hence has momentum equal to zero. In the laboratory system the fluid will have energy  $E_1 = E_0 + P^2/2M$ . If the fluid interacts with the walls of the channel in which it is moving it must *lose* energy and momentum, so that its energy is now  $E_1 - \Delta$  and its momentum is  $P - \delta$ . If we make a Galilean transformation with velocity  $-v$ , the energy will be  $E_0 - \Delta + \delta v$  and the momentum will be  $-\delta$ . Now consider the  $\epsilon'(k)$  curve. It is presumably possible to draw a straight line  $\epsilon''(k) = sk$  such that  $\epsilon''$  is just tangent to, and otherwise always under,  $\epsilon'(k)$  (we could not do this for free bosons unless  $s$  were to be zero). This line defines a velocity  $v_c = s/\hbar$ . In order to impart momentum  $\delta$  to the system the energy must therefore increase at least by an amount  $v_c\delta$ . In the above example, however, the energy increased by an amount less than  $v\delta$ . The conclusion is that if the velocity of the fluid is less than  $v_c$ , the fluid will not be able to lose any momentum to the walls of the channel, and hence it will display superfluid behavior.

We would expect from the Bogoliubov solution that  $v_c$  should be of the order of magnitude of the sound velocity. Experimentally,  $v_c$  is found to be very much less than  $v_s$ , and it is also found to depend sensitively on the diameter of the channel – especially for very narrow channels. It is clear that another type of excitation, with an energy much less than that given by (II.24b), could account for the discrepancy. Indeed, we will find such a spectrum in the one-dimensional model to be analyzed later.

Finally, we wish to emphasize another important feature of Bogoliubov’s analysis, namely that the excitation spectrum is intimately connected with the ground state wave function. This fact is important because it shows that calculating the ground state energy is not merely an academic exercise. Although  $E_0$  is a rather unimportant number (it can be measured, however) it is manifestly clear that we cannot really hope to be

able to predict the dynamics of this complicated system unless we are in a position to calculate the much simpler quantity,  $E_0$ , along with some of the important properties of the ground state, such as the two-particle correlation function which we shall discuss later.

For future reference we shall write down the Bogoliubov wave function  $\Psi'_0 = e^{-iS}\Psi_0$ .  $S$  is given by (II.21), but that expression is needlessly complicated because it contains  $a_{\underline{k}}a_{-\underline{k}}$  which vanishes when applied to  $|0\rangle$ . A little algebra will show that

$$\Psi'_0 = \exp \left\{ \sum' h(\underline{k}) a_{\underline{k}}^+ a_{-\underline{k}}^+ \right\} \Psi_0 \quad (\text{II.35})$$

where

$$\begin{aligned} h(\underline{k}) &= -\frac{1}{2g(\underline{k})} \left\{ (f(\underline{k}) - (f(\underline{k})^2 - g(\underline{k})^2)^{1/2}) \right\} \\ &= -\frac{1}{2} - \frac{1}{2}(\rho\nu(\underline{k}))^{-1}(\epsilon(\underline{k}) - \epsilon'(\underline{k})). \end{aligned} \quad (\text{II.36})$$

In (II.35) the state  $\Psi'_0$  is not normalized, and  $\Psi_0$  means the free particle ground state, i.e.,  $(a_0^+)^N|0\rangle$ . The difficulty with  $\Psi'_0$ , of course, is that it does not have a definite particle number. One way to fix this would be to replace the  $a^+$ 's by the Kromminga, Bolsterli  $b^+$ 's. This would not alter  $E_0$ . A simpler procedure would be to multiply each  $a_k^+$  by  $N^{-1/2}a_0$ . If we then write out the first few terms in (II.35) we get

$$\begin{aligned} \Psi'_0 &= (a_0^+)^N|0\rangle + N \sum'_{\underline{k}} h(\underline{k}) a_{\underline{k}}^+ a_{-\underline{k}}^+ (a_0^+)^{N-2}|0\rangle \\ &\quad + N^2/2! \sum'_{\underline{k}, \underline{q}} h(\underline{k}) h(\underline{q}) a_k^+ a_{-k}^+ a_q^+ a_{-q}^+ (a_0^+)^{N-4}|0\rangle \\ &\quad + \dots \end{aligned} \quad (\text{II.37})$$

In essence, (II.37) may be taken as the statement of the Bogoliubov *ansatz*, just as much as (II.19), for the most general wave function we could construct would be

$$\begin{aligned} \Psi &= (a_0^+)^N|0\rangle + N \sum'_{\underline{k}} h^{(2)}(\underline{k}) a_{\underline{k}}^+ a_{-\underline{k}}^+ (a_0^+)^{N-2}|0\rangle \\ &\quad + N \sum'_{\underline{k}, \underline{q}} h^{(3)}(\underline{k}, \underline{q}) a_{\underline{k}}^+ a_{\underline{q}}^+ a_{-\underline{k}-\underline{q}}^+ (a_0^+)^{N-3}|0\rangle \\ &\quad + N^2/2! \sum'_{\underline{k}, \underline{q}, \underline{p}} h^{(4)}(\underline{k}, \underline{q}, \underline{p}) a_{\underline{k}}^+ a_{\underline{q}}^+ a_{\underline{p}}^+ a_{-\underline{k}-\underline{q}-\underline{p}}^+ (a_0^+)^{N-4}|0\rangle \\ &\quad + \dots \end{aligned} \quad (\text{II.38})$$

(Notice that there can be no linear term because of momentum conservation.) The quadratic term in (II.37) is quite general, but (II.37) has no triplet or other odd power terms. Also the quartic term is of a very special kind. The Bogoliubov *ansatz* is that

$$h^{(4)}(\underline{k}, \underline{q}, \underline{p}) = \delta_{\underline{p}+\underline{k}} h^{(2)}(\underline{k}) h^{(2)}(\underline{q}), \quad (\text{II.39})$$

and so on for succeeding even powers. We could just as well have derived the Bogoliubov results by starting with (II.37) instead of with  $H_B$  in (II.19). We shall find this alternative point of view useful in discussing the hard sphere Bose gas.

### III. The Hard Core Potential

If we accept the idea that the pair approximation more or less correctly describes the ground state and low-lying states of a Bose gas with finite range interactions at low density, we are forced to admit that there is a serious gap in our understanding. We arrived at a physically meaningful result, (II.31), for  $E_0$  by starting with (II.29) as a first approximation and then making an educated guess about higher order corrections. Equation (II.29) in turn came from the Schrödinger equation, (II.10), in momentum space, wherein it was essential that the potential have a Fourier transform.

In this section we shall consider the hard core potential

$$\begin{aligned} v(r) &= \infty & \text{for } r < a \\ &= 0 & \text{for } r > a. \end{aligned} \tag{III.1}$$

Such a potential clearly has no Fourier transform, yet despite this fact we are inclined to believe that (II.31) correctly gives  $E_0$  at low density (note that the scattering length in this case is synonymous with the core diameter,  $a$ ). We shall now show how the pair approximation may be used to derive this result.

There are two reasons for being interested in the hard core potential. The first is that the potential between two helium atoms may be well described by a hard core of about 2.6 Å diameter plus an attractive tail. Clearly we cannot understand helium unless we can first understand the hard core by itself. The second reason is that of all finite range potentials we may devise (except those that are infinitesimally small), the hard core is undoubtedly the simplest. If we could not solve this problem then doubt would be cast on the previous result, (II.31).

The simplicity of the problem stems from two facts. Firstly, it is easy to demonstrate that for the hard core potential all of  $E_0$  is kinetic energy – the potential energy vanishes. Secondly, the wave function vanishes whenever two particles overlap. These two facts are given to us without any calculation and they can be of the greatest importance if we use them correctly. For a very weak potential, on the other hand, the situation is reversed. To leading order in the coupling constant,  $\lambda$ , the wave function is unity everywhere and all the energy is potential (we see this clearly from (II.29)). These two facts lie at the basis of the perturbation theory of Section II, but they are true only in the limit  $\lambda \rightarrow 0$ . As the potential increases, the proportion of kinetic energy in  $E_0$  increases and the wave function becomes more and more depressed in the overlap region. We never know precisely how much it is depressed, but our conjecture, which was really at the basis of (II.31) is that for low density and depression in the wave function is the same as for the zero energy scattering function, (II.30). Even so, we could only estimate the depression if three, four, or more particles overlapped. Finally, for the hard core case we again achieve the same simplicity as for the infinitesimal potential – the wave function

is exactly zero no matter how many particles overlap and no matter what the density may be.

To begin, ([11]) we define the domain  $R$  to be the full  $3N$  dimensional coordinate space of the particles in the volume  $V$ , and we define  $W$  to be the “allowed” region wherein no two particles overlap. The Schrödinger equation thus reads:

$$-\alpha^2 \sum_{i=1}^N \nabla_i^2 \psi(\underline{\mathbf{r}}_1, \dots, \underline{\mathbf{r}}_N) = E\psi \text{ (inside } W) \quad (\text{III.2})$$

with the boundary condition that  $\psi = 0$  on the common boundary of  $W$  and  $R - W$ , together with the usual periodic boundary condition on  $R$ . At once we see the peculiarity of the potential. The Schrödinger equation does not define  $\psi$  everywhere in  $R$ , as it would for a finite potential; the definition of  $\psi$  in  $R - W$  is quite arbitrary.

We shall use the physically reasonable definition

$$\psi \equiv 0 \text{ in } R - W. \quad (\text{III.3})$$

Equations (III.2) and (III.3) now define a continuous finite wave function everywhere in  $R$ . It is also everywhere differentiable, although the derivative is discontinuous on the boundary of  $W$  and  $R - W$ .

We define the Fourier transform of  $\psi$  in the same way as in (III.6), but because of (III.3) we have the additional relation

$$\varphi(\underline{\mathbf{k}}_1, \dots, \underline{\mathbf{k}}_N) = \int_W \psi(\underline{\mathbf{r}}_1, \dots, \underline{\mathbf{r}}_N) e^{i\Sigma \underline{\mathbf{k}}_i \cdot \underline{\mathbf{r}}_i} d^{3N}r. \quad (\text{III.4})$$

Now let us multiply both sides of (III.2) by

$$U = \exp\left(i \sum_1^N \underline{\mathbf{k}}_i \cdot \underline{\mathbf{r}}_i\right)$$

and integrate over  $W$  *only* (it would be a mistake to integrate (III.2) over  $R$ ). By virtue of (III.4), the right hand side is equal to  $E\varphi(\underline{\mathbf{k}}_1, \dots, \underline{\mathbf{k}}_N)$ . The left hand side consists of  $N$  terms, of which a typical one is

$$I_1 = -\alpha^2 \int_W (\nabla_1^2 \psi) U d^{3N}r. \quad (\text{III.5})$$

To compute  $I_1$  we must proceed cautiously. We do the integrals over  $\underline{\mathbf{r}}_2, \dots, \underline{\mathbf{r}}_N$  last. The integral over  $\underline{\mathbf{r}}_1$  may be transformed by integrating by parts:

$$I_1 = \alpha^2 \int_W (i\underline{\mathbf{k}}_1 \cdot \nabla_1 \psi) U d^3r_N - \alpha^2 \int d^3r_N \cdots \int d^3r_2 \int_S (\underline{\mathbf{n}} \cdot \nabla_1 \psi) U dS. \quad (\text{III.6})$$

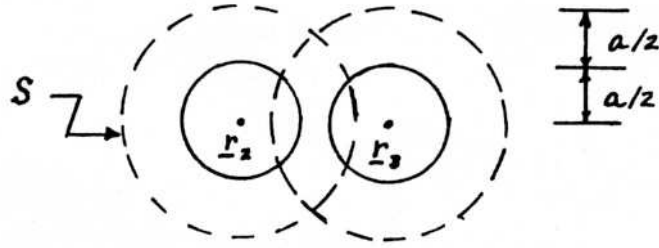
In (III.6) the surface  $S$  means the following: We hold  $\underline{\mathbf{r}}_2, \dots, \underline{\mathbf{r}}_N$  fixed and move  $\underline{\mathbf{r}}_1$  in such a way that it is always in contact with at least one other particle. Suppose for the moment that the other  $N - 1$  particles are all farther apart from each other than a distance  $2a$ . Then  $S$  would consist of  $N - 1$  parts, each associated with a sphere of

radius  $a$  about each of the fixed particles. The surface integral in (III.6) would consist of  $N - 1$  terms of which a typical one would be

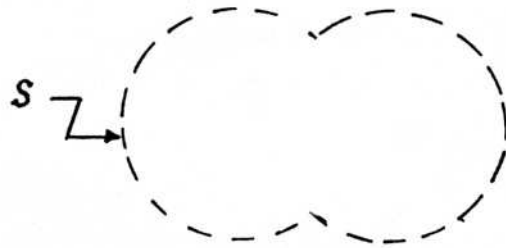
$$I_{1j} = \alpha^2 \int d^3r_N \cdots \int d^3r_2 \int d\omega_r \left( a \underline{r} \cdot \nabla_1 \psi(\underline{r}_j + \underline{r}, \underline{r}_2, \underline{r}_3, \dots, \underline{r}_N) \right) \times U(\underline{r}_j + \underline{r}, \underline{r}_2, \dots, \underline{r}_N). \quad (\text{III.7})$$

The meaning of (III.7) is that  $\underline{r}$  is a vector of length  $a$  and  $d\omega_r$  is an angular integration.

Now we come to the crucial point. Suppose the fixed particles are not so favorably disposed as in the above discussion. For concreteness, assume that  $|\underline{r}_2 - \underline{r}_3| < 2a$  as in the diagram below.



The surface  $S$ , over which  $\underline{r}_1$  is to be integrated, should properly consist only of the portion



If we used (III.7) we would overestimate the surface by including the part  $\left. \right)$  and  $\left( \right.$  which should not be included because on them particle 1 overlaps either particle 2 or 3. Nevertheless, we observe that the contribution of  $\left. \right)$ , for example, to  $I_{12}$  would automatically vanish anyway, because on this surface both  $\psi$  and its normal derivative vanish. In short,

$$\sum_{j=2}^N I_{1j}$$

is in fact always a correct expression for the surface integral in (III.6). One might worry that we might pick up a  $\delta$ -function contribution from the circles where the two dotted spheres intersect, but there is no danger of this because, while the gradient of  $\psi$  may be



discontinuous, it has no  $\delta$ -function. The same would not be true of  $\nabla^2\psi$ . We can go one step further. Strictly speaking the integrals  $d^3r_2 \cdots d^3r_N$  should be only over the region wherein  $r_2, \dots, r_N$  do not overlap each other. But when they do overlap, both  $\psi$  and its derivatives are again zero, so that for convenience we may integrate each of  $\underline{r}_2, \dots, \underline{r}_N$  over the full volume  $V$  if we wish in (III.7).

Returning to the volume integral in (III.6), we may also integrate this by parts and obtain a surface integral similar to (III.5) together with another volume integral:

$$\alpha^2 \int_W (ik_1 \cdot \nabla_1 \psi) U d^3r_N = \alpha^2 k_1^2 \int_W \psi U d^3r_N + \sum_{j=2}^N \tilde{I}_{1j} \quad (\text{III.8})$$

where

$$\begin{aligned} \tilde{I}_{1j} = -\alpha^2 \int_V d^3r_N \cdots \int_V d^3r_2 \int d\omega_r (i\mathbf{k} \cdot \overline{\mathbf{r}}a) \psi(\underline{r}_j + \underline{r}, \underline{r}_2, \dots, \underline{r}_N) \\ \times U(\underline{r}_j + \underline{r}, \underline{r}_2, \dots, \underline{r}_N) \end{aligned} \quad (\text{III.9})$$

In (III.9) we have again used the same sort of argument about the overlap region as in deriving (III.7). Notice, however, that  $\tilde{I}_{1j} = 0$  whenever any two particles touch each other. Furthermore, by virtue of (III.4), the volume integral in (III.8) is just proportional to  $\varphi$ .

The conclusion, therefore, is that

$$E\varphi = \left( \sum_1^N k_i^2 \right) \varphi + \sum_{\substack{i,j \\ i \neq j}} I_{ij}. \quad (\text{III.10})$$

The next step is to express  $I_{ij}$  in terms of  $\varphi$ . This may be done by inserting the expression (II.5b) for  $\psi$  in terms of  $\varphi$  into (III.7). All integrations may now easily be done, with the result that

$$I_{ij} = \lim_{\epsilon \rightarrow 0} (a\alpha^2/V) \sum_{\underline{p}} \varphi(\underline{k}_1, \underline{k}_2, \dots, \underline{k}_i + \underline{p}, \dots, \underline{k}_j - \underline{p}, \dots, \underline{k}_N) g(\underline{p}, \underline{k}_i, \epsilon), \quad (\text{III.11})$$

where

$$g(\underline{p}, \underline{k}, \epsilon) = \int d\omega_r e^{i\mathbf{p} \cdot \underline{r}} i(\underline{p} - \underline{k}) \cdot \underline{r}. \quad (\text{III.12})$$

The significance of  $\epsilon$  is that  $\underline{r}$  is to be regarded as a vector of length  $a + \epsilon$ . Now we must notice the following: if we evaluate (III.9) by the same method we will obtain an expression for  $\tilde{I}$  similar to (III.11). The difference would be that the corresponding  $\tilde{g}(p, k)$ , when written as in (III.12), would have the factor  $(\underline{p} - \underline{k}) \cdot \underline{r}$  replaced by  $\underline{k} \cdot \underline{r}$ . But we know that  $\tilde{I} = 0$  and hence we may if we wish omit the term  $\underline{k} \cdot \underline{r}$  in (III.12), thereby rendering  $g$  independent of  $k$ . This observation yields the result

$$g(p) = 4\pi \cos p(a + \epsilon) - [4\pi/p(a + \epsilon)] \sin p(a + \epsilon). \quad (\text{III.13})$$

Moreover, we may go one step further and drop the term

$$\sin p(a + \epsilon)/p(a + \epsilon)$$

in (III.13). The reason is that we would obtain exactly such a term if we had considered an integral similar to  $\tilde{I}$ , (III.9), but with the factor  $(i\mathbf{k} \cdot \mathbf{r})$  replaced by unity. Such an integral must vanish for the same reason that  $\tilde{I}$  vanishes and hence the last term in (III.13), when inserted into (III.11) must yield a vanishing contribution.

Combining (III.11) and (III.10), with  $g$  given by the first term of (III.13), we have an equation of the same form as (II.6). Aside from the additional complication of taking the limit  $\epsilon \rightarrow 0$ , what has happened is that  $\nu(\mathbf{p})$  has effectively been replaced by the factor  $\alpha^2 8\pi a \cos p(a + \epsilon)$ . If we wish we may recast this equation in second-quantized language since, as we explained previously, this step is nothing more than a bookkeeping convenience. Thus,

$$\lim_{\epsilon \rightarrow 0} H_\epsilon \Psi = E \Psi, \quad (\text{III.14})$$

where

$$H_\epsilon = (\hbar^2/2m) \left\{ \sum_{\mathbf{k}} k^2 a_{\mathbf{k}}^+ a_{\mathbf{k}} + (4\pi a/V) \sum_{\mathbf{k}, \mathbf{q}, \mathbf{p}} a_{\mathbf{k}+\mathbf{p}}^+ a_{\mathbf{q}-\mathbf{p}}^+ a_{\mathbf{k}} a_{\mathbf{q}} \cos p(a + \epsilon) \right\}. \quad (\text{III.15})$$

It is important to emphasize what (III.14) and (III.15) mean.  $H_\epsilon$  is a Hermitian operator that depends upon the parameter  $\epsilon$ . The state  $\Psi$  is the exact state (which we do not know) and does *not* depend upon  $\epsilon$ . The limit in (III.14) *must* be taken *after*  $H_\epsilon$  acts on  $\Psi$  — not before. The energy  $E$  is *not* the limit as  $\epsilon \rightarrow 0$  of one of the eigenvalues of  $H_\epsilon$ . Hence, although (III.14) is similar to a conventional Schrödinger equation, it cannot be used to derive a variational expression for  $E$ .

There is, too, another important point, which has sometimes been a source of confusion. Equation (III.14) was derived by assuming (III.3), and it undoubtedly has other solutions than those satisfying (III.3). These must be rejected. On the other hand, it is *not necessary to use (III.3)* explicitly in solving (III.14). In particular, if we apply the pair approximation to (III.14) there is in principle no need to use any additional properties of  $\Psi$  other than those already implicit in (III.14).

As a matter of convenience, however, it is desirable to have a simple test for whether or not any given solution of (III.14) satisfies (III.3). One way would be to take the Fourier transform of  $\Psi$  and see if (III.3) is satisfied in configuration space — but this is needlessly complicated. There does exist a test which may be applied directly in momentum space and this may be derived as follows: Let  $v(\mathbf{r})$  be any function that is positive for  $r < a$  and zero for  $r > a$ . A particular choice would be

$$\begin{aligned} \theta(r) &= 1 & r < a \\ &= 0 & r > a, \end{aligned} \quad (\text{III.16})$$

but there are, of course, many other possibilities. Consider

$$\psi'(\underline{\mathbf{r}}_1, \dots, \underline{\mathbf{r}}_N) = \left[ \sum_{\substack{i,j \\ i \neq j}} v(\underline{\mathbf{r}}_i - \underline{\mathbf{r}}_j) \right] \psi(\underline{\mathbf{r}}_1, \dots, \underline{\mathbf{r}}_N). \quad (\text{III.17})$$

Since the term in brackets,  $[ \ ]$ , is positive if and only if we are in the unphysical region  $R - W$ , and is zero in  $W$ , it follows that a necessary and sufficient condition that  $\psi$  satisfy (III.3) is that  $\psi' \equiv 0$  everywhere in  $R$ . But, as in the derivation of (II.6), it is a simple matter to express  $\psi'$  in second quantization. Thus

$$\left[ \sum_{\underline{\mathbf{k}}, \underline{\mathbf{q}}, \underline{\mathbf{p}}} a_{\underline{\mathbf{k}}+\underline{\mathbf{p}}}^+ a_{\underline{\mathbf{q}}-\underline{\mathbf{p}}}^+ a_{\underline{\mathbf{q}}} a_{\underline{\mathbf{k}}} \nu(\underline{\mathbf{p}}) \right] \Psi \equiv 0 \quad (\text{III.18})$$

is a  $N$ . and  $S$ . condition in momentum space that  $\Psi$  satisfies (III.3). Here  $\nu$  is the Fourier transform of  $v$  and if we use (III.16) it is given by

$$\nu(p) = -4\pi a/p^2 [\cos pa - \sin pa/pa]. \quad (\text{III.19})$$

It is also possible to find many necessary but not sufficient conditions by using in (III.17) a  $v(\underline{\mathbf{r}})$  that is not positive everywhere for  $r < a$ . A particularly important choice which we shall use later is  $v(r) = \delta(r - a)$  (the radial  $\delta$ -function), whence

$$\nu(p) = 4\pi a^2 \sin pa/pa. \quad (\text{III.20})$$

Before turning to the solution of (III.14), let us briefly recapitulate other similar approaches to the hard core problem. The correct expression for  $E_0$  (II.3) was first given by Lee, Huang and Yang [12] using the method of the pseudopotential. Their idea was to examine the solutions to the two-body hard core problem (which are known) and to find some effective potential (or operator) which, when inserted into the Schrödinger equation in place of the hard core potential, duplicates these solutions. At the same time it is required that this pseudopotential have a Fourier transform. They showed that the operator

$$v'\psi = 8\pi a \alpha^2 \delta(r) \partial/\partial r r \psi \quad (\text{III.21})$$

duplicates the  $S$ -wave solutions up to order  $a^2$ . One then makes the assumption that for low density the pseudopotential for the  $N$ -body problem can be obtained simply by summing (III.21) over all pairs, and when this is inserted into (II.6) one obtains an equation like our (III.15) but with the cosine factor replaced by unity and without the limiting  $\epsilon \rightarrow 0$ .

Since then many authors [13, 14, 15] have tried to find a better pseudopotential, but owing to two difficulties these have not been exact. The first is that for the two-body case they have not used the assumption (III.3) but rather assume that  $\psi$  is somehow analytically extrapolated into the forbidden region. This means that  $\psi \sim r^{-1}$  for small  $r$  and it is then difficult to find an exact pseudopotential, even for two particles. The second difficulty arises in trying to extend the method to  $N$  particles. In view of the fact that  $\psi$  does not vanish in  $R - W$ , it is necessary to take into account three, four, etc.

particle overlaps. In other words, the exact  $N$ -body pseudopotential will not be simply a two-body operator.

By using the definition (III.3), however, and by going directly into momentum space, we have been able to construct an exact equation (III.14) that involves only one- and two-body operators.

Siegert et. al. [16] have in principle derived an exact  $N$ -body pseudopotential. Unfortunately it is very difficult to deal with – unless approximations are made – because it involves non-local operators that are only defined implicitly.

In trying to solve (III.14) a naive attempt would be to use Bogoliubov's method directly. This would be disastrous because we should obtain a divergent integral (II.26) for  $E_0$ . In any event the answer so obtained could not be reliable because as we explained previously we are *not* seeking the eigenvalues of  $H_\epsilon$ . As we shall see, the correct interpretation of the  $\epsilon$  limiting procedure will eliminate the divergence. In their calculation, Lee, Huang and Yang [12] obtained a similar divergence of course. It then required a rather involved and unrigorous argument to obtain the result which we shall find directly (cf. (III.32)).

To solve (III.14) we must remember that  $\Psi$  does not depend upon  $\epsilon$ . Let us imagine  $\Psi$  written out as in (II.38). We shall assume, as in the pair theory, that the three particle term is absent and that the four-particle term is a product wave function. Notice that we do not need to assume that the higher particle terms are as in (II.37). Thus we assume that

$$\begin{aligned} \Psi = & (a_0^+)^N |0\rangle + N \sum_{\mathbf{k}}' g(\mathbf{k}) a_{\mathbf{k}}^+ a_{-\mathbf{k}}^+ (a_0^+)^{N-2} |0\rangle \\ & + \frac{1}{2} N^2 \sum_{\mathbf{k}}' \sum_{\mathbf{q}}' g(\mathbf{k}) g(\mathbf{q}) a_{\mathbf{k}}^+ a_{-\mathbf{k}}^+ a_{\mathbf{q}}^+ a_{-\mathbf{q}}^+ (a_0^+)^{N-4} |0\rangle \\ & + \dots \end{aligned} \quad (\text{III.22})$$

Equation (III.22) is the most general  $\Psi$  we could construct, except for the assumption about the three and four-particle terms. The remaining terms  $\dots$  are regarded as the corresponding exact terms in the exact  $\Psi$ . It will turn out that we shall not need to know them.

If  $\Psi$  is inserted into (III.14) we are permitted to equate the coefficients of the  $n$ -particle term on both sides of the equation. In this way we obtain a set of equations for each  $n = 0, 1, \dots$ . Unfortunately they are coupled because the quartic term in (III.15) mixes  $n - 2, n - 1, n + 1, n + 2$  as well as  $n$  itself with  $n$ . For  $n = 0$  we obtain

$$E_0/N\alpha^2 = 4\pi(N - 1/V)a + 2 \lim_{\epsilon \rightarrow 0} \sum_{\mathbf{k}}' g(\mathbf{k}) v_\epsilon(\mathbf{k}) \quad (\text{III.23})$$

where

$$v_\epsilon(\mathbf{k}) = (4\pi a/V) \cos k(a + \epsilon). \quad (\text{III.24})$$

Equation (III.23) is exact. If we can find  $g$  we have found  $E_0$ . To do this we examine the  $n = 2$  equation which will involve  $g^{(3)}$  and  $g^{(4)}$ . The former is assumed absent, while the latter is assumed to be a product. Thus,

$$\begin{aligned} \alpha^{-2} E_0 g(\underline{\mathbf{k}}) &= \left[ (N+1)(N-2)\nu(0) + 2 \lim_{\epsilon \rightarrow 0} N \sum_{\underline{\mathbf{p}}} ' v_{\epsilon}(\underline{\mathbf{p}}) g(\underline{\mathbf{p}}) \right] g(\underline{\mathbf{k}}) \\ &+ \left[ 2\mathbf{k}^2 + 4(N-2)\nu(\underline{\mathbf{k}}) \right] g(\underline{\mathbf{k}}) + 4\nu(\underline{\mathbf{k}}) N g(\underline{\mathbf{k}})^2 \\ &+ (N-1)\nu(\underline{\mathbf{k}}) + 2 \lim_{\epsilon \rightarrow 0} \sum_{\underline{\mathbf{p}}} ' \nu_{\epsilon}(\underline{\mathbf{k}} + \underline{\mathbf{p}}) g(\underline{\mathbf{p}}). \end{aligned} \quad (\text{III.25})$$

The function  $\nu(\underline{\mathbf{k}})$  means (III.24) with  $\epsilon = 0$ . Now the first term in brackets on the right side of (III.25) is equal (to order  $1/N$ ) to the right side of (III.23) and therefore cancels the left side of (III.25).

Were it not for the presence of the last term on the right side of (III.25), we should be left with a simple quadratic equation for  $g(\underline{\mathbf{k}})$ . With the last term, however, we have an integral equation for  $g$  which can in fact be solved. But an even more remarkable fact is that this term can be evaluated exactly using the true  $g(\underline{\mathbf{k}})$ , even though we do not know that function. We first use the fact for a large system  $g$  does not depend upon angles. This permits us to integrate over the angles of  $\underline{\mathbf{p}}$  in  $\nu_{\epsilon}(\underline{\mathbf{k}} + \underline{\mathbf{p}})$ . Thus, we obtain

$$\begin{aligned} F(\underline{\mathbf{k}}) &= 2 \lim_{\epsilon \rightarrow 0} \sum_{\underline{\mathbf{p}}} ' \nu_{\epsilon}(\underline{\mathbf{k}} + \underline{\mathbf{p}}) g(\underline{\mathbf{p}}) \\ &= (8\pi a/V) \lim_{\epsilon \rightarrow 0} \sum_{\underline{\mathbf{p}}} ' \left\{ (\sin pr/pr) \cos kr + (\sin kr/kr) \cos pr \right. \\ &\quad \left. - (1/pkr^2) \sin pr \sin kr \right\} g(\underline{\mathbf{p}}) \end{aligned} \quad (\text{III.26})$$

where  $r = a + \epsilon$ .  $F(\underline{\mathbf{k}})$  now consists of three factorable sums. The term involving  $\cos pr$  can be evaluated because it is just that which appears in (III.23). The term involving  $\sin pr/pr$  can likewise be evaluated if we write down the analogue of (III.23) for the equation (III.18) (using  $\nu(p)$  given by (III.20)):

$$0 = (N-1) + 2 \lim_{\epsilon \rightarrow 0} \sum_p ' \sin p(a + \epsilon)/p(a + \epsilon) g(\underline{\mathbf{p}}). \quad (\text{III.27})$$

Therefore,

$$F(\underline{\mathbf{k}}) = (E_0/N\alpha^2) \sin ka/ka - 4\pi\rho a \cos ka. \quad (\text{III.28})$$

The function  $F(\underline{\mathbf{k}})$  vanishes as  $a \rightarrow 0$  and we shall consequently drop it. We note in passing, however, that it arose from a part of the pair Hamiltonian ( $a_{\underline{\mathbf{k}}}^+ a_{-\underline{\mathbf{k}}}^+ a_{\underline{\mathbf{p}}} a_{-\underline{\mathbf{p}}} \nu(\underline{\mathbf{k}} + \underline{\mathbf{p}})$ ) not included in Bogoliubov's Hamiltonian. To retain  $F(\underline{\mathbf{k}})$  would probably be misleading

because other terms of this order have already been dropped, notably those coming from  $g^{(3)}$ .

Our result for  $g(\underline{k})$  is then:

$$g(k) = -\frac{1}{16\pi\rho a \cos ka} \left\{ k^2 + 8\pi\rho a \cos ka - (k^4 + 16\pi\rho ak^2 \cos ka)^{1/2} \right\}. \quad (\text{III.29})$$

If we now insert (III.29) into (III.23) we obtain an expression similar to (II.26) for  $E_0$ . But notice that if we mistakenly replace  $\nu_\epsilon(\underline{k})$  by  $\nu(\underline{k})$  we will obtain a divergent integral. (This was what Lee, Huang and Yang obtained before introducing their subtraction term.) It is precisely the fact that  $\nu_\epsilon$  depends upon  $\epsilon$  and  $g$  does not that makes the integral converge. To see this observe that for large  $k$ ,  $g$  behaves like

$$g(k) \sim -(2\pi\rho a/k^2) \cos ka + O(k^{-4}). \quad (\text{III.30})$$

We can then write  $E_0$  as

$$E_0 = N(\hbar^2/2m)4\pi\rho a \{1 + I_1 + I_2\}, \quad (\text{III.31})$$

where

$$I_1 = -(1/16\pi^3\rho^2 a) \lim_{\epsilon \rightarrow 0} \int_0^\infty \frac{k^2 dk}{\cos ka} \left\{ k^2 + 8\pi\rho a \cos ka - (k^4 + 16\pi\rho ak^2 \cos ka)^{1/2} - (32(\pi\rho a)^2/k^2) \cos^2 ka \right\} \cos k(a + \epsilon), \quad (\text{III.32})$$

and

$$I_2 = \lim_{\epsilon \rightarrow 0} (2/\pi)a \int_0^\infty dk \cos ka \cos k(a + \epsilon). \quad (\text{III.33})$$

Since the integral  $I_1$  is absolutely and uniformly convergent we can let  $\epsilon \rightarrow 0$  before integrating. The integral  $I_2$  is zero for any  $\epsilon \neq 0$  and hence is zero in the limit  $\epsilon \rightarrow 0$ . Finally since we are interested in  $I_1$  for small  $a$ , it is easily seen that all cosine factors may be replaced by unity thereby making the integral elementary. Thus,

$$\begin{aligned} I_1 &= (128/15\sqrt{\pi})(\rho a^3)^{1/2}, \\ I_2 &= 0, \end{aligned} \quad (\text{III.34})$$

in agreement with our previous result (II.31).

The next higher term in  $E_0$  was derived by T. T. Wu [14, 15] using an extremely involved perturbation treatment. In the context of our treatment, the next term arises from the  $g^{(3)}$  term which should properly belong in (III.25). We shall not attempt to derive Wu's result here, but shall merely quote it

$$\Delta E_0 = N(\hbar^2/2m)32\pi\rho a(4\pi/3 - \sqrt{3})\rho a^3 \ln(12\pi\rho a^3) + O(\rho a^3). \quad (\text{III.35})$$

To get the next term,  $O(\rho a^3)$ , seems to be impossible. Wu claims that it involves solving an essentially three-body problem.

#### IV. Other Methods for the Ground State Energy

We have thus far reviewed the main ideas and features of the pair-Hamiltonian approach to the ground state energy problem. It is to be admitted that we have left unmentioned the most current and sophisticated extensions of these ideas – especially the elegant “graphology” of modern perturbation theory and the so-called “Green function” method which is closely allied to it. Nevertheless, the main ideas are clear, the principal assumption being that the wave function is to a large extent a pair function in momentum space.

There are two main criticisms that can be made of this philosophy. First, while there may be some justification to momentum space pairing for low density, the justification rapidly disappears as the density is raised. Consider the hard sphere problem, for instance. The only dimensionless parameter in the problem is  $\rho a^3$  and this can be as large as  $\sqrt{2}$  (tight packing) at which point  $E_0$  becomes infinite. For liquid helium  $\rho a^3 \cong .36$  or 26 percent of the maximum. At this density, the three terms we obtained so laboriously have all the appearance of a diverging series. The third term (III.35) is about three times the second (III.34) and this in turn is about three times the first ( $4\pi\rho a$ ). Admittedly, it is possible to improve the situation somewhat by judiciously summing graphs, but it is then difficult to maintain that the original pairing assumption was valid.

The second criticism is that even for low density we have lost sight of some simple mathematics in our calculation. The leading term in  $E_0$  is  $(\hbar^2/2m)4\pi N\rho a$ . As we shall now show, this is equal to the number of pairs of particles ( $\frac{1}{2}N(N-1)$ ) times the ground state energy of an isolated pair in the large volume  $V$ , namely  $(\hbar^2/2m)(8\pi a/V)$ . This is a satisfying result, yet to obtain it we were obliged to appeal to an infinite summation of graphs in the Bogoliubov theory, or else to a complicated pseudopotential analysis in the hard core case.

To obtain the above result we integrate the equation

$$-2\alpha^2\nabla^2\psi + v\psi = E\psi \quad (\text{IV.1})$$

over the volume  $V$ . Using the fact that  $\psi$  is periodic we obtain

$$E = \int_V v(\underline{r})\psi(\underline{r})d^3r / \int_V \psi(\underline{r})d^3r. \quad (\text{IV.2})$$

Now the zero energy scattering solutions to (IV.1),  $\psi_0$ , is very nearly a periodic function if  $V$  is very large. Hence to leading order in  $V$ ,  $\psi$  may be replaced by  $\psi_0$  in (IV.2). If  $\psi_0$  is normalized to  $\psi_0 \sim 1 - a/r$  for large  $r$ , the denominator is  $V$  to leading order. But, as we explained in Section II, the numerator is then  $8\pi\alpha^2 a$ . Hence  $E = \alpha^2 8\pi a/V$ .

The preceding analysis was simplicity itself compared to the difficulties inherent in a momentum space calculation. Perhaps resort to the latter is really an unwarranted

complication – for the ground state energy at least – and configuration space is really the more appropriate framework.

One idea that immediately suggests itself is to perform a variational calculation using

$$\psi = \prod_{i < j} \varphi(\underline{r}_i - \underline{r}_j) \quad (\text{IV.3})$$

where we may write

$$\varphi(\underline{r}) = \exp(-f(\underline{r})). \quad (\text{IV.4})$$

We shall call  $\psi$  a product function in configuration space. Despite a deceptive similarity to the pair function (II.37) in momentum space, (IV.3) is really quite different from (II.37). To appreciate the plausibility of (IV.3) let us consider the three important lengths at low density:  $\ell_1 = a =$  scattering length;  $\ell_2 = \rho^{-1/3} =$  average particle spacing;  $\ell_3 = (\rho a)^{-1/2}$ . At low density  $\ell_3 \gg \ell_2 \gg \ell_1$ . To calculate the potential energy we obviously need  $\psi_0$  accurately whenever any two particles are separated a distance of the order  $\ell_1$ . We surmised before that for these distances  $\psi_0$  is proportional to the zero energy scattering function and (IV.3) can correctly describe this behavior if  $\varphi$  is of that form for small  $r \sim a$ . On the other hand, to calculate the kinetic energy, distances of the order  $\ell_3$  are important. This is because  $E_0/N \sim \ell_3^{-2}$ . The distance  $\ell_3$  is a kind of correlation length and hopefully (IV.3) can give these correlations (which extend over many particles) correctly if  $\varphi$  has the correct behavior for  $r \sim \ell_3$ .

It is to be noted that the Bose gas at low density is qualitatively different from the Fermi gas at low density. In the former  $\ell_2$  is unimportant; in the later  $\ell_2$  is important, since  $E_0/N \sim \rho^{2/3}$  for a non-interacting Fermi gas, and therefore  $\ell_3$  is unimportant. Fermi particles already have a great deal of kinetic energy with no interaction and hence the interaction may be thought of as a small perturbation. For bosons the whole energy is caused by the interaction and thus it is far more important to treat correlations carefully.

At high density, on the other hand, the above qualitative considerations become invalid. The correlations become quite complicated. Nevertheless (IV.3) still has considerable validity. By choosing  $\varphi$  carefully one could describe even a solid qualitatively. Doubtless the correlations described by  $\psi$  would be quite different from those of the true wave function, but perhaps in some average sense (the computation of  $E_0$ ) they are not too far off the mark.

The great difficulty with (IV.3), however, is that for all except weak coupling it leads to a forbiddingly difficult computation. Let us define

$$S(\underline{r}_1 - \underline{r}_2) = V^2 \int \psi^2(\underline{r}_1, \underline{r}_2, \dots, \underline{r}_N) \prod_3^N d^3 r_i$$

and

$$F(\underline{r}_1 - \underline{r}'_1) = V \int \psi(\underline{r}_1, \underline{r}_2, \dots, \underline{r}_N) \psi(\underline{r}'_1, \underline{r}_2, \dots, \underline{r}_N) \prod_2^N d^3 r_i. \quad (\text{IV.5})$$



We have assumed in (IV.5) that  $\psi$  is normalized to unity.  $S$  has significance for X-ray scattering and is called the structure factor.  $F$  is important for computing quantities involving the kinetic energy. In particular, a glance at (II.13) will show that

$$n_k = \langle a_k^+ a_k \rangle = \rho \int F(\underline{r}) e^{ik \cdot r} d^3 r. \quad (\text{IV.6})$$

The energy may be expressed in terms of  $S$  and  $F$  by

$$E/N = \frac{1}{2} \rho \int v(\underline{r}) S(\underline{r}) d^3 r - \alpha^2 \nabla^2 f(0). \quad (\text{IV.7})$$

Equation (IV.7) is correct whether we use the correct  $\psi_0$  in (IV.5) or a trial function. But with a product function, however, there is an alternative, simpler formula for  $E$ , namely

$$E/N = \rho \int S(\underline{r}) \left\{ -\alpha^2 \nabla^2 \varphi(\underline{r}) / \varphi(\underline{r}) + \frac{1}{2} v(\underline{r}) \right\} d^3 r. \quad (\text{IV.8})$$

Thus, only knowledge of  $S$  is required. The integral in (IV.8) would be the same as for a two-body problem if we replace  $S$  by  $\varphi^2$ .

At this point we are faced with two enormous difficulties. The first is to compute  $S$ , given  $\varphi$ . If  $f$  in (IV.4) is a finite range, integrable function, which means it goes to zero faster than  $r^{-3}$ , then the calculation of  $S$  is mathematically equivalent to finding the two-particle correlation function for a classical gas with an effective potential  $v = kTf$ . In the literature, such an assumption has always been made about  $f$ . It has the advantage that for low density we can make a conventional cluster expansion for  $S$  and obtain  $S$  as a simple functional of  $f$ . This functional relationship, however, soon becomes hopelessly complicated as we go to higher terms. If the density is not low we can always try to perform a Monte Carlo computation of  $S$ , but we will then have to give up trying to find the functional relationship of  $S$  to  $f$ .

There is an important drawback, however, to using a short range  $f$ . For large  $r$  the  $S$  obtained using (IV.3) will always have a different asymptotic behavior from the correct  $S$  using the correct  $\psi_0$ . We shall return to this question later when discussing the excitation spectrum.

The second difficulty comes in trying to find an optimum form for  $f$ . Even if we retain only the first two terms in a cluster expansion, it is hopeless to try to minimize (IV.8) analytically. For the hard core case, early workers guessed that  $\varphi$  should be of the form  $\varphi(r) = 1 - (a/r) \exp(-\beta(r - a))$ , where  $\beta$  is proportional to  $(\rho a)^{1/2}$ . Using the best value of  $\beta$ , the leading term in (II.3) is obtained correctly, but the second term is too large by a few percent. It is necessary to make a better guess for  $\varphi$ : one that goes like  $A(1 - (a/r))$  for small  $r$  and like  $Br^{-4}$  for large  $r$ , where  $A$  and  $B$  are constants. It appears that Hiroike [17] was the first to obtain (II.3) using such a  $\varphi$ .

To summarize, the product trial function approach appears to have considerable merit in principle, but it is nearly impossible to carry it through in practice. In addition, even if we could obtain a good estimate of  $E_0$  this way, the function  $S$  would be open to question.

The reason is that  $S(\underline{r})$  samples  $\psi$  much more sensitively than the single number  $E_0$ , and  $\psi_0$  is simply not of the form (IV.3) with a short range  $f$ .  $\psi_0$  has in it much longer range correlations than (IV.3) and, as we shall see later, these are important for X-ray scattering. It turns out that X-rays can actually measure the true  $S(\underline{r})$ .

We shall turn now to a method [18] that combines the most attractive features of pairing in momentum space together with the product *ansatz* in configuration space. We begin by defining correlation functions

$$g^n(\underline{r}_1, \dots, \underline{r}_n) = V^n \int \psi_0(\underline{r}_1, \dots, \underline{r}_N) \prod_{n+1}^N d^3 r_i / \int \psi_0(\underline{r}_1, \dots, \underline{r}_N) \prod_1^N d^3 r_i. \quad (\text{IV.9})$$

Implicit in (IV.9) is the fact that  $\psi_0$  is a positive, real function for a Bose gas [19], and hence all the  $g^N$  are positive.  $g^2(\underline{r})$  (which we shall henceforth denote by  $g$ ) is similar to  $S(\underline{r})$  but, unlike  $S$ , the energy can be expressed in terms of  $g$  alone.

If we integrate both sides of the Schrödinger equation (II.1) over all space we obtain the exact relation

$$E_0 = \frac{1}{2}(N-1)\rho \int_V g(\underline{r})v(\underline{r})d^3r. \quad (\text{IV.10})$$

The problem is then to find  $g(\underline{r})$ . For the hard core potential, (IV.10) is meaningless as it stands, but we can find an analogous expression in integrating (III.2) over  $W$ . One obtains [18]

$$E_0 = \alpha^2(N-1)\rho a^2 \int d\omega_r \partial g / \partial r |_{r=a^+} \quad (\text{IV.11a})$$

$$\rightarrow 4\pi N \rho \alpha^2 a^2 dg/dr |_{r=a^+} \quad (\text{IV.11b})$$

Equation (IV.11a) is exact, while (IV.11b) is correct in the bulk limit when  $g$  become spherically symmetric.

To find an equation for  $g$  we integrate the Schrödinger equation over all variables except 1 and 2. Thus

$$\begin{aligned} \left[ -\alpha^2 \left( \nabla_1^2 + \nabla_2^2 \right) + v_{12} \right] g_{12} &= E_0 g_{12} - 2(N-2)V^{-1} \int g_{123}^3 v_{23} d_3 \\ &\quad - \frac{1}{2}(N-2)(N-3)V^{-2} \iint g_{1234}^4 v_{34} d_3 d_4 \equiv M_{12}. \end{aligned} \quad (\text{IV.12})$$

In (IV.12) we have used the notation  $g(\underline{r}_1 - \underline{r}_2) = g_{12}$ , etc. Again, for the hard core case, the integrals in  $M$  can be interpreted as in (IV.11). The function  $M_{12}$  is unknown, but judging from the fact that it is proportional to the interaction we may suppose that it goes to zero in the weak coupling (but not necessarily weak potential) limit. For a finite range potential this means  $\rho \rightarrow 0$ . Hence if we define

$$G(\underline{r}) = \lim_{\rho \rightarrow 0} g(\underline{r}) \quad (\text{IV.13})$$

then  $G$  is the solution to the two-body zero energy scattering problem and, from (IV.10)

$$E_0 \rightarrow 4\pi N \rho a \alpha^2. \quad (\text{IV.14})$$

For a hard core potential  $G(r) = 1 - (a/r)$  and (IV.11b) agrees with (IV.14).

Certainly one advantage of the present method is that we obtain the leading term in  $E_0$  without any work, while previous methods always involved a difficult analysis.

To find the next term in  $E_0$  we require some knowledge of  $M$ . Suppose we solve (IV.12) formally for the hard core case and insert the result into (IV.10)

$$E_0/N = 4\pi \rho a \alpha^2 \left( 1 + \int_0^\infty r M(r) dr \right). \quad (\text{IV.15})$$

Presumably  $M$  has a cutoff length, and we see from (IV.15) that we need  $M$  of the order of this length. Judging by our previous discussion we anticipate that this length will be of the order of  $\ell_3 = (\rho a)^{-1/2}$  and we shall indeed find this surmise to be true.

Why does  $M$  have a cutoff length? It has one because of what might be called independence at large distances (ILD). Presumably when  $\underline{\mathbf{r}}_1$  is very far removed from  $\underline{\mathbf{r}}_2$  and  $\underline{\mathbf{r}}_3$  then

$$g_{123}^3 \rightarrow P(\underline{\mathbf{r}}_1) Q(\underline{\mathbf{r}}_2, \underline{\mathbf{r}}_3),$$

i.e.,  $g^3$  factors. But, from the fact that

$$\int_V g_{123}^3 d_1 = V g_{23},$$

it follows that  $P = 1$  and  $Q = g$  to leading order in the volume. Likewise  $g_{1234}^4 \rightarrow g_{12}g_{34}$  when 1 and 2 are far from 3 and 4. If we insert these asymptotic forms into the definition of  $M$ , and use (IV.10) we find that  $M \rightarrow 0$  when 1 is far from 2.

Therefore, in order to find the leading term in the integral in (IV.15) we need the first correction to the asymptotic forms just given. We claim (although we cannot prove this) that these are given, for low density at least, by the superposition *ansatz*:

$$g_{123}^3 = s(1 - w_{12})(1 - w_{13})(1 - w_{23}) \quad (\text{IV.16})$$

$$g_{1234}^4 = t \prod_{i < j=1}^4 (1 - h_{ij}). \quad (\text{IV.17})$$

Here  $s$  and  $t$  are constants and  $w$  and  $h$  are functions to be determined from the relations

$$\int g_{123}^3 d_3 = V g_{12} \quad \text{and} \quad \iint g_{1234}^4 d_3 d_4 = V^2 g_{12}.$$

If we write

$$g_{12} = (1 - u_{12})/(1 - \delta) \quad (\text{IV.18a})$$

$$\delta = \int u/V, \quad (\text{IV.18b})$$

where  $u$  is the finite part of  $g$  and is defined to vanish for large  $r$ , we can find  $s, t, w$  and  $h$  in terms of  $u$  and  $\delta$

$$\begin{aligned} s &= 1 + 3\delta + O(V^{-1}) \\ t &= 1 + 6\delta + O(V^{-1}) \\ w_{12} &= u_{12} + g_{12} \int u_{13} u_{23} d_3 / V + (V^{-1}) \\ h_{12} &= u_{12} + 2g_{12} \int u_{13} u_{23} d_3 / V + (V^{-1}). \end{aligned} \quad (\text{IV.19})$$

The reason we were careful to retain the terms in (IV.19) of order  $V^{-1}$  is that the first and third terms in  $M$  are both of order  $N$ . They cancel to this order, as we explained before, and leave a residue of order unity. This residue comes from three sources in the last integral: the fact that  $g_{1234}^4$  goes asymptotically to  $g_{12}g_{34} + O(V^{-1})$ ; the contribution when 3 or 4 is close to 1 or 2; and the presence of the factor  $(N-2)(N-3)$  instead of  $N(N-1)$ .

If we insert (IV.19) into (IV.12) and pass to the bulk limit we obtain an integro-differential equation:

$$\left[ -\alpha^2 \left( \nabla_1^2 + \nabla_2^2 \right) + v_{12} \right] g_{12} = \rho g_{12} \{ 2K_{12} - \rho L_{12} \} \quad (\text{IV.20a})$$

where

$$K_{12} = \int u_{13} g_{23} u_{23} d_3 \quad (\text{IV.20b})$$

and

$$L_{12} = \iint u_{23} u_{24} \left\{ g_{14} g_{23} - \frac{1}{2} u_{14} u_{23} \right\} g_{34} v_{34} d_3 d_4. \quad (\text{IV.20c})$$

Equation (IV.20) is our final result. Although our expression for  $M$ , which came from (IV.16) and (IV.17), was justified only for low density we claim that (IV.16) and (IV.17) are in general reasonable approximations. Take  $g^3$ , for example. It is known to be positive and asymptotically goes like  $g$ . Also  $g^3$  should become very small (zero for the hard core case) when all three particles overlap. The *ansatz*, (IV.16), has all these properties. Moreover, the superposition *ansatz* clearly is related to the product trial function approach. The difference is that instead of assuming that  $\psi_0$  is a product, we merely assume a product form for the three and four-body correlation functions. This, it seems to us, is much less of a leap into the unknown. Lastly, the superposition *ansatz* determines  $M$  and this in turn determines  $g$  for large distances (for low density). But for small distances  $g$  is determined by the two-body Schrödinger equation — a fact that is obviously in keeping with the pair assumption in momentum space.

The solution of (IV.20) is obviously a job for a computer, and we shall mention later the result of one such computation that has been performed. But let us just ask for the solution to (IV.20) in the low density limit. To this end we reiterate the statement that

we need the right side of (IV.20a) only for large distances. We may therefore replace the first factor  $g$  on the right hand side by unity. Also in  $K$  we may replace  $g_{23} v_{23}$  by  $\delta^3(\underline{\mathbf{r}}_2 - \underline{\mathbf{r}}_3)2e/\rho$  where  $E_0/N = e$ . In  $L$  we may make a similar replacement and in addition we can replace the factor in braces  $\{ \}$  by unity. Thus

$$[-2\alpha^2\nabla^2 + v(r)](1 - u(r)) = 4e u(r) - 2e\rho \int u(\underline{\mathbf{r}} - \underline{\mathbf{z}})u(\underline{\mathbf{z}})d^3z. \quad (\text{IV.21})$$

The claim is that for low density (IV.21) should give the same result as (IV.20). However,  $e$  appears as a parameter in (IV.21) and therefore (IV.10) will become a transcendental equation for  $e$ .

Were it not for the term  $v(r)g(r)$ , Equation (IV.21) could be solved by Fourier transforms. Nevertheless, (IV.21) can be solved to leading order by judiciously going back and forth between configuration and momentum space. It is a technical exercise and details will be found in reference [18]. The result is that for small distances ( $r < \rho^{-1/3}$ )

$$g(r) = 1 - u(r) = (e/4\pi\rho a \alpha^2)\psi_0(r) \quad (\text{IV.22a})$$

where  $\psi_0$  is the zero energy scattering solution. For large distances ( $r > \rho^{-1/3}$ )  $u$  is given by

$$u(r) = (4e/\pi^2\rho \alpha^2 r) \int_0^1 dz z^2(1 - z^2)^{1/2} \exp[-2(e/\alpha^2)^{1/2}r z]. \quad (\text{IV.22b})$$

Matching (IV.22a) and (IV.22b) for  $r \sim \rho^{-1/3}$  we obtain

$$E_0/N = e = 4\pi\rho a \alpha^2 \{1 + (128/15\sqrt{\pi})(\rho a^3)^{1/2} + \dots\}, \quad (\text{IV.23})$$

in agreement with our previous calculations.

Certain features of our  $g(r)$  are noteworthy. For small distances  $\sim \ell_1$ ,  $g$  is proportional to the two-body scattering function. This is a correct feature that was very difficult to obtain in the Bogoliubov formalism, although it was relatively simple to obtain using a product trial function. For large distances  $\sim \ell_3$ ,  $g$  is given by a universal function, (IV.22b), which depends only on the energy (or scattering length) as its only parameter. This was more or less a feature of the Bogoliubov function as well as of the  $S(r)$  derived from a product function, but in the latter case it involved a difficult computation to find  $S$ , even if  $f(r)$  were given, and an even more difficult task to find the long range behavior of the optimum  $f(r)$ . As we mentioned previously, it took some years before it became clear that  $f(r)$  should go as  $r^{-4}$  for large  $r \sim \ell_3$ , yet in (IV.22b) this feature is unambiguously obtained.

Another important advantage of (IV.20) is that we can obtain the hard core result on the same footing as for a finite potential – no pseudopotential being required. In fact the solution to (IV.20) is easier to obtain for the hard core potential than for any finite potential.

There have been further attempts to establish (IV.20) as a useful general approximation scheme. In the above analysis it was shown to be correct for finite range potentials at low density. Another weak coupling situation is the charged Bose gas at *high* density.

It appears that in this case Bogoliubov's theory gives the leading term in the energy correctly ([20], [5]), although this assertion has not been proved rigorously. If one defines  $r_s = (3/4\pi\rho)^{1/3} e^2(m/\hbar^2)$ , where  $e$  is the charge of each particle, then for small  $r_s$  the energy per particle in Rydbergs ( $R_H = me^4/2\hbar^2$ ) is

$$E_0/NR_H = Ar_s^{-3/4} \quad (\text{charged Bose gas}) \quad (\text{IV.24})$$

where

$$A = (2/\pi)6^{1/4} \int_0^\infty \{p^2(p^4 + 2)^{1/2} - p^4 - 1\} dp = -0.803. \quad (\text{IV.25})$$

We have verified [21] that (IV.20) gives this result, (IV.24), in the same limit.

Another example where (IV.20) acquits itself well is for the exactly soluble Bose gas problem ([22]) which we shall discuss in the next section. In this case the exact  $E_0$  is known for all values of the coupling constant. Equation (IV.20) was solved for this case [23] on a computer and it was found that the *worst* error in  $E_0$  occurred for infinite coupling constant, as expected, and was only 19 percent. It was also found that for *infinite* coupling constant the  $g(r)$  given by (IV.20) and the exact  $g(r)$  were in remarkably close agreement. That (IV.20) predicts  $g(r)$  correctly, and not merely  $E_0$ , is strong evidence in its favor.

## V. An Exactly Soluble Model

With various approximation schemes before us, it would certainly be advantageous to have at least one problem of the type (II.1) that can be solved exactly. We should then be able to verify whether or not the previously mentioned qualitative ideas are correct.

Such model problem is the one-dimensional Bose gas with a pair-wise repulsive  $\delta$ -function potential ([22]). Using units in which  $\hbar^2/2m = 1$ , the Schrödinger equation is

$$\left\{ -\sum_1^N \partial^2/\partial x_i^2 + 2c \sum_{i<j} \delta(x_i - x_j) \right\} \psi = E\psi. \quad (\text{V.1})$$

Hence  $2c \geq 0$  is the amplitude of the  $\delta$ -function. If  $L$  is the length of the line then  $\rho = N/L$ . It is well known that a  $\delta$ -function potential is equivalent to the following boundary conditions whenever any two particles touch each other (irrespective of the value of the remaining  $N - 2$  coordinates):

$$(\partial/\partial x_j - \partial/\partial x_k)\psi|_{x_j=x_k^+} - (\partial/\partial x_j - \partial/\partial x_k)\psi|_{x_j=x_k^-} = 2c\psi|_{x_j=x_k}. \quad (\text{V.2})$$

We also note that we are seeking symmetric solutions to (V.1) and hence if we know  $\psi$  in  $R_1$

$$R_1 : 0 \leq x_1 \leq \cdots \leq x_N \leq L, \quad (\text{V.3})$$

we know  $\psi$  everywhere by symmetric extension. Thus our equations become

$$\left\{ - \sum_1^N \partial^2 / \partial x_i^2 \right\} \psi = E\psi \text{ inside } R_1 \quad (\text{V.4})$$

$$(\partial / \partial x_{j+1} - \partial / \partial x_j) \psi|_{x_{j+1}=x_j} = c\psi|_{x_{j+1}=x_j}. \quad (\text{V.5})$$

Moreover, the original periodic boundary conditions can be interpreted as

$$\begin{aligned} \psi(0, x_2, \dots, x_N) &= \psi(x_2, \dots, x_N, L) \\ \partial / \partial x \psi(x, x_2, \dots, x_N)|_{x=0} &= \partial / \partial x \psi(x_2, \dots, x_N, x)|_{x=L}. \end{aligned} \quad (\text{V.6})$$

To solve these equations, consider the function

$$\varphi(x_1, \dots, x_N) = \text{Det} | \exp(i k_i x_j) | \quad (\text{V.7})$$

where  $k_1, \dots, k_N \equiv \{k\}$  are any set of  $N$  distinct numbers. Now define  $\psi$  by

$$\psi = \prod_{j>i} (\partial / \partial x_j - \partial / \partial x_i + c) \varphi. \quad (\text{V.8})$$

It is readily verified that  $\psi$  satisfies (V.5) automatically, as well as (V.4) with

$$E = \sum_1^N k_i^2. \quad (\text{V.9})$$

It is (V.6) which determines the members  $\{k\}$  and it may be shown that this is equivalent to the  $N$  simultaneous equations

$$(-1)^{N-1} \exp(-i k_j L) = \exp \left[ i \sum_{s=1}^N \theta(k_s - k_j) \right], \quad (\text{V.10})$$

where

$$\theta(k) = -2 \tan^{-1}(k/c), \quad -\pi < \theta < \pi \quad \text{for real } k. \quad (\text{V.11})$$

Equation (V.10) may be rewritten as

$$\delta_j \equiv (k_{j+1} - k_j)L = \sum_{s=1}^N [\theta(k_s - k_j) - \theta(k_s - k_{j+1})] + 2\pi n_j \quad (\text{V.12})$$

for  $j = 1, \dots, N - 1$ . Equation (V.12) is  $N - 1$  simultaneous equations for the  $\delta_j$ ; when they are found, the individual  $k$ 's may be obtained from (V.10). The  $n_j$  in (V.12) are integers, and it can be shown that for any choice of the  $n_j$  such that all  $n_j \geq 1$  there is a solution to (V.12) with real  $\delta_j \geq 0$ . Presumably these solutions are unique and are the only solutions to (V.10); at least this is true if  $N = 2$ . These  $n$ 's are therefore the quantum numbers of the system.

If we pass now to the bulk limit,  $N \rightarrow \infty$ , the ground state will be obtained when all  $n_j = 1$ , because this choice clearly minimizes (V.9). It may be verified that all the  $k$ 's

must lie between  $-\pi\rho$  and  $\pi\rho$ , which means that the spacing between the  $k$ 's decreases as  $N \rightarrow \infty$ . If we set

$$f(k_j) = 1/\delta_j \quad (\text{V.13})$$

then  $Lf(k)$  = the number of  $k$ 's between  $k$  and  $k + dk$ . Furthermore, we denote by  $K$  the common value of  $k_N$  and  $-k_1$ . Using Poisson's formula, (V.10) may be converted into an integral equation:

$$2c \int_{-K}^K f(p) dp / [c^2 + (p - k)^2] = 2\pi f(k) - 1, \quad (\text{V.14})$$

with

$$\int_{-K}^K f(k) dk = \rho \quad (\text{V.15})$$

being the condition that the total number of particles be  $N$ . This latter condition determines  $K$ . The ground state energy is then

$$E_0 = (N/\rho) \int_{-K}^K f(k) k^2 dk. \quad (\text{V.16})$$

At this point it is convenient to introduce the dimensionless coupling constant

$$\gamma = c/\rho, \quad (\text{V.17})$$

in terms of which we may write

$$E_0 = N\rho^2 e(\gamma). \quad (\text{V.18})$$

Equations (V.14) and (V.15) can easily be solved on a computer for all values of  $\gamma \geq 0$ . Graphs for  $K(\gamma)$ ,  $e(\gamma)$  and  $f(k, \gamma)$  are given in Figures 1, 3 and 2 respectively of reference [22a]. The results, briefly, are these

$$\begin{aligned} \text{small } \gamma : \quad & e(\gamma) = \gamma - (4/3\pi)\gamma^{3/2} \\ & K(\gamma) = 2\rho\gamma^{1/2} \\ & f(k, \gamma) = (2\pi\rho\gamma)^{-1}(4\rho^2\gamma - k^2)^{1/2} \end{aligned} \quad (\text{V.19})$$

$$\begin{aligned} \text{large } \gamma : \quad & e(\gamma) = (\pi^2\gamma^2/3)(\gamma + 2)^{-2} \\ & K(\gamma) = \pi\rho\gamma(\gamma + 2)^{-1} \\ & f(k, \gamma) = (\gamma + 2)/2\pi\gamma. \end{aligned} \quad (\text{V.20})$$

We may inquire how Bogoliubov's theory fares for this problem. This theory yields (V.19) for  $e(\gamma)$  for *all*  $\gamma$ , a result which is in fair agreement with the correct  $e(\gamma)$  up to  $\gamma = 2$  and then becomes quite useless. While the true  $e(\gamma)$  is a monotonically increasing function of  $\gamma$ , with an asymptotic value of  $\pi^2/3$ , (V.19) is actually negative for  $\gamma > (3\pi/4)^2$ .



Equation (IV.20), on the other hand, gives a result in excellent agreement with the correct  $e(\gamma)$ . The first two terms (V.19) are obtained exactly from (IV.20); to derive them (IV.21) may be used instead, as explained before. For infinite  $\gamma$  (the worst case) (IV.20) predicts an  $e$  that is too small by only 19 percent.

When  $\gamma$  is infinite, the wave functions, (V.8), are given by

$$\psi = \text{Det} |\exp(i k_i x_j)| \quad (\text{V.21})$$

where each  $k_i$  is of the form:

$$\begin{aligned} k &= (2\pi/L) \times (\text{integer}), & (N \text{ odd}) \\ &= (2\pi/L) \times (\text{integer}) + \pi/L, & (N \text{ even}). \end{aligned} \quad (\text{V.22})$$

For the ground state the  $k$ 's run between  $-\pi\rho$  and  $\pi\rho$ . Another way to express  $\psi_0$  (for any  $N$ ) is to recognize (V.21) as a Vandermonde determinant, whence

$$\psi_0 = \prod_{i < j} \sin(\pi/L) |x_j - x_i| \quad (\text{V.23})$$

for *all* values of the  $x_i$  in  $(0, L)$ . For this  $\psi_0$ , the function  $g^2(x_1, x_2)$ , (IV.9), can be computed exactly [24].

The solution to (IV.20) is in excellent agreement with this result.

Turning now to the excitation spectrum, let us first consider the infinite  $\gamma$  case, where the  $k$ 's are given by (V.22). The spectrum will be recognized as the same as that of a one-component Fermi gas.

An elementary excitation consists in increasing one of the momenta from  $q < K = \pi\rho$  to  $k > K$ . The energy is then

$$\epsilon(k, q) = k^2 - q^2, \quad (\text{V.24})$$

and the momentum of the state is

$$p(k, q) = k - q. \quad (\text{V.25})$$

The difficulty with this description is that it is completely different from what we had been led to expect on the basis of the pair Hamiltonian calculation. For one thing there is no unique  $\epsilon(p)$  curve. For another, each excitation may take place only once, whereas a boson type excitation can be repeated as often as desired.

In order to make this spectrum appear boson-like, let us define *two* types of elementary excitations: for type I we increase  $k_N$  from  $K$  to  $K + p$  (where  $p > 0$ ). The momentum of the state is  $p$  and the energy is

$$\epsilon_1(p) = (K + p)^2 - K^2 = p^2 + 2\pi\rho p. \quad (\text{V.26})$$

For type II we increase one of the momenta from  $K - p + 2\pi/L$  (where  $0 < p < K$ ) to  $K + 2\pi/L$ . Here the momentum is again  $p$  and

$$\epsilon_2(p) = 2\pi\rho p - p^2 \quad (\text{V.27})$$

A type II excitation is defined *only* for momentum less than  $\pi\rho$ . With this description we have achieved our aim, but at the expense of introducing two  $\epsilon(p)$  curves. Any type I excitation can be repeated as often as desired providing we agree always to take the last available  $k$  less than  $K$  and increase it by  $p$ . Similarly, with the same proviso, a type II excitation is boson-like. In addition, both I and II excitations may occur simultaneously. In fact the excitation in (V.24) may be thought of as a simultaneous type I and II excitation with momenta  $p - k$  and  $K - q$ , respectively. It will be seen that provided we make a *finite* number of excitations by the above rule the energies and momenta will be additive to order  $1/N$ . Thus if we make  $n$  type I excitations with momenta  $p_1, \dots, p_n$  and  $m$  type II excitations with momenta  $q_1, \dots, q_m$ , the energy as given by (V.26) and (V.27) would be

$$E = \sum_{j=1}^n \epsilon_1(p_j) + \sum_{j=1}^m \epsilon_2(q_j), \quad (\text{V.28})$$

while the momentum would be

$$P = \sum_{j=1}^n p_j + \sum_{j=1}^m q_j. \quad (\text{V.29})$$

Now if we examine the state we would obtain with these excitations we will find that the *true* energy of the state agrees with (V.28) to order  $1/N$  while the *true* momentum is exactly given by (V.29).

There is one *caveat*, however. In achieving this boson description of the excitations we have, in reality, counted each state twice. If the rules above are carefully examined it turns out that a state with  $n$  type I excitations with momentum  $p = 2\pi m/L$  is identical to the state with  $m$  type II excitations of momentum  $p = 2\pi m/L$ . The spectrum is therefore really much more complicated than we had imagined. If we give up the double spectrum point of view in order to avoid the double counting, then we would have to regard a type II excitation, for example, as essentially an infinite number of type I excitations with vanishing small momentum,  $2\pi/L$ . Not only is this unnatural, but the energy would then be given incorrectly. From (V.26) we would conclude that  $\epsilon_2(p) = 2\pi\rho p$ , where as the correct expression is (V.27).

When  $\gamma$  is not infinite the same qualitative conclusions apply. It will be appreciated that increasing one of the  $k$ 's is the same as putting all but one of the  $n_j$ 's in (V.12) equal to unity. For a type I excitation the singular  $n$  is  $n_{N-1}$  and this is set equal to  $qL/2\pi$ . For a type II excitation the singular  $n$  is one of the  $n_j$ 's (where  $N/2 < j < N-1$ ) and this is set equal to 2. The difficulty with the finite  $\gamma$  case is that when the  $n$ 's are changed in this way *all* the  $k$ 's are shifted — not merely one of them. This shift can be computed from (V.12) and one can again obtain two  $\epsilon(p)$  functions. The details are given in reference [22b]. It is found that as  $\gamma \rightarrow 0$ ,  $\epsilon_1(p) \rightarrow p^2$  (the free boson function) while  $\epsilon_2(p) \rightarrow 0$  for all  $p$ . But for every  $\gamma$  there are always *two*  $\epsilon(p)$  curves.

Bogoliubov's theory, on the other hand, predicts only *one*  $\epsilon(p)$  curve:

$$\epsilon(p) = p(p^2 + 4\gamma\rho^2)^{1/2}, \quad (\text{Bogoliubov}). \quad (\text{V.30})$$

It turns out that for small  $\gamma$ , (V.30) is quite close to the true  $\epsilon_1(p)$  (cf. Fig. 4 of Reference [22b]). The  $\epsilon_2(p)$  curve is entirely missing from Bogoliubov's theory.

## VI. Elementary Excitations and Quasi-Particles

The words elementary excitations and quasi-particles tend to be used interchangeably in the literature, but to the extent that it is possible to define these quantities, at least two definitions are possible.

The first, which we shall call *elementary excitations*, refer to a bookkeeping description, or spectroscopy, of the true excitation energies of the system. These energies (measured from  $E_0$ ) are always real positive numbers since the Hamiltonian is Hermitian. Also, since the total momentum commutes with the Hamiltonian, with each state,  $i$ , we may associate an energy  $E_i$  and momentum  $\underline{P}_i$ . For each, distinct value of  $\underline{P}$  we pick out one of the energies that are associated with that particular value of  $\underline{P}$  and call it  $\epsilon_1(\underline{P})$ . Since there will always be an infinite number of energy levels for each  $\underline{P}$ , we may repeat the process and get several such sets,  $\epsilon_j(\underline{P})$  where  $j = 1, \dots, m$ . These sets will be called elementary excitations if for almost every "low lying state" (admittedly a difficult concept to define), with energy  $E$  and momentum  $\underline{P}$  it is possible to find *uniquely*  $m$  sets of non-negative integers,  $n_j(\underline{p})$ , such that

$$\underline{P} = \sum_{\underline{p}} \sum_{j=1}^m \underline{p} n_j(\underline{p}) \quad (\text{VI.1})$$

and

$$E = \sum_{\underline{p}} \sum_{j=1}^m \epsilon_j(\underline{p}) n_j(\underline{p}) + 0(1/N). \quad (\text{VI.2})$$

Conversely, we require that for *every* choice of the  $m$  sets  $n_j(\underline{p})$ , the sums in (VI.1) and (VI.2) correspond to a pair in the spectrum.

We emphasize that the elementary excitation energies mean no more than stated above. In no sense is it implied that the corresponding wave functions have any simple relationship to each other. Moreover, there is no theorem that proves the possibility of describing the low lying states in this way. The one case, discussed in Section V, that we can solve completely, has a spectrum that almost, but not quite, fits into this pattern. The difficulty is that the sets  $n_j(\underline{p})$ , ( $j = 1, 2$ ), corresponding to a given state are not unique.

It is important to realize that an elementary excitation can *not* be defined as the lowest excitation energy for a given momentum. This is because a reasonable  $\epsilon(\underline{p})$  curve — one which has the additivity properties above — need not have a positive second derivative with respect to  $p$ . Nevertheless, Feynman [25, 26] has argued that for small  $\underline{p}$

there should be only one  $\epsilon(\underline{p})$  and that it should be given essentially by the variational energy of the wave function

$$\psi_{\underline{p}}(\underline{r}_1, \dots, \underline{r}_N) = \left[ \sum_{j=1}^N \exp(i \underline{p} \cdot \underline{r}_j) \right] \psi_0(\underline{r}_1, \dots, r_N), \quad (\text{VI.3})$$

where  $\psi_0$  is the exact ground state function. This turns out to be

$$\epsilon(\underline{p}) = (\hbar^2/2m)p^2[1 + \rho S(\underline{p})]^{-1} \quad (\text{VI.4})$$

where  $S(\underline{p})$  is the Fourier transform of the  $S(\underline{r})$  given in (IV.5). Now, Feynman and Cohen (cf. Appendix B of Reference [26]) argue that for small  $\underline{p}$ , the expansion of  $S$  is

$$S(\underline{p}) = -\rho^{-1} + A p, \quad (\text{VI.5})$$

where  $A$  is some constant which, if the first term (VI.5) is correct, would be inversely proportional to the velocity of sound. There does, in fact, exist [27] an almost rigorous proof that

$$\lim_{\underline{p} \rightarrow 0} S(\underline{p}) = -\rho^{-1} \quad (\text{VI.6})$$

for a Bose gas. For the two particle distribution function of a classical gas, on the other hand, it is a well known fact that

$$\lim_{p \rightarrow 0} S(\underline{p}) = -\rho^{-1} + kT \chi, \quad (\text{VI.7})$$

where  $\chi$  is the isothermal compressibility. It is therefore clear that the  $S(\underline{p})$  derived from a product trial function, (IV.3), with a finite range  $f$ , (IV.4), could not possibly be correct for small momentum. In addition, the fact that the second term in (VI.5) is linear – and not quadratic – in  $p$  means that for large  $r$ ,  $S(r) \sim r^{-\epsilon}$  where  $5 < \epsilon < 3$ . This is in agreement with the inverse fourth power behavior we obtained previously.

The reason for postulating the existence of elementary excitations is that were they to exist and be susceptible to calculation, then from them one could calculate the free energy of the system for low temperature. The canonical free energy,  $F$ , would be given by the well known boson formula:

$$F - E_0 = kT \sum_{\underline{p}} \sum_{j=1}^m \ln(1 - \exp(-\epsilon_j(\underline{p})/kT)). \quad (\text{VI.8})$$

For the one dimensional model of Section V,  $F$  can be calculated exactly in the  $\gamma = \infty$  limit because the spectrum is then the same as for a noninteracting Fermi gas. If we apply (VI.8) to *either* (V.26) *or* (V.27) alone, we indeed obtain the correct result for  $F - E_0$  at low temperature. But because (VI.9) instructs us to add together the  $j = 1$  and  $j = 2$  contributions, it would give a result twice the correct one.

It would seem then, that while the elementary excitation idea has some heuristic appeal, it is really an awkward method at best for calculating the free energy. In any

event it could only give the free energy for very low temperatures. If the free energy is to be computed, a more direct approach must be found.

A different concept is that of a *quasi-particle*. It is useful for calculating the result of a scattering experiment and is defined in terms of the propagator relevant to that experiment. Let us define the (advanced) propagator

$$\begin{aligned} G(\underline{k}, t) &= N^{-1} \langle \rho_{\underline{k}}(t) \rho_{-\underline{k}} \rangle, & t > 0 \\ &= 0, & t < 0 \end{aligned} \quad (\text{VI.9})$$

where  $\rho_{\underline{k}}$  is defined in (II.16) and

$$\rho_{\underline{k}}(t) = e^{iHt/\hbar} \rho_{\underline{k}} e^{-iHt/\hbar}. \quad (\text{VI.10})$$

The expectation value in (VI.9) is with respect to a thermal average, but for simplicity we shall consider only zero temperature, whence (VI.9) is a ground state expectation value. The time Fourier transform of  $G$  is

$$G(\underline{k}, \omega) = \int_0^\infty G(\underline{k}, t) e^{i\omega t} dt \quad (\text{VI.11})$$

and is analytic for  $\omega$  in the upper half plane. If we expand (VI.11) in terms of intermediate states  $|n\rangle$ , with energy  $\hbar\omega_n$  relative to  $E_0$  (these states must all have momentum  $\hbar\underline{k}$ ), then

$$G(\underline{k}, \omega) = i N^{-1} \sum_n |\rho_{\underline{k},n}|^2 (\omega - \omega_n)^{-1}, \quad (\text{VI.12})$$

where

$$\rho_{\underline{k},n} = \langle 0 | \rho_{\underline{k}} | n \rangle, \quad (\text{VI.13})$$

$\langle 0 |$  being the ground state. From (VI.12) we see that  $G(\underline{k}, \omega)$  is in fact analytic in the entire  $\omega$  plane, except for singularities on the positive real axis. For a finite system these singularities are poles at  $\omega_n$ . When we pass to the bulk limit these poles become dense and presumably take on the character of branch cuts and poles. In any event we can hopefully define a distribution  $S(\underline{k}, \omega)$  such that for any piecewise “smooth” function  $f(\omega)$

$$\lim_{N \rightarrow \infty} N^{-1} \sum_n |\rho_{\underline{k},n}|^2 f(\omega_n) = \int_0^\infty S(\underline{k}, \omega) f(\omega) d\omega. \quad (\text{VI.14})$$

If  $S$  turns out to be a reasonably piecewise smooth function of  $\omega$  then

$$S(\underline{k}, \omega) = \frac{1}{2\pi} [G_+(\underline{k}, \omega) - G_-(\underline{k}, \omega)], \quad (\text{VI.15})$$

where  $G_+$  and  $G_-$  are the respective limits of  $G$  from above and below the real axis. An interesting sum-rule is

$$\int_0^\infty S(\underline{k}, \omega) d\omega = N^{-1} \langle \rho_{\underline{k}} \rho_{-\underline{k}} \rangle = (1 + \rho S(\underline{k})). \quad (\text{VI.16})$$

Now, for a non-interacting Bose gas we would have

$$G(\underline{k}, t) = \exp(-i\omega(\underline{k})t), \quad t > 0 \quad (\text{VI.17})$$

with  $\omega(\underline{k}) = \hbar k^2/2m$ . Presumably (and there is no guarantee of this) for a gas with weak interactions we can find a time  $t_1$ , which is not too small to avoid transients, and a time  $t_2$ , which is not too large, such that (VI.17) is still true in the time interval  $(t_1, t_2)$ , i.e.,

$$G(\underline{k}, t) = \exp(-i\bar{\omega}(\underline{k})t), \quad t_1 < t < t_2, \quad (\text{VI.18})$$

where  $\bar{\omega}$  will now have a real part,  $\omega_0$ , and a negative imaginary part  $-\Gamma$ . If such a behavior were true, it *could* (but not necessarily) be accounted for by assuming that  $G(\underline{k}, \omega)$  had an analytic continuation from above the positive real axis into the lower half plane *and* that the analytic continuation had a simple pole at  $\omega_0 - i\Gamma$ . If so we would say that this pole *defines* a quasi-particle of energy  $\hbar\omega_0$  and a lifetime proportional to  $\Gamma^{-1}$ . Quasi-particles therefore decay, while elementary excitations, as defined above, do not. Clearly, however, even if the analytic continuation is possible and if the pole exists, there must also be other singularities below the real axis. As the interaction increases in strength, it becomes senseless to single out this one pole for special treatment.

It has been generally asserted, however, that if the interaction is not too strong then the quasi-particle energy  $\hbar\omega_0(\underline{k})$  and the  $\epsilon(\hbar\underline{k})$  that we defined before are approximately equal. There is very little mathematical justification for this premise, but if we accept it we are also entitled to look for poles in other propagators. For example, there is the advanced one-particle propagator, which is most conveniently described in second quantized language

$$\begin{aligned} G_A(\underline{k}, t) &= -i \langle a_{\underline{k}}(t) a_{\underline{k}}^{\dagger} \rangle, \quad t > 0 \\ &= 0, \quad t < 0 \end{aligned} \quad (\text{VI.19})$$

and the retarded one-particle propagator

$$\begin{aligned} G_R(\underline{k}, t) &= 0, \quad t > 0 \\ &= \langle a_{\underline{k}}^{\dagger} a_{\underline{k}}(t) \rangle, \quad t < 0. \end{aligned} \quad (\text{VI.20})$$

The time dependence is as in (VI.10).  $G_A$  and  $G_R$  differ from (VI.9) primarily in that in  $G_A$  the intermediate states have  $N + 1$  particles, while in  $G_R$  they have  $N - 1$  particles. Nevertheless, the same arguments can be made about cuts and quasi-particle poles on the second Riemann sheet. (In this case, however, we define the quasi-particle energy by adding or subtracting the chemical potential,

$$E_0(N + 1) - E_0(N),$$

from the position of the poles.) Hopefully, the quasi-particle poles of (VI.19) and (VI.20) have the same energy as that of (VI.9). If we were dealing with a proper relativistic field theory and poles in  $G_A$  and  $G_R$  would have to be at the same place for a given  $\underline{k}$ . But for our problem such symmetry is lacking and we may expect the two quasi-particle energies defined by (VI.19) and (VI.20) to be different. Is one to be considered more elementary than the other? Is it conceivable that the two  $\epsilon(\underline{p})$  curves that we found for the one-dimensional gas are approximately these two poles? Unfortunately, while we know the ground state wave functions for this system it has not in general been possible to calculate the necessary  $N$ -fold integrals to determine  $G$ .

The one case in which the propagator can be calculated exactly is when  $\gamma = \infty$  (cf. (V.17)). Here  $G$  (VI.9) can be found because when we insert wave functions defined by (V.21) into (VI.13) we may do the  $N$ -fold integral of the product of the two determinants over all space, without worrying about changes in sign as we go from region  $R_1$  to some other of the  $N!$  possible sub-regions. This means that our boson  $G$  will turn out to be the same as that for a one-dimensional non-interacting Fermi system. The result is that

$$G(k, \omega) = (i/N) \sum_p' [\omega - \beta(k^2 + 2p|k|)]^{-1}, \quad (\text{VI.21})$$

where  $\beta = \hbar/2m$  and the sum on  $p$  is such that  $|p| \leq K = \pi \rho$  and  $|p+k| > K$ . Replacing the sum by an integral in the usual way, we obtain in the bulk that

$$G(k, \omega) + (4\pi i \beta \rho |k|)^{-1} \ln \frac{\omega - \omega_1}{\omega - \omega_2}, \quad (\text{VI.22})$$

where

$$\begin{aligned} \omega_1/\beta &= (|k| + K)^2 - K^2 \\ \omega_2/\beta &= |K^2 - (|k| - K)^2|. \end{aligned} \quad (\text{VI.23})$$

It is interesting to note that upper branch point,  $\omega_1$ , is  $(1/\hbar)\epsilon_1$  found before (V.26). The lower branch point similarly corresponds to  $\epsilon_2$  (V.27) for  $k < 2K$ .

We observe that for this case  $G$  has a cut on the positive real axis, as expected, but it is a *finite* cut. Moreover,  $G$  is indeed analytically continuable through the cut but it has *no poles on the second sheet*. The question, which is so far unresolved, is whether or not a pole does exist for finite  $\gamma$ ? Does the pole move out to infinity as  $\gamma$  increases, or does it never exist at all?

The  $S(k, \omega)$  we obtain in this case (V.15) is

$$\begin{aligned} S(k, \omega) &= (4\pi\beta\rho|k|)^{-1} & \omega_2 < \omega < \omega_1 \\ &= 0 & \text{otherwise.} \end{aligned} \quad (\text{VI.24})$$

The importance of  $G$  for scattering is that from it one can calculate  $S$ . Suppose we scatter either X-rays or cold neutrons from the Bose gas. Hopefully we can treat the individual scattering events by the Born approximation (first order perturbation theory), in which case [28]

$$\partial^2 \sigma / \partial \Omega \partial e_f = N(m^2/8\pi^3 \hbar^5) (P_f/P_i) |V(\underline{k})|^2 S(\underline{k}, \omega). \quad (\text{VI.25})$$

The left hand side of (VI.25) is the differential scattering cross section per unit solid angle,  $\Omega$ , and per unit outgoing energy  $e_f$ . In the right hand side,  $P_f$  and  $P_i$  are the outgoing and incoming momenta, respectively,  $\hbar \underline{k} = \underline{P}_f - \underline{P}_i$  and  $\hbar \omega = e_i - e_f$ .  $V(\underline{k})$  is the Fourier transform of the elementary interaction potential between the scattering particles and the particles of the gas. It should be noted that even if it is agreed that the Born approximation is appropriate for a single scattering, it has not been proved that

the Born approximation can be applied to the entire gas at once (as in (VI.25)) in the bulk limits  $N \rightarrow \infty$ .

For a fixed momentum transfer,  $\hbar\mathbf{k}$ ,  $S$  determines the inelastic cross section. This can be measured with neutrons, but in the case of X-rays it is impossible to resolve  $S$  for each value of  $\omega$ . All that can be measured is the integrated value of  $S$ , (VI.16), which means that X-rays measure the structure factor  $S(\mathbf{k})$ . Unfortunately there is a limit to how low  $k$  can be made experimentally. Nevertheless, it does appear that for liquid helium the right hand side of (VI.16) does vanish as  $k \rightarrow 0$ , in conformity with our prediction, (VI.6).

It is found experimentally with liquid helium that for a fixed  $\mathbf{k}$ ,  $S$  has a pronounced peak at a certain  $\omega$  associated with that  $\mathbf{k}$ . This result would *tend* to confirm (VI.18) as well as the notion of a quasi-particle pole. On the other hand, it does not prove the existence of a pole. Indeed, from our calculation on the one-dimensional gas we see from (VI.24) that for small  $k$  the cross section is *strongly* peaked about  $\omega = 2\pi\rho k$ . Nevertheless, there is no quasi-particle pole in this case.

It would appear from our formula, (VI.12), that calculating  $G$  involves considerable knowledge of the excited state wave function, as well as of their energies. Such an approach is much too complicated and, fortunately, there is a simpler method. Consider the original Hamiltonian (II.1) with the addition of an impurity particle of mass  $M$ , position  $\underline{y}$ , and interaction potential with the Bose particles  $\lambda u(\underline{y} - \underline{x})$ . The total Hamiltonian is then

$$H = -\hbar^2/2m \sum_1^N \nabla_i^2 - \hbar^2/2M \nabla_{\underline{y}}^2 + \sum_{i < j} v(\underline{r}_i - \underline{r}_j) + \lambda \sum_{j=1}^N u(\underline{y} - \underline{x}_j). \quad (\text{VI.26})$$

If we compute the insertion energy,  $\Delta E$  (= difference in ground state energy with and without the impurity), up to second order in  $\lambda$  we easily obtain

$$\begin{aligned} \Delta E &= -(i\lambda^2\rho/\hbar L) \sum_{\mathbf{k}} |\mu(\mathbf{k})|^2 G(\mathbf{k}, -\omega), \\ &= -(i\lambda^2\rho/2\pi\hbar) \int d^3k |\mu(\mathbf{k})|^2 G(\mathbf{k}, -\omega). \end{aligned} \quad (\text{VI.27})$$

Here,  $\omega = \hbar k^2/2M$  and  $\mu$  is the Fourier transform of  $u$ . Now, let us suppose that by some independent method we can calculate the ground state energy of (VI.26) to second order in  $\lambda$  only, but for *arbitrary*  $u$  and  $M$ . We have in mind the method of Section IV (Eq. (IV.9) *et seq.*), but we shall not pursue the calculation here. Since  $M$  is arbitrary we will then have an expression for  $G$  for all  $\mathbf{k}$  and all negative real  $\omega$ .  $G$  may then be extended to positive  $\omega$  by analytic continuation, and a test of whether or not the approximation for  $\Delta E$  was sensible is whether or not the continued  $G$  is free of singularities except on the positive, real  $\omega$  axis.

Thus, the calculation of the desired  $S$  can be reduced to a ground state energy problem. In a sense we have come full circle because we have already observed, in connection with



the Bogoliubov approximation, that the ground state ought to contain a good deal of information about the excited states. What we have said above is that from the mathematical point of view the shift in the ground state energy caused by an impurity particle is as good a probe of the system as the scattering of neutrons.

If one dislikes the idea of analytically continuing an approximate function to find the jump across its cut on the positive, real axis (VI.15), then there does exist a formula that relates  $G$  on the negative axis (where we have some confidence in the approximation) directly to experiment, namely

$$\int_0^{\infty} S(\underline{k}, \omega')(\omega' + \omega)^{-1} d\omega' = iG(\underline{k}, -\omega), \quad (\text{VI.28})$$

for positive  $\omega$ . Thus, the quantity obtained by computing  $\Delta E$  is directly the Stieltjes transform of the scattering cross section.

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