discussed in I, this feature appears already in a perturbation evaluation of the energy, as has been emphasized by Huang and Yang.[4] The rigidity against particle excitation manifests itself in the peculiar excitation spectrum which, as evaluated in this paper for a hard-sphere gas, has the essential features of the phonon-roton spectrum deduced by Landau from experiment. The energy of the system cannot be evaluated, except at very low density, by perturbation methods based on an expansion in powers of $(\rho a^3)^{\frac{1}{2}}$. As we have shown, however, reasonably accurate nonperturbation methods can be used for densities such as those of He^4.

These methods are being at present extended to a study of the λ-transition region in He^4 which will be published separately.

VII. ACKNOWLEDGMENTS

The authors are deeply indebted to Professor C. N. Yang for valuable discussions on the methods used by himself and Professor T. D. Lee in their studies on the boson system.[5]

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PHYSICAL REVIEW VOLUME 106, NUMBER 6 JUNE 15, 1957

Eigenvalues and Eigenfunctions of a Bose System of Hard Spheres and Its Low-Temperature Properties

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(Received March 19, 1957)

It is shown that the pseudopotential method can be used for an explicit calculation of the first few terms in an expansion in power of $(\rho a^3)^{\frac{1}{2}}$ of the eigenvalues and the corresponding eigenfunctions of a system of Bose particles with hard-sphere interaction. The low-temperature properties of the system are discussed.

THIS paper is concerned with the low-temperature properties of a dilute system of Bose particles with hard-sphere interactions, at a low but finite density. An explicit mathematical calculation is made of the energies and wave functions of the ground state and the low-lying excited states. The results confirm the usual notion of phonon waves as the only low-lying excitation, and the idea of momentum space ordering. One concludes from the calculation that such a system does show superfluidity and exhibit the two-fluid behavior at low temperatures.

It may be appropriate here to describe the motivation underlying the study of a system of hard spheres. One would like, of course, to study the general many-body problem with any potential of interaction between the particles. Such a program can be formalistically carried out. It is, however, generally recognized that to draw any definite physical conclusions from such a general program is very difficult. If one makes approximations on the general problem in order to arrive at concrete results, one usually encounters the great difficulty of defining and justifying the validity of the approximation made. We therefore start instead from the concrete model of hard-sphere interactions, which is sufficiently simple so that one might hope to be able to discuss the validity of the method of approach.

The interaction between real He atoms contains besides a hard repulsive core, also an attractive interaction outside of the core. This attractive interaction is responsible for many properties of the He liquid. For example, the ground state of a system of He atoms is known to have a negative energy corresponding to a binding energy per He atom of $(k\times 7°)$, as determined from the experimental vapor pressure curve near the absolute zero of temperature. Such a bound system owes its origin, of course, to the attractive force. The strength of the attractive force also determines the density of the He atoms in the ground state. Now at this density the total attractive potential that a He atom experiences from its neighbors is expected not to fluctuate very much. This fact suggests the following approximate picture: One replaces the attractive interparticle forces by a constant uniform negative external potential that acts on the individual particles, the repulsive core is retained, and the system is kept by an external pressure at a density equal to that of the ground state of He. Many qualitative features of the behavior of this hypothetical model may then be expected to resemble those of real He. Since the uniform external potential does not influence the system except to give it a negative total energy, one may consider simply a system of hard spheres at a given density and in the end add the external potential separately. This kind of reasoning is essentially contained in the work

of London[1] on the density and the energy of liquid He in the ground state.

In Secs. 1 and 2 the method of the pseudopotential[2,3] is applied to the problem. It is seen that the energy per particle in the ground state and the energy level spectrum near the ground state can be very easily obtained as power series expansions in the parameter $(\rho a^3)^{\frac{1}{2}}$, where ρ is the particle density and a the hard-sphere diameter. That the expansion parameter should be $(\rho a^3)^{\frac{1}{2}}$ was already pointed out before.[4] The ground state energy per particle calculated with the present method agrees with that given in reference 4. The excited levels immediately above the ground state represent "phonon" states. The excitation spectrum is the same as that of Bogoliubov's.[5]

In Sec. 3 the same method is used to calculate the wave functions for the ground state, and the pair distribution function for the ground state. The results are compared with the work of Feynman[6] and of Penrose and Onsager.[7] It emerges from these results that one can define a "correlation length" which characterizes the spatial extension of the correlation introduced by the hard-sphere interactions.

Section 4 is devoted to a critical discussion of the validity of the method of the pseudopotential in the present problem. The order of magnitude of the expected corrections to the present calculation is analyzed.

In Sec. 5 the physical properties of a dilute system of a gas of hard spheres are discussed briefly on the basis of the energy spectrum obtained in Sec. 2. The energy spectrum near the ground state is shown to be that of a collection of "phonons." The properties of the system, such as the existence of a normal fluid and a superfluid component, can therefore be inferred immediately from the work of Landau,[8] Kramers,[9] and others.[9]

In Sec. 6 the concept of a "correlation length" introduced in Sec. 3 is further emphasized, and related to London's idea[10] of an order in momentum space. The question of the flow of the superfluid is discussed by the method of Sec. 1. It is indicated that the superfluid flow is irrotational, as was pointed out by Onsager and Feynman.[11]

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1. GROUND STATE ENERGY

We use mostly the same notation as that of reference 2 but choose units so that $\hbar=1$, $2m=1$, and recall that the Hamiltonian of a system of hard spheres can be replaced in certain approximations by the pseudopotential Hamiltonian [see Eqs. (32) and (33) of reference 2]:

$$H=-\sum_{i=1}^{N}\nabla_i^2+V,$$
$$V=8\pi a\sum_{i<j}\delta(\mathbf{r}_i-\mathbf{r}_j)\frac{\partial}{\partial r_{ij}}r_{ij}. \tag{1}$$

By using the language of quantized fields, the pseudopotential V can be recast in the form [see Eq. (38) of reference 2]:

$$V=4\pi a\int d^3\mathbf{r}_1 d^3\mathbf{r}_2\psi^*(\mathbf{r}_1)\psi^*(\mathbf{r}_2)\delta(\mathbf{r}_1-\mathbf{r}_2)\frac{\partial}{\partial r_{12}}\times[r_{12}\psi(\mathbf{r}_1)\psi(\mathbf{r}_2)]. \tag{2}$$

We shall not enter here into a discussion of the region of validity of the use of the pseudopotential, a subject that we shall come back to in Sec. 4. In the present section and the next section it will be shown that the pseudopotential (2) leads directly and simply to an expression of the ground state energy per particle of the Bose gas and to the energy spectrum near the ground state.

It was already observed and emphasized in reference 2 that the pseudopotential V, when operating on a wave function that is not singular at $r_{ij}=0$, is equivalent to the operator

$$V'=4\pi a\int d^3\mathbf{r}_1 d^3\mathbf{r}_2\psi^*(\mathbf{r}_1)\psi^*(\mathbf{r}_2)\delta(\mathbf{r}_1-\mathbf{r}_2)\psi(\mathbf{r}_1)\psi(\mathbf{r}_2). \tag{3}$$

It was further observed that using the potential (3) leads to divergences which arise from the singularities of the correct wave function. The use of the correct pseudopotential V, however, does not lead to any divergencies. For clarity we shall adopt the following procedure in the present paper. The potential V' will first be used to compute the ground state energy per particle. It will be found that the expression obtained is divergent, as expected. It will then be easy to see that substituting the correct pseudopotential V, [Eq. (2)], for the potential V', [Eq. (3)], in the calculation leads very simply to a subtraction procedure which yields a correct finite result.

By expanding ψ into free-particle waves as was done in reference 2, we obtain

$$V'=\Omega^{-1}4\pi a\sum_{\alpha,\beta,\mu,\nu}a_\alpha^* a_\beta^* a_\mu a_\nu\delta(\mathbf{k}_\alpha+\mathbf{k}_\beta-\mathbf{k}_\mu-\mathbf{k}_\nu), \tag{4}$$

where a_α^* and a_α are, respectively, the creation and

annihilation operators of the free-particle states with momentum $\mathbf{k}_\alpha$, and $\Omega=L^3$ is the volume of the cube in which the N particles move. The delta symbol $\delta(\mathbf{k}_\alpha+\mathbf{k}_\beta-\mathbf{k}_\mu-\mathbf{k}_\nu)$ appearing in (4) is a Kronecker delta function. It is essential that the boundary condition at the edge of the box be taken to be the usual periodicity condition [compare reference 17]. The diagonal elements of (4) are

$$\langle n|V'|n\rangle=\Omega^{-1}4\pi a(2N^2-N-\textstyle\sum_\alpha n_\alpha^2), \tag{5}$$

where n_α is the occupation number $a_\alpha^* a_\alpha$. Equation (5) has already been obtained in reference 2. Subtracting a constant term $4\pi a\rho(N-1)$ from expression (5), one obtains

$$\langle n|V'|n\rangle-4\pi a\rho(N-1)$$
$$=8\pi a\rho\sum_{\alpha\neq 0} n_\alpha-\frac{4\pi a}{\Omega}\Big(\sum_{\alpha\neq 0} n_\alpha\Big)^2-\frac{4\pi a}{\Omega}\sum_{\alpha\neq 0} n_\alpha, \tag{6}$$

with $\rho=N/\Omega$. If one takes a system for which the density ρ is fixed and for which N and Ω both approach infinity, Eq. (6) reduces to[12]

$$\langle n|V'|n\rangle-4\pi a\rho N=8\pi a\rho\sum_{\alpha\neq 0} n_\alpha. \tag{7}$$

The off-diagonal matrix elements of the potential V' cause transitions in which two particles of momenta $\mathbf{k}_\alpha$ and $\mathbf{k}_\beta$ collide and go into the states $\mathbf{k}_\mu$ and $\mathbf{k}_\nu$. The periodicity boundary condition that we took insures that the matrix element is nonvanishing only if momentum is conserved: $\mathbf{k}_\alpha+\mathbf{k}_\beta=\mathbf{k}_\mu+\mathbf{k}_\nu$. The value of such an off-diagonal matrix element is equal to

$$(4\pi a/\Omega)[n_\alpha n_\beta(n_\mu+1)(n_\nu+1)]^{\frac{1}{2}}. \tag{8}$$

The crucial point is now to observe that as the total number of particles N approaches infinity, each of the n_α's is finite except n_0, which is $N-\sum_{\alpha\neq 0} n_\alpha$. For large values of N, the off-diagonal matrix elements fall into three categories in magnitude:

(1) Those in which two of the four momenta $\mathbf{k}_\alpha$, $\mathbf{k}_\beta$, $\mathbf{k}_\mu$, $\mathbf{k}_\nu$ are equal to 0. Such matrix elements are proportional to $8\pi a\rho$.

(2) Those for which only one of the four momenta $\mathbf{k}_\alpha$, $\mathbf{k}_\beta$, $\mathbf{k}_\mu$, $\mathbf{k}_\nu$ is equal to 0. Such matrix elements are smaller than those of the first category by a factor $N^{-\frac{1}{2}}$.

(3) Those for which none of the four momenta $\mathbf{k}_\alpha$, $\mathbf{k}_\beta$, $\mathbf{k}_\mu$, $\mathbf{k}_\nu$ is 0. Such matrix elements are smaller than those of the category (1) by a factor N^{-1}.

[12] The neglect of the second and third terms of the right hand side of (6) as compared to the first term is consistent with the power series expansion of the energy in the parameter $(\rho a^3)^{\frac{1}{2}}$. It is shown later [see (41)] that

$$N^{-1}\langle\sum_{\alpha\neq 0} n_\alpha\rangle\sim(\rho a^3)^{\frac{1}{2}},$$

where the expectation value is taken with respect to the *perturbed* ground state of the total system.

Starting from the free-particle ground state, by first considering only matrix elements of category (1), we would obtain the dominant term of the energy of the system. The matrix elements of categories (2) and (3) will later be shown in Sec. 4 to give rise to higher order corrections. To calculate the dominant term of energy, we thus need *only consider those free-particle states S which are connected to the free-particle ground state, directly or indirectly, through off-diagonal matrix elements of category* (1), i.e., matrix elements that represent the scattering of two particles of momenta $\mathbf{k}$ and $-\mathbf{k}$ into the ground state or vice versa. Evidently a state in S is specified by l_1 pairs of particles each with momenta $\mathbf{k}_1$ and $-\mathbf{k}_1$, l_2 pairs of particles each with momenta $\mathbf{k}_2$ and $-\mathbf{k}_2$, etc., and $N-2\sum l_i$ particles with momentum zero. We denote such a state by

$$|l_1, l_2, \cdots\rangle. \tag{9}$$

In terms of the annihilation operators $a_\mathbf{k}$, where $\mathbf{k}\neq 0$ ranges over *half* of the momentum space, we can write down the diagonal matrix elements (7) for the pseudopotential V' between the states of S:

$$4\pi a\rho N+16\pi a\rho\sum{}' a_\mathbf{k}^* a_\mathbf{k}, \tag{10}$$

where $\sum'$ represents a summation over *half* of the $\mathbf{k}$ space with $\mathbf{k}\neq 0$. The off-diagonal matrix elements of V' are given by those of

$$8\pi a\rho\sum{}' B_0(k), \tag{11}$$

where

$$B_0(\mathbf{k})=\begin{bmatrix}0&1&0&0&\\1&0&2&0&\\0&2&0&3&\\0&0&3&0&\\&&&&\cdots\end{bmatrix}, \tag{12}$$

in the standard representation in which $a_\mathbf{k}^* a_\mathbf{k}$ is diagonal:

$$a_\mathbf{k}^* a_\mathbf{k}=\begin{bmatrix}0&0&0&0&\\0&1&0&0&\\0&0&2&0&\\0&0&0&3&\\&&&&\cdots\end{bmatrix}. \tag{13}$$

One has evidently the commutation relations

$$0=[B_0(\mathbf{k}),a_{\mathbf{k}'}]=[B_0(\mathbf{k}),a_{\mathbf{k}'}^*] \quad \text{if} \quad \mathbf{k}\neq\mathbf{k}'. \tag{14}$$

The Hamiltonian $H'=-\sum\nabla_i^2+V'$ between the states of S is then

$$H'=4\pi a\rho N+2\sum{}'(k^2+k_0^2)[a_\mathbf{k}^* a_\mathbf{k}+y_\mathbf{k}B_0(\mathbf{k})], \tag{15}$$

where

$$k_0^2=8\pi a\rho, \tag{16}$$

$$y_\mathbf{k}=\tfrac{1}{2}k_0^2(k^2+k_0^2)^{-1}. \tag{17}$$

The summation $\sum'$ in (15) is a sum of mutually commuting operators. Its lowest eigenvalue is therefore the sum of the lowest eigenvalues of the individual

terms. It will be shown in Appendix I that the eigenvalues of

$$a^*a+yB_0$$

are

$$\lambda_m=-\tfrac{1}{2}+(m+\tfrac{1}{2})(1-4y^2)^{\frac{1}{2}}, \tag{18}$$

with $m=0, 1, 2, \cdots$. One thus obtains the lowest eigenvalue of the Hamiltonian (15):

$$\begin{aligned}E_0'&=4\pi a\rho N+\sum'(k^2+k_0^2)[-1+(1-4y_k^2)^{\frac{1}{2}}]\\&=4\pi a\rho N-\sum'[k^2+k_0^2-k(k^2+2k_0^2)^{\frac{1}{2}}].\end{aligned} \tag{19}$$

The above expression contains a spurious term which makes the sum divergent. This is because we have used V' instead of the correct pseudopotential V. The situation is easily remedied by identifying the spurious term and subtracting it.

The correct interaction V, Eq. (2), expressed in momentum space, reads

$$\begin{aligned}V=\lim_{r\to 0}4\pi a\Omega^{-1}\frac{\partial}{\partial r}\{r\sum_{\mu,\nu}\exp[\tfrac{1}{2}i(\mathbf{k}_\mu-\mathbf{k}_\nu)\cdot\mathbf{r}]\\\times\sum_{\alpha,\beta}a_\alpha^*a_\beta^*a_\mu a_\nu\delta(\mathbf{k}_\alpha+\mathbf{k}_\beta-\mathbf{k}_\mu-\mathbf{k}_\nu)\}.\end{aligned} \tag{20}$$

It can be seen that the replacement of (4) by (20) does not affect in any essential way the general arguments that led to the Hamiltonian (15), which is now replaced by

$$\begin{aligned}H=4\pi a\rho N+2\sum'(k^2+k_0^2)a_k^*a_k\\+\tfrac{1}{2}k_0^2\operatorname*{Lim}_{r\to 0}\frac{\partial}{\partial r}\{r\sum_{k\neq 0}e^{i\mathbf{k}\cdot\mathbf{r}}B_0(\mathbf{k})\}.\end{aligned} \tag{21}$$

Using this Hamiltonian, the calculation of E_0 proceeds in the same way as before except that in the final expression (19), the simple sum over $\mathbf{k}$ is replaced by a limiting process, namely

$$\begin{aligned}E_0=4\pi a\rho N-\tfrac{1}{2}\operatorname*{Lim}_{r\to 0}\frac{\partial}{\partial r}\{r\sum_{k\neq 0}e^{i\mathbf{k}\cdot\mathbf{r}}[k^2+k_0^2\\-k(k^2+2k_0^2)^{\frac{1}{2}}]\}.\end{aligned} \tag{22}$$

The mathematical problem of evaluating this expression is similar to the corresponding problems encountered in reference 2. It can be shown without difficulty that

$$E_0=4\pi a\rho N-\sum'\left[k^2+k_0^2-k(k^2+2k_0^2)^{\frac{1}{2}}-\frac{k_0^4}{2k^2}\right]. \tag{23}$$

The sum can easily be evaluated in the limit $\Omega\to\infty$:

$$\begin{aligned}E_0=4\pi a\rho N+\frac{\Omega k_0^5}{4\pi^2}\int_0^\infty dy y^2\Big[-1-y^2\\+y(y+2)^{\frac{1}{2}}+\frac{1}{2y^2}\Big],\end{aligned} \tag{24}$$

or

$$E_0=4\pi aN\rho\left[1+\frac{128}{15\sqrt{\pi}}(a^3\rho)^{\frac{1}{2}}\right], \tag{25}$$

a result which was first obtained in reference 4 by the "binary collision expansion method."

Another way of proving that the correct pseudopotential V of Eq. (1) leads to the convergent expression (23) while V' leads to the divergent one [Eq. (19)] is the following: Treating the pseudopotential V or V' as a perturbation, one can calculate the ground state energy E_0 as a power series expansion in a. This was the procedure followed in reference 2. In the order a^2, using the potential V', one obtains a divergent expression. Using the correct pseudopotential V, however, one obtains zero in the order a^2. [See Eq. (53) below. Notice that $a/L=0$ in the limit $L\to\infty$.] Except for the order a^2, V and V' give the same results. [We stay here within the approximation of neglecting small off-diagonal matrix elements. As will be discussed in Sec. 4, this approximation is equivalent to retaining the maximum power of N to each order of a.] To obtain the energy expression when V is used, one therefore need only take the divergent expression (19) for the case of V' and expand it in powers of a and strike out the term a^2. Now

$$\sum'[k^2+k_0^2-k(k^2+2k_0^2)^{\frac{1}{2}}]=\sum'\left[\frac{k_0^4}{2k^2}-\frac{k_0^6}{2k^4}+\cdots\right],$$

$$k_0^2=8\pi a\rho.$$

Striking out the term a^2 therefore means subtracting from the summand $k_0^4/2k^2$, leading immediately to (23). We shall return to this discussion in Sec. 4.

2. ENERGY LEVELS NEAR THE GROUND STATE; PHONON SPECTRUM

The method of the last section can also be applied to discuss the energy of a state with a nonvanishing momentum. We start from an unperturbed state $|\mathbf{q}\rangle$ in which all particles have momentum zero except one, which has momentum $\mathbf{q}$. The set of unperturbed states, denoted by S', connected to $|\mathbf{q}\rangle$ by large off diagonal matrix elements are all of the form

$$|\mathbf{q};l_q;l_1,l_2,\cdots\rangle, \tag{26}$$

which means that there is a particle of momentum $\mathbf{q}$, and in addition, there are l_q pairs of particles $\mathbf{q}, -\mathbf{q}$; l_1 pairs $\mathbf{k}_1, -\mathbf{k}_1$; l_2 pairs $\mathbf{k}_2, -\mathbf{k}_2$; etc., with $\mathbf{k}_i\neq\mathbf{q}$. The rest of the particles, $(N-2\sum l_i-1)$ in number, have momentum $\mathbf{k}=0$. The total momentum of every state in S' is $\mathbf{q}$. The Hamiltonian H' for the states S' is very similar to that for the states S given before by Eq. (15). It is

$$\begin{aligned}H'=4\pi a\rho N+2\sum_{k\neq q}'(k^2+k_0^2)[a_k^*a_k+y_kB_0(\mathbf{k})]\\+2(q^2+k_0^2)[N_q+y_qB_1(\mathbf{q})]+8\pi a\rho+q^2,\end{aligned} \tag{27}$$

where

$$N_{\mathbf{q}}=\begin{pmatrix}0&0&0&0&\\0&1&0&0&\\0&0&2&0&\\0&0&0&3&\\&&&&\cdots\end{pmatrix} \tag{28}$$

has diagonal values equal to $l_{\mathbf{q}}$, and

$$B_1(\mathbf{q})=\begin{pmatrix}0&(1\times2)^{\frac{1}{2}}&0&\\(1\times2)^{\frac{1}{2}}&0&(2\times3)^{\frac{1}{2}}&\\0&(2\times3)^{\frac{1}{2}}&0&\\&&&\cdots\end{pmatrix}. \tag{29}$$

The matrix $B_0(\mathbf{k})$ is given by Eq. (12). The eigenvalue of $N+yB_1$ is discussed in Appendix I. The lowest eigenvalue is

$$-1+[1-4y^2]^{\frac{1}{2}}. \tag{30}$$

The difference of the lowest eigenvalue of (27) and that of (15) is the energy of excitation into a state of momentum $\mathbf{q}$. From (30) and (18) it is evidently equal to[13]

$$E_{\mathbf{q}}-E_0=q(q^2+2k_0^2)^{\frac{1}{2}}=q(q^2+16\pi a\rho)^{\frac{1}{2}}. \tag{31}$$

It will be shown in Appendix II that the wave function in coordinate space for the state we just discussed, i.e., for the lowest excited state with momentum $\mathbf{q}$, is to the order of approximation considered equal to

$$\sum_{j=1}^{N} e^{i\mathbf{q}\cdot\mathbf{r}_j}\Psi_0,$$

where Ψ_0 is the wave function of the ground state. This means that these excitations are density fluctuations (i.e., sound waves, or phonons), as has been discussed by Bijl[14] and Feynman.[6]

The velocity v of sound waves of infinite wavelength is directly related to the macroscopic compressibility, which can in turn be computed from the energy expression Eq. (25) for the ground state. In fact, remembering that in our units $m=\frac{1}{2}$, one has

$$v=\left(2\frac{dp}{d\rho}\right)^{\frac{1}{2}}, \quad \text{and} \quad p=\rho^2\frac{d}{d\rho}(E_0/N). \tag{32}$$

Equations (25) and (32) together give

$$v=(16\pi a\rho)^{\frac{1}{2}}[1+16\pi^{-\frac{1}{2}}(a^3\rho)^{\frac{1}{2}}]. \tag{33}$$

The first term of (33) agrees with the velocity that one computes from (31) for the sound waves with momentum $\mathbf{k}=0$, as it should. The second term in (33) represents a correction term that is beyond the accuracy of (31).

In an entirely similar way, one can solve other eigenvalues and eigenstates of the Hamiltonian (1), by considering the excited states of (15) and (27) and also considering the states connected to an unperturbed state that contains more than one particle having nonvanishing momentum. This is discussed in detail in Appendix I. The eigenvalues for these states can be shown to be

$$E=E_0+\sum_{\mathbf{k}\neq0} m_{\mathbf{k}}k(k^2+16\pi a\rho)^{\frac{1}{2}}, \tag{34}$$

with the corresponding total momentum

$$\mathbf{P}=\sum m_{\mathbf{k}}\mathbf{k}, \quad m_{\mathbf{k}}=0,\ 1,\ 2,\ \cdots. \tag{35}$$

They represent therefore states with $m_{\mathbf{k}}$ phonons of momentum $\mathbf{k}$.

3. WAVE FUNCTIONS AND THE PAIR DISTRIBUTION FUNCTION

The ground state wave function Ψ_0 of the Hamiltonian (15) can be written in terms of the free-particle states $|l_1,l_2,\cdots\rangle$ [Eq. (9)] as

$$\Psi_0=\sum_{l_i=0}^{\infty} A(l_1,l_2,\cdots)\,|l_1,l_2,\cdots\rangle, \tag{36}$$

with $A(l_1,l_2,\cdots)$ representing the probability amplitudes. The value of $A(l_1,l_2,\cdots)$ is found to be (see Appendix I)

$$A(l_1,l_2,\cdots)=C\prod_i{}'[-\alpha(\mathbf{k}_i)]^{l_i}, \tag{37}$$

where

$$\alpha(\mathbf{k})=(8\pi a\rho)^{-1}[k^2+8\pi a\rho-k(k^2+16\pi a\rho)^{\frac{1}{2}}], \tag{38}$$

and C is a normalization constant given by

$$C=\prod_i{}'[1-\alpha^2(\mathbf{k}_i)]^{\frac{1}{2}}. \tag{39}$$

In Eqs. (37) and (39) the product $\prod_i'$ extends over half of the $\mathbf{k}$ space with $\mathbf{k}_i\neq0$.

Upon using Eq. (37), it is easy to compute the average occupation number $\langle n_{\mathbf{k}}\rangle$ of the free-particle states with momentum $\mathbf{k}$ for the ground state wave function Ψ_0. One finds

$$\langle n_{\mathbf{k}}\rangle=\frac{\alpha^2(\mathbf{k})}{1-\alpha^2(\mathbf{k})} \quad \text{for} \quad \mathbf{k}\neq0, \tag{40a}$$

and

$$\langle n_{\mathbf{k}=0}\rangle=N\left[1-\frac{8}{3\sqrt{\pi}}(\alpha^3\rho)^{\frac{1}{2}}\right], \tag{40b}$$

where N is the total number of particles and $\langle\ \rangle$ means taking the average over the ground state of the system. For an ideal Bose system the ground state of the system is characterized by the fact that all particles are in the free-particle ground state. In the present case, owing to the interactions, particles are excited from the state, $\mathbf{k}=0$, into various free-particle states

[13] To calculate the excitation energy $(E_{\mathbf{q}}-E_0)$, the identical result is obtained by using either V' [Eq. (3)] or the correct pseudopotential V [Eq. (2)].

[14] A. Bijl, Physica 7, 869 (1940).

with $\mathbf{k}\neq 0$. Let f be the total fractional number of particles excited. We find for the ground state of the entire system, this fraction is

$$f\equiv N^{-1}\sum_{\mathbf{k}\neq 0}\langle n_{\mathbf{k}}\rangle=\frac{8}{3\sqrt{\pi}}(\rho a^3)^{\frac{1}{2}}. \tag{41}$$

It is important to note that the occupation number of the free-particle ground state $\langle n_{\mathbf{k}=0}\rangle$ is proportional to N while all the other free-particle states have finite occupation numbers as $N\to\infty$. The significance of these free-particle state occupation numbers in the discussion of a Bose system with interactions has recently been pointed out and emphasized by Penrose and Onsager.[7]

Another important quantity is the pair distribution function $D(r_{12})$, defined by

$$D(r_{12})\equiv\rho^{-2}\langle\psi^*(\mathbf{r}_1)\psi^*(\mathbf{r}_2)\psi(\mathbf{r}_2)\psi(\mathbf{r}_1)\rangle. \tag{42}$$

The pair distribution function $D(r)$ describes the relative probability for finding two particles at a distance r apart. The normalization of the function is so chosen that $D(r)\to 1$ as $r\to\infty$. By using Eqs. (36)–(39), the function $D(r)$ can be readily evaluated. It is

$$D(r)=[1+G(r)]^2+[1+F(r)]^2-1-4f[G(r)+F(r)], \tag{43}$$

where

$$F(r)=\frac{1}{8\pi^3\rho}\int\frac{\alpha^2(\mathbf{k})}{1-\alpha^2(\mathbf{k})}e^{i\mathbf{k}\cdot\mathbf{r}}d^3\mathbf{k},$$
$$G(r)=-\frac{1}{8\pi^3\rho}\int\frac{\alpha(\mathbf{k})}{1-\alpha^2(\mathbf{k})}e^{i\mathbf{k}\cdot\mathbf{r}}d^3\mathbf{k}, \tag{44}$$

with f and $\alpha(\mathbf{k})$ given by Eq. (41) and Eq. (38). To study the behavior of these two functions F and G, it is convenient to introduce a "correlation length" r_0, defined as

$$r_0\equiv(8\pi a\rho)^{-\frac{1}{2}}. \tag{45}$$

r_0 is the inverse of k_0 introduced in Eq. (16). For $r\gg r_0$, the functions F and G approach, respectively,

$$F(r)\to+\frac{1}{\pi^2\rho r_0 r^2}$$
and (46)
$$G(r)\to-\frac{1}{\pi^2\rho r_0 r^2},$$

while for small distances $r\ll r_0$,

$$F(r)\to f=\frac{8}{3\sqrt{\pi}}(\rho a^3)^{\frac{1}{2}}$$
and (47)
$$G(r)\to-\frac{a}{r}+\frac{8}{\sqrt{\pi}}(\rho a^3)^{\frac{1}{2}}.$$

Correspondingly, we see that for $r\ll r_0$,

$$D(r)\to\left(1-\frac{a}{r}\right)^2+O\left(\frac{a}{r_0}\right)$$

and for $r\gg r_0$,

$$D(r)\to 1+O\left(\frac{1}{r^4}\right). \tag{48}$$

Thus the correlation length r_0 characterizes the extension of the correlation between particles introduced by the hard-sphere interaction. Qualitative discussion of the physical implications of this correlation length will be given in Sec. 6.

It is of interest to compare the present result with the work of Feynman.[6] The function $S(\mathbf{k})$ in Feynman's paper can be defined in terms of the Fourier transform of $D(r)$ as

$$S(\mathbf{k})\equiv 1+\rho\int D(r)e^{i\mathbf{k}\cdot\mathbf{r}}d^3\mathbf{k}. \tag{49}$$

From Eq. (44), one finds

$$S(\mathbf{k})=k(k^2+16\pi a\rho)^{-\frac{1}{2}}[1+O(\rho a^3)^{\frac{1}{4}}],\quad(\mathbf{k}\neq 0). \tag{50}$$

Substitution into the Feynman-Bijl relation[6,14] for the phonon energy,

$$E_{\mathbf{k}}-E_0=k^2/S(\mathbf{k}) \tag{51}$$

leads to

$$E_{\mathbf{k}}-E_0=k(k^2+16\pi a\rho)^{-\frac{1}{2}}, \tag{52}$$

in agreement with Eq. (31). This is not surprising since we shall see in Appendix II that the wave functions of the excited states have the form used by Feynman and Bijl from which Eq. (51) was derived.[6]

4. CRITICAL DISCUSSION OF THE VALIDITY OF THE PSEUDOPOTENTIAL METHOD FOR THE PRESENT PROBLEM

The method used in the present paper evokes many questions concerning its validity. In particular the following points need be analyzed:

(1) It has been emphasized in reference 2 that the pseudopotential (1) is in general accurate only to the order a^2, and that as applied to the ground state energy it is only accurate to the order a^3. The approximations involved include the neglect of the D-wave scattering and the genuine triple collisions as explained in Fig. 2 of reference 2. In the present paper we have used the pseudopotential (1) to calculate quantities which certainly involve contributions from infinitely high powers of a. How could one then be sure that such use of the pseudopotential is justified? Also, in reference 2 the energy per particle for the ground state was calculated

up to a^3. The result was

$$\frac{E_0}{N}=\frac{4\pi a(N-1)}{L^3}\left\{1+2.37\frac{a}{L}+\frac{a^2}{L^2}\left[(2.37)^2+\frac{\xi}{\pi^2}(2N-5)\right]\right\}, \quad (53)$$

$$\xi=\sum_{l,m,n=-\infty}^{\infty}\frac{1}{(l^2+m^2+n^2)^2}; \quad (l,m,n)\neq(0,0,0).$$

If one keeps $\rho=N/\Omega$ constant and allows $\Omega=L^3$ to approach ∞, expression (53) diverges as $N^{\frac{1}{3}}$. How does one reconcile this divergence with the finite result obtained in Sec. 1 of the present paper?

(2) Even assuming the validity of the use of the pseudopotential (1), how can one justify the neglect of the small off-diagonal matrix elements (8)?

(3) What is the nature of the series expansion of which (25) gives the first two terms? What is the limit of validity of the phonon spectrum (31)?

We start with a discussion of point (1) by examining the divergence of formula (53). If the expansion is carried out to higher orders of a, one can express the energy per particle E_0/N as a power series in a/L. The coefficient of $(a/L)^m$, $m\geqq 3$, is a polynomial in N:

$$\frac{1}{NL^2}\left(\frac{a}{L}\right)^m[AN^\nu+BN^{\nu-1}+\cdots+Z],$$

where $A, B, \cdots Z$ are numerical constants independent of a, L, or N, and ν is an integer depending on m, giving the maximum power of N that occurs in the coefficient of $(a/L)^m$. Of the terms in the polynomial, the most divergent one in the limit $N\to\infty$ at constant ρ is

$$\frac{1}{NL^2}\left(\frac{a}{L}\right)^m AN^\nu. \quad (A,\ \nu=\text{functions of } m). \quad (54)$$

Now in the discussion of Sec. 1 the guiding principle was that to each order of a, only the term with the maximum power for N be retained. The calculation that leads to (25) is therefore a calculation of the sum of the terms (54). This calculation shows that for the order $(a/L)^m$, the maximum exponent of N is

$$\nu=m \quad (m\geqq 3),$$

as one verifies immediately by expanding (23) in powers of a. The power series for E_0/N can therefore be written in the following way:

$$\frac{E_0}{N}-4\pi a\rho=\frac{1}{NL^2}\left[A\left(\frac{aN}{L}\right)^3+A'\left(\frac{aN}{L}\right)^4+A''\left(\frac{aN}{L}\right)^5+\cdots+B\left(\frac{aN}{L}\right)^3\frac{1}{N}+B'\left(\frac{aN}{L}\right)^4\frac{1}{N}+B''\left(\frac{aN}{L}\right)^5\frac{1}{N}+\cdots+C\left(\frac{aN}{L}\right)^3\frac{1}{N^2}+\cdots+\cdots\right], \quad (55)$$

where terms of the form (54) are written in the first line. The calculation that leads to (25) consists of summing the first line of the foregoing expression, and the result shows that this series, namely

$$\frac{1}{NL^2}\left[A\left(\frac{aN}{L}\right)^3+A'\left(\frac{aN}{L}\right)^4+\cdots\right],$$

approaches the finite limit

$$\frac{1}{NL^2}\frac{4\pi\times 128}{15\sqrt{\pi}}\left(\frac{Na}{L}\right)^{\frac{5}{2}}=4\pi a\rho\frac{128}{15\sqrt{\pi}}(a^3\rho)^{\frac{1}{2}},$$

as $Na/L\to\infty$.

It is clear that D-wave scattering introduces terms that contain higher powers of a for given powers of N. Triple collisions give rise to terms also of such nature. Therefore, their inclusion does not affect the first line of (55), but only subsequent lines.

It seems reasonable to expect that the sum of the terms in the second line of (55), i.e.,

$$\frac{1}{NL^2}\frac{1}{N}\left[B\left(\frac{aN}{L}\right)^3+B'\left(\frac{aN}{L}\right)^4+\cdots\right]$$

would also converge to a finite number of the limit $aN/L\to\infty$. This can happen only if the series in the square bracket approaches $(aN/L)^4$ as $aN/L\to\infty$. In that case the second line of (55) reduces to an expression of the form

$$(\text{constant})\rho^2a^4,$$

indicating that the expansion (25) is in powers of $(a^3\rho)^{\frac{1}{2}}$.

One arrives at the same conclusion in discussing question (2) mentioned at the beginning of this section. If one attempts to include the next dominant off-diagonal matrix elements, the additional perturbation energy is of the form

$$\Delta E=\sum(\text{matrix element})^2/(\text{energy difference}).$$

The matrix elements are of the order $N^{-\frac{1}{2}}a\rho$ and connects the ground state with states in which three phonons $\mathbf{k}_1$, $\mathbf{k}_2$, $\mathbf{k}_3$ are present, where $\mathbf{k}_1+\mathbf{k}_2+\mathbf{k}_3=0$. One therefore has a sum of the form

$$\Delta E=\sum\delta(\mathbf{k}_1+\mathbf{k}_2+\mathbf{k}_3)\frac{(a\rho)^2N^{-1}}{E(\mathbf{k}_1,\mathbf{k}_2,\mathbf{k}_3)}.$$

Using the energy spectrum for the phonons calculated in Sec. 2, one obtains

$$\Delta E=(a\rho)^2N^{-1}L^6\int d\mathbf{k}_1d\mathbf{k}_2F((a\rho)^{\frac{1}{2}},\mathbf{k}_1,\mathbf{k}_2).$$

By a dimensional argument one obtains

$$\Delta E=(a\rho)^2N^{-1}L^6(a\rho)^2(\text{constant})=(\text{constant})Na^4\rho^2,$$

indicating again that the expansion (25) is in powers of $(a^3\rho)^{\frac{1}{2}}$.

The surmise that the expansion (25) is in powers of $(a^3\rho)^{\frac{1}{2}}$ is in agreement with a conclusion already drawn[4] from the "binary collision expansion method."

We now come to the third point raised at the beginning of this section: the limit of validity of the formulas (25) and (31). The above discussions indicate that they represent the first terms of expansions in $(a^3\rho)^{\frac{1}{2}}$. As has been pointed out before,[4] such expansions are probably asymptotic expansions which even may not converge. For the phonon spectrum (31) the limit of validity,

$$ka \ll 1, \tag{56}$$

has to be imposed in addition to the condition

$$(a^3\rho)^{\frac{1}{2}} \ll 1.$$

Condition (56) is necessary for the validity of the pseudopotential (1).

We conclude this section by stating that to develop a systematic expansion method starting from the pseudopotential method of the present paper seems difficult, because the inclusion of triple collision terms presents grave obstacles. On the other hand, in the "binary collision expansion method"[4] triple and higher order collision terms can be automatically included. A systematic approach starting from the "binary collision expansion method" appears hopeful.

5. "TWO-FLUID MODEL" AND THE LOW-TEMPERATURE PROPERTIES OF THE HARD-SPHERE SYSTEM

In Sec. 2 we obtained the low-lying energy levels of a Bose system of hard spheres. The levels can be described as those of a collection of phonons with a spectrum given by (34). If one examines, by a method similar to the one already used, the low-lying energy levels of a corresponding Fermi-Dirac system, one finds that the energy level density near the ground state is infinitely greater than in the Bose case. The scarcity of low-lying energy levels in the Bose case has long been recognized[15] as the reason for the superfluid behavior of liquid helium. Feynman[15] has given arguments to show that for a Bose system of interacting particles such scarcity is to be expected. The results of Secs. 1 and 2 of the present paper confirms this conclusion in the case of a dilute hard sphere gas by an explicit mathematical treatment.

Knowing the spectrum of the phonons (i.e., of the low-lying states), one can easily obtain the specific heat of the system at low temperatures. Furthermore, by the reasoning developed by Landau,[8] Kramers,[9] and others[9] one can conclude that the system shows a two-fluid[16] behavior. According to these authors the ground state of the system is looked upon as a pure "superfluid." The low-lying excited states are looked upon as a mixture of "superfluid" and "normal fluid" components, with the collection of phonons constituting the "normal fluid" component. The "normal fluid" thus can be said to be moving against a "background superfluid." With such an identification of the two fluids, one can use all the formulas which the previously mentioned authors have established for the two-fluid model, and one can compute the density of the normal fluid, the velocity of second sound, and the magnitude of the fountain effect at very low temperatures. We shall not go into these discussions in detail as we have nothing new to add to the reasonings already developed in the literature quoted. It is to be noticed, however, that the present explicit mathematical treatment of a definite model allows one to visualize very clearly the fact that a phonon does carry a momentum equal to $\hbar\mathbf{k}$, where $\mathbf{k}$ is its wave number, and that by a superposition of phonon waves one does obtain a mass transport of the Bose particles.

6. MOMENTUM SPACE ORDER, CORRELATION LENGTH, AND SUPERFLUID FLOW

The method of Secs. 1 and 2 can be applied easily to the case where one starts from an unperturbed state in which almost all particles are in a given state of momentum $\mathbf{k}_0 \neq 0$. The lowest perturbed eigenstate there describes a background superfluid flow with velocity $2\mathbf{k}_0$ (notice that the mass per particle is $\frac{1}{2}$). The excited states represent various phonon states in such a background superfluid.

Is it possible to start from an unperturbed state in which a finite fraction of the particles occupy each of two different momentum states? In other words, is it possible to have an interpenetration of two superfluid velocities? The answer is no, because the method of Sec. 1 leads in this case to very large perturbations, indicating[17] that the unperturbed state is very far from an eigenstate.

The condensation of nearly all particles into a single free-particle momentum state is what London[10] called momentum space ordering. The foregoing discussion and the wave function and eigenvalues found in Secs. 1, 2, and 3 give explicit demonstrations of this concept for the special model of a dilute Bose system of hard spheres.

The influence of the order in momentum space does not, however, extend over infinite spatial distances. If it did, there would not be the possibility of superfluid flow, but only uniform motion of the superfluid as a whole. We shall in the following give a qualitative

[15] See, e.g., R. P. Feynman, in *Progress in Low Temperature Physics*, edited by C. J. Gorter (North Holland Publishing Company, Amsterdam, 1955), Vol. 1, p. 17.

[16] L. Tisza, J. phys. radium **1**, 164 (1940).

[17] For the same reason it is important to take periodic boundary conditions, as we remarked in Sec. 1. If one had chosen, e.g., the boundary condition $\Psi=0$ on the surface of the box, the unperturbed ground state would have an unphysical density variation across the box, so that the hard-sphere interaction would not be a small perturbation.

discussion[18] of the superfluid flow in the present model and of the stability of the flow. *The discussion is to be regarded as suggestive, rather than mathematically conclusive.*

We first notice that the number of particles within one correlation distance $r_0=k_0^{-1}=(8\pi a\rho)^{-\frac{1}{2}}$ is

$$\sim\rho r_0^3\sim(\rho a^3)^{-\frac{1}{2}}\gg 1.$$

The number of excited particles among these is computable from the fraction (41), and is a finite number of the order of 1. The correlation distance is therefore the distance within which the momentum space ordering is strongly effective.

In order to allow for a variation of the superfluid velocity, we divide the system into small boxes each of which is of the dimension of the correlation length, within which the ordering in momentum space forces practically all the particles to have the same momentum. The correlation between two different boxes is, however, not so strong, with the result that the superfluid velocity may vary from one small box to the other. This suggests that one makes use of the method of Secs. 1, 2, and 3, but takes the individual particle wave functions to be

$$e^{i\varphi+i\mathbf{k}\cdot\mathbf{r}}, \tag{57}$$

which form a complete set. Here, φ is a function of $\mathbf{r}$ (independent of $\mathbf{k}$) and $\nabla\varphi$ varies little within each small box. Expanding the second quantized wave function into these individual particle waves,

$$\psi(\mathbf{r})=\sum_{\mathbf{k}} a_{\mathbf{k}}e^{i\varphi+i\mathbf{k}\cdot\mathbf{r}},$$

one can calculate the matrix elements of the kinetic energy and the pseudopotential for the various eigenstates of the occupation numbers $a_{\mathbf{k}}^*a_{\mathbf{k}}$. It is then seen that the pseudopotential has the same matrix elements as in Sec. 1, and that the diagonal matrix elements of the kinetic energy is also the same as in Sec. 1 except for a uniform increment of the amount

$$\rho\int(\nabla\phi)^2d\tau. \tag{58}$$

To give a physical meaning to $\nabla\varphi$, we notice that in each small box $\nabla\varphi$ may be taken as a constant vector. It is then evident that for the ground state in each small box the momentum of the superfluid is equal to $\nabla\varphi$ per particle. In other words,

$$\mathbf{v}_s=2\nabla\phi. \tag{59}$$

The expression (58) then gives simply the kinetic energy of the superfluid flow, which according to (59) is irrotational.

Neglecting the off-diagonal matrix elements of the kinetic energy, one could solve for the excited states too. The excited states are again describable as the states of phonon waves. The off-diagonal matrix elements of the kinetic energy then give rise to a possible transfer of momentum and energy from the superfluid background flow into the phonon waves.

The above discussion leads to the conclusion that the superfluid flow is described by a condensation of almost all particles [i.e., other than a fraction $\sim(\rho a^3)^{\frac{1}{2}}$] into the single-particle state (57). This is clearly exactly what London[10] meant by a macroscopic quantum state. It is clear that from the single-valuedness of φ one would obtain a quantization of the vortices, an interesting conclusion that has been discussed in detail by Onsager and by Feynman.[11]

One of us (K. Huang) would like to thank Dr. J. Robert Oppenheimer for the hospitality extended him during his stay at the Institute for Advanced Study.

APPENDIX I

In this Appendix, we discuss the eigenvalues and eigenfunctions of the matrix

$$M_s=N+yB_s, \tag{A1}$$

where

$$N=\begin{bmatrix}0&0&0&0&\cdot\\0&1&0&0&\cdot\\0&0&2&0&\cdot\\0&0&0&3&\cdot\\\cdot&\cdot&\cdot&\cdot&\cdots\end{bmatrix}, \tag{A2}$$

and

$$B_s=\begin{bmatrix}0&[1\times(s+1)]^{\frac{1}{2}}&0&\cdot\\[1\times(s+1)]^{\frac{1}{2}}&0&[2(s+2)]^{\frac{1}{2}}&\cdot\\0&[2(s+2)]^{\frac{1}{2}}&0&\cdot\\\cdot&\cdot&\cdot&\cdots\end{bmatrix}. \tag{A3}$$

Let ψ be an eigenstate, with

$$M_s\psi=\lambda\psi, \tag{A4}$$

and

$$\psi=\begin{bmatrix}A_0\\A_1\\A_2\\\cdot\\\cdot\\\cdot\end{bmatrix}. \tag{A5}$$

By substituting ψ into (A4), we have

$$nA_n+y\{A_{n-1}[n(n+s)]^{\frac{1}{2}}+A_{n+1}[(n+1)(n+s+1)]^{\frac{1}{2}}\}=\lambda A_n.$$

It is convenient to introduce A_n' defined by

$$A_n'=\left[\frac{n!}{(n+s)!}\right]^{\frac{1}{2}}A_n. \tag{A6}$$

The difference equation for the A_n' becomes

$$(n-\lambda)A_n'+y[nA_{n-1}'+(n+s+1)A_{n+1}]=0, \tag{A7}$$

[18] See similar discussions by Onsager and Feynman, reference 11.

which can be readily solved by defining a generating function

$$H(z)\equiv\sum_{n=0}^{\infty}A_n'z^n. \tag{A8}$$

From (A7), we obtain the differential equation for H as

$$\frac{dH}{dz}[z+yz^2+y]=H\left[\lambda-yz-\frac{sy}{z}\right]. \tag{A9}$$

In order that ψ be normalizable we must have

$$\sum_{n=0}^{\infty}|A_n|^2=\text{finite},$$

which in turn implies that in the complex z plane except for $z=0$, $H(z)$ has no singularity inside the unit circle $|z|<1$. Thus, the eigenvalues of M_s are immediately determined. They are

$$\lambda_m=-\tfrac{1}{2}(1+s)+(\tfrac{1}{2}+m+\tfrac{1}{2}s)(1-4y^2)^{\frac{1}{2}}, \tag{A10}$$

with $m=0, 1, 2, \cdots$.

The corresponding eigenstates are given by Eqs. (A5) and (A6), with

$$A_n'=\text{coefficient of } z^n \text{ in } H_m(z), \quad (n\geq 0).$$

The generating function $H_m(z)$ is

$$H_m(z)=z^{-s}(z+\alpha)^{m+s}(1+\alpha z)^{-(m+1)}, \tag{A11}$$

with

$$\alpha=(2y)^{-1}[1-(1-4y^2)^{\frac{1}{2}}]. \tag{A12}$$

In particular, for $s=0$ and $m=0$

$$\lambda=-\tfrac{1}{2}+\tfrac{1}{2}(1-4y^2)^{\frac{1}{2}}, \tag{A13}$$

and the corresponding unnormalized A_n are

$$A_n=(-\alpha)^n, \quad (n=0, 1, 2\cdots), \tag{A14}$$

which yields Eq. (37).

The Hamiltonians (15) and (27) are related to the matrices M_s with $s=0$ and $s=1$. Consider now the more general case of starting with any unperturbed state which has $s_{\mathbf{k}}$ free particles with momentum $\mathbf{k}$. (Without loss of generality we can restrict the momentum $\mathbf{k}$ to range over only half of the $\mathbf{k}$ space.) Using the same arguments as that of Sec. 1, it is easy to see that the dominant part of the Hamiltonian H, Eq. (1), connects this state with other states which has in addition to these $s_{\mathbf{k}}$ particles also $l_{\mathbf{k}}$ pairs of particles each of momentum $\mathbf{k}$ and $-\mathbf{k}$, etc. Thus the Hamiltonian reduces to

$$H'=4\pi a\rho N+2\sum_{\mathbf{k}\neq 0}{}'(k^2+k_0^2)[N_{\mathbf{k}}+y_{\mathbf{k}}B_s(\mathbf{k})+\tfrac{1}{2}s_{\mathbf{k}}], \tag{A15}$$

where k_0^2 and $y_{\mathbf{k}}$ are given by Eqs. (16) and (17). The sum $\sum'$ extends over half of the $\mathbf{k}$ space with $\mathbf{k}\neq 0$. From the solution (A.10), we obtain immediately the complete phonon spectrums which are listed in Eqs. (34) and (35).

APPENDIX II

In this Appendix, we discuss the properties of the wave functions in the configuration space. From Eqs. (36) and (37), the ground state wave function Ψ_0 can be written in the configuration space as

$$\Psi_0=C\sum_{n=0}^{N/2}\chi_n, \tag{A16}$$

where

$$\chi_n=\Omega^{-N/2}\left[\frac{(N-2n)!}{N!}\right]^{\frac{1}{2}}N^n\sum f(r_{12})f(r_{34})\cdots, \quad (n\neq 0) \tag{A17}$$

and C is the normalization constant. The functions χ_n represent the part in which n pairs of particles are excited. In (A17), the sum extends over all different combinations of selecting n pairs made of $2n$ different particles among a total of N particles. Each term in the sum is a product of n functions $f(r_{ij})$ with the distances between these n pairs as arguments. Altogether there are

$$\frac{N!}{(N-2n)!n!2^n}$$

terms in the sum. The function $f(r)$ is

$$f(r)=-\frac{1}{8\pi^3\rho}\int\alpha_{\mathbf{k}}e^{i\mathbf{k}\cdot\mathbf{r}}d^3\mathbf{k}, \tag{A18}$$

with

$$\alpha_{\mathbf{k}}=(8\pi a\rho)^{-1}[k^2+8\pi a\rho-k(k^2+16\pi a\rho)^{\frac{1}{2}}].$$

Its behaviors at large and small distances are as follows:

$$f(r)\to -a/r \quad \text{as} \quad r\to 0, \tag{A19}$$

and

$$f(r)\to -(2\pi^{\frac{5}{2}}a^{\frac{1}{2}}\rho^{\frac{3}{2}}r^4)^{-1} \quad \text{as} \quad r\to\infty.$$

Using the ground state wave function Ψ_0 in the configuration space, it is also possible to obtain directly the pair distribution function $D(r_{12})$ [Eq. (43)] by integrating over the remaining spatial coordinates $\mathbf{r}_3, \cdots, \mathbf{r}_n$.

Our ground state wave function Ψ_0 satisfies the boundary condition,

$$\Psi_0=0 \quad \text{at} \quad r_{ij}=a, \tag{A20}$$

only *approximately*. Its violation of this boundary condition, however, has an effect on the energy spectrum only in higher orders of $(\rho a^3)^{\frac{1}{2}}$. To see this more clearly, let us consider the wave function

$$\Psi_0'=C'\Omega^{-N/2}\prod_{i<j}[1+f(r_{ij})], \tag{A21}$$

which satisfies the required boundary conditions. We

can obtain Ψ_0 from the above wave function by expanding the above product in powers of f and then omitting all terms in which the coordinate of any particle, say $\mathbf{r}_i$, occurs more than once. For example, a term like

$$f(r_{12})f(r_{13}) \tag{A22}$$

must be omitted. The difference between Ψ_0' and Ψ_0, therefore, consists of terms like (A22), which expresses a correlation among more than two particles. Such terms belong to a higher order of $(a^3\rho)^{\frac{1}{2}}$ than we have considered. For example, upon Fourier-analyzing (A22), we find that it is of the form of a sum over three momenta $\mathbf{k}_1$, $\mathbf{k}_2$, $\mathbf{k}_3$, subject to $\mathbf{k}_1+\mathbf{k}_2+\mathbf{k}_3=0$. Such terms arise from a calculation of order a^4, as shown in Sec. 4.

The wave function for the one-phonon state can be obtained directly from (A11). By an argument similar to the above one, it can be shown that upon neglecting terms of higher orders in $(\rho a^3)^{\frac{1}{2}}$ the wave function $\Psi_\mathbf{q}$ of one phonon with momentum $\mathbf{q}$ in the configuration space is

$$\Psi_\mathbf{q}=\sum_{i=1}^{N} e^{i\mathbf{q}\cdot\mathbf{r}_i}\Psi_0, \tag{A23}$$

where Ψ_0 is the ground state wave function [Eq. (A16) or Eq. (A21)]. Thus it is to be expected that the Feynman-Bijl relations [Eq. (52)] correlating the excitation energy of a phonon with the pair distribution function is satisfied for a dilute system of hard spheres with Bose statistics.