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Energy Levels of a Bose-Einstein System of Particles with Attractive Interactions*

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An N -body Bose-Einstein system of particles with long-range attraction and hard-sphere repulsion between particles is considered. It is shown that if the constants of the interaction have values within a certain range it is possible to calculate the ground-state energy of the system as a function of Ω/N , where Ω is the volume of the box containing the system, in the limit $N \rightarrow \infty, \Omega \rightarrow \infty$, with $N/\Omega = \rho$ fixed. The results show that the system can possess an N -body bound state, which has an equilibrium density and negative energy, and that the interactions can be saturating. Excited states are also considered. It is shown that low-lying excitations consist purely of phonons, whose velocity agrees with that computed from the macroscopic compressibility, furnished by the ground-state energy. The formula for the general excited energy levels suggests that thermodynamically the system may have a "gas" phase and two "liquid" phases, the transition between the two "liquid" phases being the analog of the Bose-Einstein condensation of the ideal gas. Thermodynamic considerations are, however, not contained in this paper.

I. INTRODUCTION

THE present investigation concerns a system of a large number N of interacting Bose-Einstein particles, enclosed in a box of very large volume Ω , which is externally fixed. Eventually we let $N \rightarrow \infty, \Omega \rightarrow \infty$, with the ratio N/Ω fixed. The two-body interaction contains a hard-sphere repulsion of diameter a , plus a long-range attraction. The attraction shall be so weak that it may not be sufficient to cause a two-body bound state, but strong enough to cause an N -body bound state. That is, the N -body system may possess an equilibrium density, at which the total energy is negative. If this total energy is of the form $Nf(N/\Omega)$, we say that the interaction is saturating.

The possible existence of an N -body bound state makes the present problem qualitatively different from one in which the interactions are purely repulsive. It is physically clear where the difference lies. In the case of purely repulsive interactions, it is imperative that, by external means, we fix the volume Ω at some finite value, if we wish the system to have a nonzero energy in the ground state. For, if there were no containing box, the system would expand in space indefinitely,

approaching an infinitely rarefied ideal gas. This is no longer true when there are attractive interactions which are capable of producing an N -body bound state with an equilibrium density ρ_0 . If the volume Ω is fixed at such a value that $N/\Omega > \rho_0$, the system would first tend to expand when Ω is increased from this value, just as in the former case. However, when Ω is made to increase further, until $N/\Omega = \rho_0$, the presence of the box becomes immaterial (apart from the trivial limitation the box places on the center-of-mass motion of the system). Any further increase of Ω beyond this point leaves the energy and the density ρ_0 of the system unaffected. We may illustrate the difference between the two cases discussed by the qualitative plot of energy per particle E/N as a function of Ω/N in Fig. 1. At a point such as P on the diagram, the system exists in the same internal state as at O . The only difference is that at P the center of mass of the system has more space to move in. For a sufficiently large system ($N \rightarrow \infty, \Omega \rightarrow \infty$) the energy at P is the same as at O . It might also be noted in passing that at the point P , because of the center-of-mass motion of the entire system, the probability of finding *any one* particle at any position inside the box should be a constant throughout the box, apart from boundary effects, which become negligible as $N \rightarrow \infty, \Omega \rightarrow \infty$.

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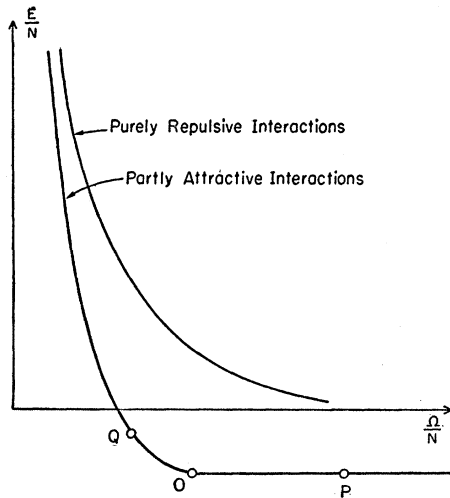


FIG. 1. Qualitative behavior of the energy per particle of an N -body system as a function of available volume per particle, as expected on a physical basis.

The foregoing discussion suggests that it is sufficient to calculate the energy of the system for $N/\Omega \geq \rho_0$. In other words, we must approach the density ρ_0 from the high-density side. The present calculation follows this suggestion, and is an extension of previous calculations concerning the N -body Bose-Einstein system with hard-sphere interactions.¹⁻³ It is recalled that these calculations are based on the smallness of the parameter $(\rho a^3)^{1/2}$, where $\rho = N/\Omega$. In order to make use of similar methods for the present case, it is necessary that the additional attractive interactions are such as to make the equilibrium density ρ_0 satisfy the condition $(\rho_0 a^3)^{1/2} \ll 1$. It is not intuitively obvious whether it is at all possible to choose the parameters of the attractive interaction to satisfy this condition; that it is possible is the main result of this paper.

The present paper represents an initial effort which aims to answer the following questions:

(a) Is there a range of values of the parameters of a saturating potential, within which one can calculate the energy levels, in particular bound states, of the system in a well-defined scheme of approximations?

(b) Does the system under consideration possess properties that are qualitatively similar to some of the properties of liquid helium, in particular, the property that there exist the thermodynamic phases: gas, liquid I, and liquid II?

The first question is answered in the affirmative by the following calculations. To answer the second question completely requires a knowledge of the thermodynamic properties of the system, which has not been included in this paper. The results of this paper, however, do indicate that the answer would also be yes.

¹ K. Huang and C. N. Yang, Phys. Rev. **105**, 767 (1957).

² Lee, Huang, and Yang, Phys. Rev. **106**, 1135 (1957).

³ T. D. Lee and C. N. Yang, Phys. Rev. **112**, 1419 (1958).

II. DEFINITION OF THE MODEL

1. Two-Body Potential

In our problem the two-body interaction between the particles of the system is represented by a central potential $v(r)$, where r is the interparticle distance. It is infinite for $r \leq a$. For $r > a$ it is negative, characterized by a range parameter r_0 and a depth parameter v_0 . We require that⁴

$$v_0^{1/2} a \ll 1. \quad (1)$$

Since $v_0^{1/2}$ is of the order of the average wave number of a particle inside the attractive well, condition (1) allows the representation of the hard-sphere part of the interaction by a pseudopotential, as discussed in reference 1. We write, accordingly,

$$v(r) = 8\pi a \delta(r) \frac{\partial}{\partial r} r + w(r), \quad (2)$$

where $w(r)$ is the attractive part of the interaction and the meaning of the differential operator $(\partial/\partial r)r$ has been explained in references 1 and 2. To simplify calculations we choose $w(r)$ such that its Fourier transform is a step function:

$$w_{\mathbf{k}} \equiv \int d\mathbf{r} e^{i\mathbf{k} \cdot \mathbf{r}} w(r) = \begin{cases} -8\pi(a+b) & \text{if } |\mathbf{k}| < k_0 \\ 0 & \text{if } |\mathbf{k}| > k_0. \end{cases} \quad (3)$$

The number $a+b$ may be interpreted to be the zero-energy scattering length of the attractive part of the potential. This choice of the Fourier transform leads to the following potential in ordinary space:

$$w(r) = -v_0 [3j_1(k_0 r)/k_0 r], \quad v_0 \equiv (32\pi^2/3)(a+b)k_0^3, \quad (4)$$

where j_1 is a spherical Bessel function. The total potential is this plus a hard core of diameter a . A plot of it is given in Fig. 2. The range parameter may be defined as

$$r_0 \equiv 4.5/k_0. \quad (5)$$

At large distances the potential oscillates about zero, as a result of the sharp cutoff in momentum space. The oscillations are however quite small, and unlikely to produce spurious effects.

In terms of k_0 , b , and a , the requirement (1) may be re-expressed as follows:

$$k_0 a [1 + (b/a)]^{1/2} \ll 1. \quad (6)$$

The potential binds a two-body system when the range is larger than a quarter wavelength of the relative motion in the lowest S state. This means that $(k_0/4.5) \lesssim 4v_0^{1/2}$, or $k_0(a+b) \gtrsim (1/54\pi^2)$.

2. N -Body Hamiltonian

Let $a_{\mathbf{k}}^\dagger$, $a_{\mathbf{k}}$ be, respectively, the usual creation and annihilation operators for plane wave states, with

⁴ We choose units so that $\hbar = 1$, $2m = 1$, m being the mass of a particle.

commutator

$$[a_k, a_p^\dagger] = \delta_{kp}. \tag{7}$$

As usual let

$$\psi(\mathbf{r}) \equiv \Omega^{-\frac{1}{2}} \sum_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{r}} a_{\mathbf{k}}, \tag{8}$$

where the sum extends over all vectors \mathbf{k} whose components are $2\pi\Omega^{-\frac{1}{2}}$ times an integer (positive, negative, or zero). The plane wave single-particle states therefore obey periodic boundary conditions with respect to the box of volume Ω . The N -body Hamiltonian is

$$H = \int d\mathbf{r} (\nabla\psi^\dagger) \cdot (\nabla\psi) + \frac{1}{2} \int d\mathbf{r}_1 d\mathbf{r}_2 \psi^\dagger(\mathbf{r}_1) \psi^\dagger(\mathbf{r}_2) v(r_{12}) \psi(\mathbf{r}_1) \psi(\mathbf{r}_2), \tag{9}$$

where $r_{12} = |\mathbf{r}_1 - \mathbf{r}_2|$. In terms of a_k^\dagger and a_k , we may write

$$H = \sum_{\mathbf{k}} k^2 a_{\mathbf{k}}^\dagger a_{\mathbf{k}} + \frac{1}{2\Omega} \sum_{\mathbf{k}}' v_{\mathbf{k}} \sum_{\mathbf{p}, \mathbf{q}} a_{\mathbf{p}+\mathbf{k}}^\dagger a_{\mathbf{q}-\mathbf{k}}^\dagger a_{\mathbf{p}} a_{\mathbf{q}}, \tag{10}$$

where

$$v_{\mathbf{k}} \equiv \int d\mathbf{r} e^{i\mathbf{k}\cdot\mathbf{r}} [8\pi a \delta(\mathbf{r}) + w(r)] = \begin{cases} 8\pi a & \text{if } |\mathbf{k}| > k_0 \\ -8\pi b & \text{if } |\mathbf{k}| < k_0. \end{cases} \tag{11}$$

The summation over \mathbf{k} in (10), indicated by a prime, includes a limiting process that takes into account the effects of the differential operator $(\partial/\partial\mathbf{r})\mathbf{r}$ in the pseudopotential. It is defined in the following way: If $f(\mathbf{k})$ is a matrix element arising from (10), then

$$\sum_{\mathbf{k}}' f(\mathbf{k}) \equiv \lim_{r \rightarrow 0} \frac{\partial}{\partial r} [r \sum_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{r}} f(\mathbf{k})]. \tag{12}$$

Suppose that $f(\mathbf{k}) \rightarrow Ak^{-2} + g(k)$ for $k \rightarrow \infty$, where $g(k)$ vanishes more rapidly than k^{-3} ; then it follows from (12) that

$$\sum_{\mathbf{k}}' f(\mathbf{k}) = \sum_{\mathbf{k}} [f(\mathbf{k}) - Ak^{-2}]. \tag{13}$$

For such $f(\mathbf{k})$ the definition (12) is equivalent to a simple subtraction procedure. It is sufficient to consider those $f(\mathbf{k})$ having the property postulated, for we shall not encounter any other case. We may therefore take (13) as the definition of the operation \sum' .

The model having been defined, our task is to diagonalize (10), requiring that all states be eigenstates of $\sum a_{\mathbf{k}}^\dagger a_{\mathbf{k}}$ belonging to the eigenvalue N , in the limit

$$N \rightarrow \infty, \quad \Omega \rightarrow \infty, \quad \text{with } N/\Omega \equiv \rho \text{ fixed.} \tag{14}$$

3. Orders of Magnitudes

We summarize here the range of values of the parameters of the problem within which the calculation is to be carried out. The parameters occurring in the

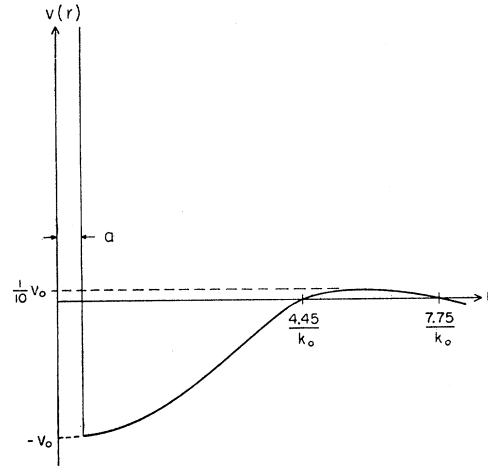


FIG. 2. The two-body potential used in the present calculation.

problem are four:

$$a, \quad b, \quad k_0, \quad \rho.$$

We shall define orders of magnitudes of dimensionless combinations of these parameters by the following table:

Order:	0	1
Parameters:	$\begin{cases} 1 \\ k_0 a / (\rho a^3)^{\frac{1}{2}} \\ (b/a) / (k_0 a) \end{cases}$	$\begin{cases} (\rho a^3)^{\frac{1}{2}} \\ k_0 a \\ b/a \end{cases}$

(15)

Second- and higher-order quantities are given by products of powers of the lower-order quantities. It is therefore not necessary to list them explicitly.

It may be instructive to re-express the assignment (15) in terms of the lengths of the problems. There are four independent lengths:

- a = scattering length of hard sphere,
 - b = total scattering length at zero energy,
 - r_0 = range of attraction $\sim k_0^{-1}$,
 - r_p = average interparticle distance $\sim \rho^{-\frac{1}{2}}$.
- (16)

To these one might add a fifth, which is not independent of the ones above, but convenient to introduce:

$$r_c = (a\rho)^{-\frac{1}{2}} = \text{correlation length of hard-sphere repulsion.} \tag{17}$$

It is recalled that in reference 3, this length emerges as the approximate distance from a particle, beyond which the probability of finding another particle becomes unaffected by the hard-sphere interaction. (i.e., in the case of pure hard-sphere interactions, the pair correlation function is essentially unity for distances larger than r_c .) In terms of these lengths, the orders of magnitudes set down by (15) may be illustrated by the scale in Fig. 3, which is self-explanatory.

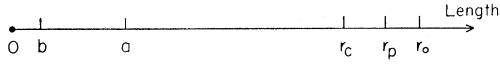


FIG. 3. Scale of lengths in the present problem. These lengths are defined in Eq. (16).

The following calculations are carried out up to and including the first order, unless the first-order calculation gives a vanishing result. In the latter case the calculation is carried out to the lowest nonvanishing order.

The consistency of the assignment of orders of magnitude shall be demonstrated by calculation. The motivation for such an assignment is given in the next section.

III. A SIMPLE CALCULATION

This section is not logically necessary. It is here only for the sake of clarity, as it provides a physical motivation for the way the calculation is to be made, and it points out some of the difficulties that have to be overcome. Let us recall that for the case of purely hard-sphere interactions, the ground-state energy per particle is²

$$\frac{E_0}{N} = (4\pi a\rho) + (4\pi a\rho) \frac{128}{15} \left(\frac{\rho a^3}{\pi} \right)^{\frac{1}{2}} \quad (\text{hard spheres}). \quad (18)$$

The first term is simply the diagonal matrix element of the interaction Hamiltonian, taken in the unperturbed ground state. The second term is the result of summing selected terms from every order of perturbation theory.

Let us now perform the following calculation: Take as unperturbed states the eigenfunctions in the case of purely hard-sphere interactions. Treat the attraction as a perturbation and calculate the energy in first-order perturbation theory. The energy shift is thus $4\pi\rho$ times the zero-energy scattering length of the attractive potential, i.e., $-4\pi(a+b)\rho$. Adding this to the unperturbed energy, which is (18), we obtain

$$\frac{E_0}{N} = -(4\pi b\rho) + (4\pi a\rho) \frac{128}{15} \left(\frac{\rho a^3}{\pi} \right)^{\frac{1}{2}}. \quad (19)$$

If one makes a plot of this as a function of ρ^{-1} , one gets a curve shown in Fig. 4. The fine dotted lines represent, respectively, the two terms in (19), and their sum is the solid curve. There is a minimum at ρ_0 , which has the value given by

$$\left(\frac{\rho_0 a^3}{\pi} \right)^{\frac{1}{2}} = \frac{5b}{64a}, \quad (20)$$

at which density the energy per particle is

$$\epsilon_0 = -(4\pi/3)\rho_0 b. \quad (21)$$

Since the hard-sphere calculation is valid only if $(\rho a^3)^{\frac{1}{2}} \ll 1$, the formula (20) is valid only if $b/a \ll 1$. If we require $b/a \sim (\rho a^3)^{\frac{1}{2}} \ll 1$, then the calculation is consistent in the neighborhood of $\rho = \rho_0$.

The portion of the curve for $\rho < \rho_0$ must be discarded. Take the point P' , for example. It obviously does not represent the lowest state of the system, for point P has a lower energy, and does represent a state of the system. Namely, it is the state O , except that it does not completely fill the box containing the system. This is possible because at O the curve of E/N has zero slope with respect to ρ . *The state O can therefore exist without external pressure.* We conclude that the energy per particle as a function of ρ^{-1} follows the curve QOP in Fig. 4. An N -body bound state is formed at the point O . The equilibrium density is given by ρ_0 of (20), and the binding energy per particle, ϵ_0 of (21). The interaction saturates.

Except for minor modifications, the results above are in fact correct, as a more exact calculation later shows.

It is however instructive to ask: What is wrong with the foregoing consideration? Some criticisms are given below. They serve the purpose of pointing out some of the difficulties that have to be overcome in a better calculation: (a) One notes that (20) and (21) are independent of k_0 . This cannot be accurate because one should expect the binding energy to decrease when the range of the attraction is decreased. (b) If one wants to do better than the results (20) and (21), and go to the second order in perturbation theory, the result diverges. Furthermore, a summation of selected terms from every order of perturbation theory also fails, if one selects the same type of terms which in the hard-sphere calculation led to the order $(\rho a^3)^{\frac{1}{2}}$.

The last-mentioned difficulty may be seen as follows. If we recall that the calculation which led to the $(\rho a^3)^{\frac{1}{2}}$ term in (18) consists of diagonalizing the operator

$$(k^2 + 8\pi a\rho) a_{\mathbf{k}}^\dagger a_{\mathbf{k}} + 4\pi a\rho (a_{\mathbf{k}}^\dagger a_{-\mathbf{k}}^\dagger + a_{\mathbf{k}} a_{-\mathbf{k}}),$$

then it is immediately obvious that applying the same method to the attractive part of the interaction requires the diagonalization of

$$(k^2 - 8\pi b\rho) a_{\mathbf{k}}^\dagger a_{\mathbf{k}} - 4\pi b\rho (a_{\mathbf{k}}^\dagger a_{-\mathbf{k}}^\dagger + a_{\mathbf{k}} a_{-\mathbf{k}}),$$

where $|\mathbf{k}| < k_0$. As long as $8\pi b\rho$ is finite, no matter how small, there exists a k such that $k^2 - 8\pi b\rho < 0$. For such a k the above operator can be shown to possess no real eigenvalue that belongs to a normalizable wave function.

The foregoing discussion has served the purpose of illustrating the central idea behind the calculation that is to follow, and pointed out the difficulties of the problem. We shall show in the following sections that these difficulties can be overcome, and that the result of a better calculation turns out to be not materially different from what has been obtained here.

IV. SYSTEMATIC CALCULATIONS

1. Reduction of the Hamiltonian

The notation employed in the following is, whenever possible, the same as that of references 2 and 3. We consider an unperturbed state which is specified by the occupation numbers $\{m_k\}$ of the single-particle levels, with the requirements that

- (a) The level $\mathbf{k}=0$ is occupied by ξN particles
 $(0 < \xi \leq 1)$,
 (b) No other level may be occupied by a finite fraction of all the particles.

Since the total number of particles is N , we have

$$\sum_{\mathbf{k} \neq 0} m_{\mathbf{k}} = (1 - \xi)N. \quad (23)$$

For brevity we shall call a level "macroscopically occupied," if its occupation number is a finite fraction of all the particles. The unperturbed states which we consider have the property that no level other than $\mathbf{k}=0$ may be macroscopically occupied. Obviously this terminology has meaning only in the limit $N \rightarrow \infty$.

The unperturbed state $\{m_k\}$ is connected by matrix elements of the Hamiltonian (10) to other unperturbed states through repeated interactions. The most general state which is reachable from $\{m_k\}$ through repeated interactions has occupation numbers denoted by $m_k + \delta_k$. More explicitly the occupation numbers are listed in the following table:

Level	Occupation number
0	$\xi N - \sum_{\mathbf{k} \neq 0} \delta_{\mathbf{k}}$
$\mathbf{k} \ (\mathbf{k} \neq 0)$	$m_{\mathbf{k}} + \delta_{\mathbf{k}}$

To excite δ_k particles into the state \mathbf{k} , the interaction has to be applied δ_k times. It is shown in reference 2 that the expectation value of $\sum \delta_k$ with respect to the *perturbed state* is of order $N(\rho a^3)^{\frac{1}{2}}$ for the case of hard sphere interactions. It is therefore a small number compared to N . In the present case it will be later shown that

$$\begin{aligned} \langle \sum_{k > k_0} \delta_k \rangle &\sim N(\rho a^3)^{\frac{1}{2}}, \\ \langle \sum_{0 < k < k_0} \delta_k \rangle &\sim N(\rho b^3)^{\frac{1}{2}}, \end{aligned} \quad (25)$$

where the expectation values are taken with respect to the perturbed state. Assuming this fact now simplifies the classification of terms in the Hamiltonian. The collection of states of the type (24), satisfying (22), (23), spans a subspace S of the Hilbert space. The consistency of (25) with the calculation means that the interactions do not transform a state in S to one outside it. We shall first restrict the Hamiltonian to the sub-

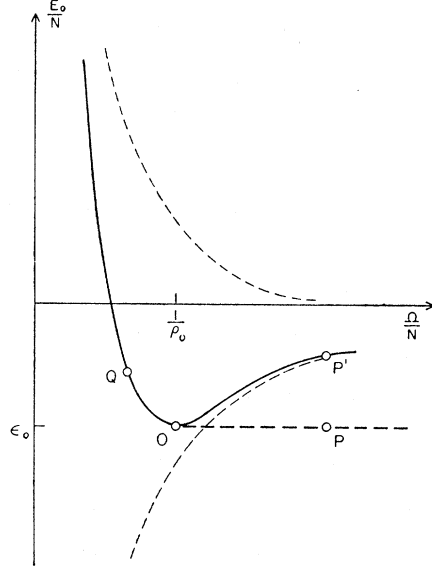


FIG. 4. Ground-state energy per particle, as a function of available volume per particle. The upper dotted curve represents contributions from the hard-sphere interaction, and the lower dotted curve, from the attraction. The sum of these give the solid curve QOP' . The straight heavy dotted line OP , however, represents states of the system at an energy lower than those on OP' . The state at P is the state O , not filling the whole volume. This is possible because in state O the system requires no external pressure to maintain its density ρ_0 , since $\partial E/\partial \rho = 0$ at this point. The lowest state of the system is therefore represented by the curve QOP .

space S , and later show the consistency of this restriction.

Let $n_0 \equiv \xi N - \sum \delta_k$, and $n_k \equiv m_k + \delta_k$ (obviously $n_0 = a_0^\dagger a_0$ and $n_k = a_k^\dagger a_k$). The diagonal matrix element of the Hamiltonian (10) with respect to a state in S is

$$k^2 n_k + \frac{1}{2} v_0 \rho N + n_0 \Omega^{-1} \sum_{\mathbf{k} \neq 0} n_{\mathbf{k}} v_{\mathbf{k}} + \frac{1}{2} \Omega^{-1} \sum_{\substack{\mathbf{k} \neq \mathbf{p} \\ \mathbf{k}, \mathbf{p} \neq 0}} n_{\mathbf{k}} n_{\mathbf{p}} v_{\mathbf{k}-\mathbf{p}},$$

which can be rewritten as follows:

(diagonal matrix element)

$$= C + \sum_{\mathbf{k} \neq 0} (k^2 + \xi \rho v_{\mathbf{k}} + \gamma_{\mathbf{k}}) n_{\mathbf{k}} + V_0', \quad (26)$$

where C and $\gamma_{\mathbf{k}}$ are numbers depending only on $\{m_{\mathbf{k}}\}$:

$$C \equiv -4\pi b \rho N + (1 - \xi) \rho \sum_{\mathbf{k} \neq 0} v_{\mathbf{k}} m_{\mathbf{k}} - \frac{1}{2} \Omega^{-1} \sum_{\substack{\mathbf{k} \neq \mathbf{p} \\ \mathbf{k}, \mathbf{p} \neq 0}} m_{\mathbf{k}} m_{\mathbf{p}} v_{\mathbf{k}-\mathbf{p}}, \quad (27)$$

$$\gamma_{\mathbf{k}} \equiv \Omega^{-1} \sum_{\mathbf{p} \neq 0, \mathbf{k}} (v_{\mathbf{p}-\mathbf{k}} - v_{\mathbf{p}}) m_{\mathbf{p}}, \quad (28)$$

while V_0' depends on the state in which the diagonal element is taken (it is therefore an operator):

$$V_0' \equiv \frac{1}{2} \Omega^{-1} \sum_{\substack{\mathbf{p} \neq \mathbf{k} \\ \mathbf{p}, \mathbf{k} \neq 0}} \delta_{\mathbf{p}} \delta_{\mathbf{k}} v_{\mathbf{p}-\mathbf{k}} - \Omega^{-1} \left(\sum_{\mathbf{k} \neq 0} \delta_{\mathbf{k}} \right) \left(\sum_{\mathbf{p} \neq 0} v_{\mathbf{p}} \delta_{\mathbf{p}} \right). \quad (29)$$

We now turn to the nondiagonal matrix elements of H in the subspace S . These matrix elements naturally fall into three classes, exactly as in reference 2: namely those that create or annihilate (i) two particles of $\mathbf{k}=0$, (ii) one particle of $\mathbf{k}=0$, and (iii) no particle of $\mathbf{k}=0$. They are, respectively, proportional to ξN , $(\xi N)^{\frac{1}{2}}$, and 1. The interaction Hamiltonian is accordingly decomposed into three terms, $V_1+V_2+V_3$, in an obvious way:

$$V_1 = \frac{1}{2}\Omega^{-1} \sum'_{\mathbf{k} \neq 0} v_{\mathbf{k}} (a_{\mathbf{k}}^\dagger a_{-\mathbf{k}}^\dagger a_0 a_0 + a_{\mathbf{k}} a_{-\mathbf{k}} a_0^\dagger a_0^\dagger), \quad (30)$$

$$V_2 = \Omega^{-1} \sum'_{\mathbf{k} \neq 0} v_{\mathbf{k}} \sum_{\mathbf{p} \neq 0, \mathbf{k}} (a_{\mathbf{p}-\mathbf{k}}^\dagger a_{\mathbf{k}}^\dagger a_{\mathbf{p}} a_0 + a_0^\dagger a_{\mathbf{p}}^\dagger a_{\mathbf{k}} a_{\mathbf{p}-\mathbf{k}}), \quad (31)$$

$$V_3 = \frac{1}{2}\Omega^{-1} \sum'_{\mathbf{k} \neq 0} v_{\mathbf{k}} \sum_{\mathbf{p}, \mathbf{q}} a_{\mathbf{p}-\mathbf{k}}^\dagger a_{\mathbf{q}+\mathbf{k}}^\dagger a_{\mathbf{p}} a_{\mathbf{q}}, \quad (32)$$

where the sum $\sum_{\mathbf{p}, \mathbf{q}}$ is a sum over \mathbf{p} and \mathbf{q} , subject to the condition $\mathbf{p} \neq 0, \mathbf{k}$, and $\mathbf{q} \neq 0, -\mathbf{k}$.

In V_1 there appears $a_0 a_0$ and $a_0^\dagger a_0^\dagger$ whose matrix elements in the subspace S are, respectively,

$$\begin{aligned} [(n_0-1)n_0]^{\frac{1}{2}} &= n_0 + O(1/\xi N), \\ [(n_0+2)(n_0+1)]^{\frac{1}{2}} &= n_0 + O(1/\xi N). \end{aligned}$$

In V_2 there appear a_0 and a_0^\dagger , whose matrix elements in the subspace S are, respectively,

$$n_0^{\frac{1}{2}}, \quad (n_0+1)^{\frac{1}{2}} = n_0^{\frac{1}{2}} + O(1/\xi N).$$

Therefore if in V_1 and V_2 we replace all a_0 and a_0^\dagger by $n_0^{\frac{1}{2}}$, their matrix elements are not affected in the limit $N \rightarrow \infty$, except when $\xi=0$. But if $\xi=0$, V_1 and V_2 both vanish anyway. Accordingly we prescribe the replacement

$$a_0^\dagger, \quad a_0 \rightarrow n_0^{\frac{1}{2}}. \quad (33)$$

This *does not* mean that the interaction no longer conserves the number of particles, because we make this replacement only when we are restricted to the subspace S . The number of particles of the system is necessarily constant and equal to N , for this is a property explicitly imposed on all states in S by the relation (23).

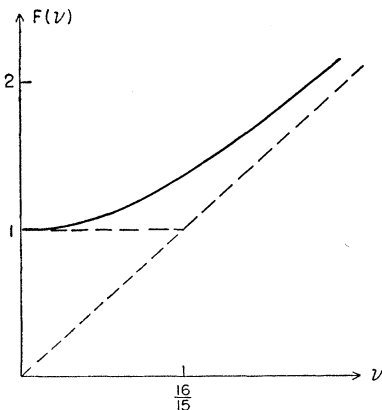


FIG. 5. Plot of the function $F(v)$, which appears in Eq. (41).

It is convenient to further decompose V [with the replacement (33)], in the following manner:

$$\begin{aligned} V_1 &= \frac{1}{2}n_0\Omega^{-1} \sum'_{\mathbf{k} \neq 0} v_{\mathbf{k}} (a_{\mathbf{k}}^\dagger a_{-\mathbf{k}}^\dagger + a_{\mathbf{k}} a_{-\mathbf{k}}) \\ &= \frac{1}{2}(\rho\xi - \Omega^{-1} \sum_{\mathbf{p} \neq 0} \delta_{\mathbf{p}}) \sum'_{\mathbf{k} \neq 0} v_{\mathbf{k}} (a_{\mathbf{k}}^\dagger a_{-\mathbf{k}}^\dagger + a_{\mathbf{k}} a_{-\mathbf{k}}) \equiv \tilde{V}_1 + V_1', \end{aligned}$$

where

$$\begin{aligned} \tilde{V}_1 &\equiv 4\pi a \rho (\xi - N^{-1} \sum_{0 < k < k_0} m_{\mathbf{p}}) \sum'_{k > k_0} (a_{\mathbf{k}}^\dagger a_{-\mathbf{k}}^\dagger + a_{\mathbf{k}} a_{-\mathbf{k}}) \\ &\quad - 4\pi a \Omega^{-1} (\sum_{0 < p < k_0} n_{\mathbf{p}}) \sum'_{k > k_0} (a_{\mathbf{k}}^\dagger a_{-\mathbf{k}}^\dagger + a_{\mathbf{k}} a_{-\mathbf{k}}) \\ &\quad - 4\pi b \rho \xi \sum_{0 < k < k_0} (a_{\mathbf{k}}^\dagger a_{-\mathbf{k}}^\dagger + a_{\mathbf{k}} a_{-\mathbf{k}}), \quad (34) \end{aligned}$$

$$\begin{aligned} V_1' &\equiv 8\pi b \rho N^{-1} (\sum_{k \neq 0} \delta_{\mathbf{k}}) \sum_{0 < k < k_0} (a_{\mathbf{k}}^\dagger a_{-\mathbf{k}}^\dagger + a_{\mathbf{k}} a_{-\mathbf{k}}) \\ &\quad - 4\pi a \rho N^{-1} (\sum_{k > k_0} \delta_{\mathbf{k}}) \sum'_{k > k_0} (a_{\mathbf{k}}^\dagger a_{-\mathbf{k}}^\dagger + a_{\mathbf{k}} a_{-\mathbf{k}}). \quad (35) \end{aligned}$$

Let us introduce a new quantum number x for the unperturbed state, defined by

$$N^{-1} \sum_{0 < k < k_0} m_{\mathbf{k}} \equiv (1-\xi)x, \quad (0 \leq x \leq 1) \quad (36)$$

and define

$$f(\xi, x) \equiv \xi + (1-\xi)x. \quad (36')$$

The number x is the fraction of excited particles [i.e., the fraction of $(1-\xi)N$] that occupies levels with $0 < k < k_0$. It is to be noted that the number of momentum states with $0 < k < k_0$, denoted by $N'(k_0)$, is a small fraction of N . In fact,

$$\frac{N'(k_0)}{N} = \frac{k_0^2}{6\pi^2 \rho} = \frac{k_0 a \left[\frac{(k_0 a)^2}{\rho a^3} \right]}{6\pi^2 \rho}, \quad (37)$$

which, according to the classification of (15), is a small quantity of the first order. The unperturbed states with $\xi < 1$ and $x \neq 0$ means that a finite fraction of all the particles are jammed into the small sphere $k < k_0$. However, this can still be consistent with the requirement that no single level other than $\mathbf{k}=0$ is macroscopically occupied.

We now rewrite the Hamiltonian (10) as follows:

$$\begin{aligned} H &= C + \sum'_{k > k_0} [(k^2 + 8\pi a \rho \xi + \gamma_{\mathbf{k}}) n_{\mathbf{k}} \\ &\quad + 4\pi a \rho f(\xi, x) (a_{\mathbf{k}}^\dagger a_{-\mathbf{k}}^\dagger + a_{\mathbf{k}} a_{-\mathbf{k}})] + V, \quad (38) \end{aligned}$$

where C , $\gamma_{\mathbf{k}}$, $f(\xi, x)$ are, respectively, defined by (27), (28), and (36), and

$$\begin{aligned} V &\equiv \sum_{0 < k < k_0} \{ [k^2 + \gamma_{\mathbf{k}} - 8\pi b \rho \xi - 4\pi a \Omega^{-1} \sum'_{p > k_0} (a_{\mathbf{p}}^\dagger a_{-\mathbf{p}}^\dagger \\ &\quad + a_{\mathbf{p}} a_{-\mathbf{p}})] n_{\mathbf{k}} - 4\pi b \rho \xi (a_{\mathbf{k}}^\dagger a_{-\mathbf{k}}^\dagger + a_{\mathbf{k}} a_{-\mathbf{k}}) \} \\ &\quad + V_0' + V_1' + V_2 + V_3, \quad (39) \end{aligned}$$

where V_0', V_1', V_2, V_3 are defined, respectively, by (29), (30), (31), and (32). The procedure of calculation is to regard the term V in (38) as a perturbation. Its contributions to the energy levels are of order higher than first order [as defined by (15)]. It is therefore important only for quantities which have no first-order term. That this is true is shown in subsection 4 of this section.

2. Properties Near Ground States

By ground states we mean the state specified by $\xi=1$. This is the state which is obtained from the free-particle ground state by adiabatically "turning on" the interactions. The Hamiltonian (38) now reads

$$H = -4\pi b\rho N + \sum_{k>k_0}' [(k^2 + 8\pi a\rho)n_k + 4\pi a\rho(a_k^\dagger a_{-k}^\dagger + a_k a_{-k})] + V. \tag{40}$$

Neglecting V , we can immediately write down the lowest eigenvalue of the above, since the answer has already been given in reference 2. Call the lowest eigenvalue E_0 . Then

$$\frac{E_0}{N} = -4\pi b\rho + (4\pi a\rho) \frac{128}{15} \left(\frac{\rho a^3}{\pi}\right)^{\frac{1}{2}} F(\nu), \tag{41}$$

where $\nu \equiv k_0 / (16\pi a\rho)^{\frac{1}{2}}$, and

$$F(\nu) = \frac{15}{2} \left[\frac{1}{3}(1+\nu^2)^{\frac{3}{2}} - \frac{1}{5}(1+\nu^2)^{\frac{5}{2}} + \frac{1}{6}\nu^3 + \frac{1}{5}\nu^5 \right]. \tag{42}$$

Figure 5 shows a graph of $F(\nu)$. The formula (41) for E_0/N differs from the result (19) of a more simple-minded calculation only by the presence of the factor $F(\nu)$, which does not make any qualitative difference. As a function of $\rho^{-1} = \Omega/N$, E_0/N has the same shape as that shown in Fig. 4 if $k_0 a / \pi < b/a$. Otherwise the curve is everywhere positive and the system does not bind. The conditions for binding is therefore $b > 0$ and $k_0 a / \pi < b/a$, which we assume. The minimum of the curve occurs at $\rho = \rho_0$, where ρ_0 is now the root of the transcendental equation (with $z = k_0^2 / 16\pi a\rho$):

$$(1+z^{-1})^{\frac{1}{2}} (1 - \frac{1}{2}z + z^2) - z^2 = \frac{5\pi b}{16 a k_0 a}, \tag{43}$$

which may be solved graphically. The result is not qualitatively different from that obtained by approximating $F(\nu)$ by the heavy dotted curve of Fig. 5, which means that for the range of parameters we are interested in (i.e., the case of binding) we may take

$$F(\nu) \cong 1. \tag{44}$$

We shall use this approximation, for it avoids clumsy graphical solutions. With (44) one obtains the same

results as (20) and (21):

$$\left(\frac{\rho_0 a^3}{\pi}\right)^{\frac{1}{2}} \cong \frac{5 b}{64 a}, \tag{45}$$

$$\left(\frac{E_0}{N}\right)_{\rho=\rho_0} \cong -\left(\frac{5}{64}\right)^2 \frac{4\pi^2 b}{3a^2 a}.$$

The more accurate results from (43) give slightly smaller values for ρ_0 and $-E_0$. Everything we have said about (19) may be said here again, in particular the statements that (a) the calculation is consistent in the neighborhood of $\rho = \rho_0$, and (b) the lowest energy is represented by the curve QOP of Fig. 4. For (b) to be true, it must be shown that for $\rho > \rho_0$ no other state has a lower energy than $E_0(\rho)$, and that for $\rho < \rho_0$ no state has a lower energy than $E_0(\rho_0)$. It will be shown in the next section that this is so, if $k_0 \gg (b\rho)^{\frac{1}{2}}$, (as we have assumed), while for values of k_0 that are too small, this may not be so.

From (40) we can also find the energies of very low-lying excited states. The excitation spectrum, which corresponds to the phonon spectrum in the hard-sphere calculation (2), is easily found to be [this is derived in (73)]

$$E_{\mathbf{k}} - E_0 = \begin{cases} k(k^2 + 16\pi a\rho)^{\frac{1}{2}} & \text{if } |\mathbf{k}| > k_0 \\ 0 & \text{if } |\mathbf{k}| < k_0, \end{cases} \tag{46}$$

where the state corresponding to the eigenvalue $E_{\mathbf{k}}$ has a total momentum \mathbf{k} . For $|\mathbf{k}| < k_0$, (46) implies that the excitation energy is of an order higher than that which has been calculated. To calculate it requires taking V into account in (40). This will be done in subsection 4 of this section. However, we can deduce what the answer must be in the limit $|\mathbf{k}| \rightarrow 0$, by noting that there must exist long-wavelength density fluctuations of the system (phonons), whose energy is kc where c is the sound velocity. Remembering that the mass of a particle is $\frac{1}{2}$, we have

$$c = (-2\partial P / \partial \rho)^{\frac{1}{2}},$$

where P is the pressure of the system at absolute zero:

$$P = \rho^2 \frac{\partial}{\partial \rho} \left(\frac{E_0}{N}\right). \tag{47}$$

Combining the above yields

$$\frac{c^2}{4\rho} = \left(\frac{\partial}{\partial \rho} + \frac{1}{2}\rho \frac{\partial^2}{\partial \rho^2}\right) \frac{E_0}{N}, \tag{48}$$

and performing the indicated operations on (41) gives indeed a number of higher order:

$$c = (16\pi a'\rho)^{\frac{1}{2}}, \tag{49}$$

where

$$a'/a = 16(\rho a^3/\pi)^{1/2} G(\nu) - (b/a), \tag{50}$$

$$G(\nu) = \frac{1}{2}[(1+\nu^2)^{1/2} + (1+\nu^2)^{-1/2}], \tag{51}$$

which is a positive-definite function. It is obvious from (48) and Fig. 4 that for $\rho \geq \rho_0$, c is real and positive. At $\rho = \rho_0$ we have, using the approximate formula (45),

$$c \cong (4\pi\rho_0 b)^{1/2}.$$

What is not known through these considerations is whether at low k , sound waves are the *only* excitations. That such is the case will be shown by explicit higher-order calculation, which of course verifies (49).

It is not hard, at this point, to *guess* that a higher-order calculation must yield for the excitation spectrum the following:

$$E_{\mathbf{k}} - E_0 = \begin{cases} k(k^2 + 16\pi a\rho)^{1/2} & \text{if } |\mathbf{k}| > k_0 \\ k(k^2 + 16\pi a'\rho)^{1/2} & \text{if } |\mathbf{k}| < k_0. \end{cases} \tag{52}$$

This enables us to find the pair correlation function $D(\mathbf{r})$ of the system at absolute zero by using Feynman's formula,⁵

$$S(\mathbf{k}) = k^2 / (E_{\mathbf{k}} - E_0), \tag{53}$$

where $S(\mathbf{k})$ is the Fourier transform of the pair correlation function. We obtain from (52)

$$S(\mathbf{k}) = \begin{cases} k(k^2 + 16\pi a\rho)^{-1/2} & \text{if } |\mathbf{k}| > k_0 \\ k(k^2 + 16\pi a'\rho)^{-1/2} & \text{if } |\mathbf{k}| < k_0. \end{cases} \tag{54}$$

A qualitative plot of $S(\mathbf{k})$ is shown in Fig. 6. The behavior of $D(\mathbf{r})$ at small distances is determined by the behavior of $S(\mathbf{k})$ for large k . From (54) it is seen that at small distances $D(\mathbf{r})$ is the same as that of the hard-sphere gas, discussed in reference 2. Namely:

$$D(\mathbf{r}) \xrightarrow{r \rightarrow 0} \left(1 - \frac{a}{r}\right)^2.$$

At large distances the behavior of $D(\mathbf{r})$ is governed by the behavior of $S(\mathbf{k})$ for small k , in which the attractive part of the interaction plays an important role. A qualitative sketch of $D(\mathbf{r})$ is shown in Fig. 7. At $r > r_c$, the correlation length of the hard-sphere interaction, the function rapidly approaches unity. At $r > r_0$, the range of the attractive interaction, the function oscillates about a constant value, which by proper normalization may be made unity. It qualitatively possesses the form one expects of a system with short-range repulsive and long-range attractive interactions. The correctness of (54), being a guess at the present moment, will be proved later by higher-order calculations.

⁵ R. P. Feynman, Phys. Rev. **94**, 262 (1954). The justification for using Feynman's formula is given in reference 2.

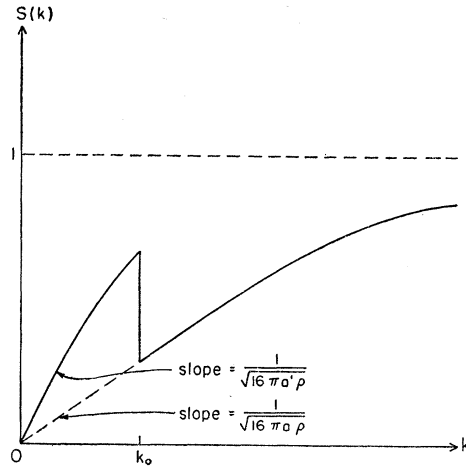


FIG. 6. Fourier transform of the pair correlation function at absolute zero. The number a' is defined in (50).

3. Excited States

Neglecting V , we can again diagonalize the Hamiltonian (38). For a given set of $\{m_{\mathbf{k}}\}$ we are to calculate that eigenvalue of (38) which reduces to $\sum k^2 m_{\mathbf{k}}$ in the absence of interactions. We are therefore calculating the energy of that perturbed state which arises from the free-particle state specified by $\{m_{\mathbf{k}}\}$, when the interactions are adiabatically "turned on." The general answer can be immediately written down; but it is too complicated to be of interest, because the quantity $\gamma_{\mathbf{k}}$, defined in (28), in general depends on the details of the set of integers $\{m_{\mathbf{k}}\}$. We shall first introduce a simplification.

We shall not consider the most general set of occupation numbers $\{m_{\mathbf{k}}\}$ satisfying the requirements (22); but we consider more restrictive sets. Namely, we impose these further restrictions on $\{m_{\mathbf{k}}\}$:

(a) The occupation of levels \mathbf{k} for $0 < |\mathbf{k}| < k_0$ is essentially uniform. That is,

$$m_{\mathbf{k}} \sim 6\pi^2 \rho (1 - \xi)x / k_0^3 \quad \text{if } 0 < |\mathbf{k}| < k_0. \tag{55}$$

(b) The occupation number $m_{\mathbf{k}}$ for $|\mathbf{k}| > k_0$, considered as a function of \mathbf{k} , changes by a negligible amount when $|\mathbf{k}|$ changes by k_0 .

The motivation of this restriction is (37), which shows that the sphere of radius k_0 contains a very small number of levels, compared to N . States not satisfying these restrictions may be expected to be of little importance for the thermodynamic properties of the system to the accuracy of the present calculation, because they describe spatial correlation effects over distances longer than the range of the attraction. With these restrictions, both $\gamma_{\mathbf{k}}$ and C become greatly

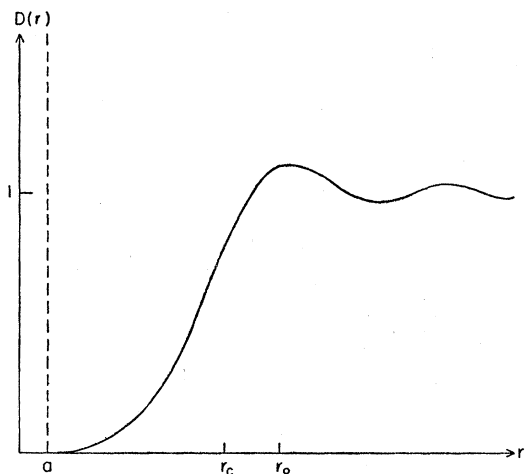


FIG. 7. Qualitative sketch of the pair correlation function at absolute zero. The lengths r_0 , r_c are defined in (16).

simplified, as shown in the Appendix:

$$\frac{C}{N} \cong -4\pi b\rho + 4\pi a\rho(1-\xi)^2 \left[\left(1 + \frac{b}{a}\right)(1-x)^2 - \frac{b}{a} \right], \quad (56)$$

$$\gamma_{\mathbf{k}} \cong \begin{cases} 8\pi a\rho(1-\xi)x & \text{if } |\mathbf{k}| > k_0 \\ 0 & \text{if } |\mathbf{k}| < k_0. \end{cases}$$

They depend on the occupation numbers $\{m_{\mathbf{k}}\}$ only through the two parameters ξ and x , which are defined by (23) and (36).

With (56) and the neglect of V , the Hamiltonian is

$$C + \sum'_{k>k_0} \{ [k^2 + 8\pi a\rho f(\xi, x)] n_{\mathbf{k}} + 4\pi a\rho f(\xi, x) (a_{\mathbf{k}}^\dagger a_{-\mathbf{k}}^\dagger + a_{\mathbf{k}} a_{-\mathbf{k}}) \}.$$

The eigenvalue corresponding to the free-particle state $\{m_{\mathbf{k}}\}$ is

$$\frac{E\{m_{\mathbf{k}}\}}{N} = -4\pi b\rho + 4\pi a\rho \left\{ g(\xi, x) + \frac{128}{15} \left(\frac{\rho a^3}{\pi} \right)^{\frac{1}{2}} F(\nu) \right. \\ \left. \times [f(\xi, x)]^{\frac{1}{2}} \right\} + \frac{1}{N} \sum_{k>k_0} k [k^2 + 16\pi a\rho f(\xi, x)]^{\frac{1}{2}} m_{\mathbf{k}} \\ + (\text{contribution from } V), \quad (57)$$

where $F(\nu)$ is defined in (42), $f(\xi, x)$ in (36), and

$$g(\xi, x) \equiv (1-\xi)^2 \left[\left(1 + \frac{b}{a}\right)(1-x)^2 - \frac{b}{a} \right]. \quad (58)$$

The formula (57) formally reduces to that given in reference 3 for the hard-sphere gas, if we put $k_0=0$, $x=0$, and $b=-a$.

In (57) the contribution from V can be calculated only for states very near the ground state ($\xi \cong 1$). The

answer, derived in the next section, is

$$(\text{contribution from } V) = N^{-1} \sum_{0 < k < k_0} k^2 (k^2 + 16\pi a\rho)^{\frac{1}{2}} m_{\mathbf{k}} \\ (\text{for } \xi \cong 1), \quad (59)$$

where a' is defined in (50). For general ξ , the calculation becomes too difficult. It is sufficient for the present purpose to take the zero-order answer:

$$(\text{contribution from } V) \cong N^{-1} \sum_{0 < k < k_0} k^2 m_{\mathbf{k}} \\ = \frac{2}{3} (1-\xi) x k_0^2. \quad (60)$$

The last expression results from the assumptions (55). This formula is in conformity with (59), since $16\pi a\rho' \ll k_0^2$.

For given values of ξ , x , we have the inequality

$$N^{-1} E\{m_{\mathbf{k}}\} \geq \epsilon_{\xi, x}(\rho), \quad (61)$$

where

$$\epsilon_{\xi, x}(\rho) = -4\pi b\rho + 4\pi a\rho \left\{ g(\xi, x) + \frac{128}{15} \left(\frac{\rho a^3}{\pi} \right)^{\frac{1}{2}} F(\nu) \right. \\ \left. \times [f(\xi, x)]^{\frac{1}{2}} \right\} + k_0 [k_0^2 + 16\pi a\rho f(\xi, x)]^{\frac{1}{2}} (1-\xi)(1-x) \\ + \frac{2}{3} (1-\xi) x k_0^2. \quad (62)$$

When $\xi=1$, denote it by $\epsilon_1(\rho)$. The function $\epsilon_1(\rho)$ is independent of x . In fact $\epsilon_1(\rho) = E_0/N$. For fixed ξ , x , the quantity $\epsilon_{\xi, x}(\rho)$ as a function of ρ is an envelope of all energy levels belonging to given values of ξ, x . In order to investigate whether any $E\{m_{\mathbf{k}}\}$ can be smaller than E_0 , it is sufficient to ask whether $\epsilon_{\xi, x}(\rho)$ can be smaller than $\epsilon_1(\rho)$.

Let us first look at some limiting cases:

For $\xi=1$ (no particle excited):

$$\epsilon_1(\rho) = 4\pi a\rho \left[-\frac{b}{a} + \frac{128}{15} \left(\frac{\rho a^3}{\pi} \right)^{\frac{1}{2}} F(\nu) \right].$$

For $\xi=0$, $x=0$ (all N particles excited to levels above k_0)

$$\epsilon_{0,0}(\rho) = 4\pi a\rho [1 - (b/a)] + k_0^2 \cong 4\pi a\rho + k_0^2.$$

For $\xi=0$, $x=1$ (all N particles excited to levels below k_0):

$$\epsilon_{0,1}(\rho) = -8\pi b\rho + (4\pi a\rho) \frac{128}{15} \left(\frac{\rho a^3}{\pi} \right)^{\frac{1}{2}} F(\nu) + \frac{2}{3} k_0^2.$$

The function ϵ_1 has a minimum at ρ_0 given by (45). The function $\epsilon_{0,0}$ is a monotonically increasing function of ρ , which is everywhere greater than ϵ_1 . The function $\epsilon_{0,1}$ has a minimum at $\rho > \rho_0$; but it is everywhere much larger than ϵ_1 if $k_0^2/(a\rho)^{\frac{1}{2}} \sim 1$ as we assume, for then

$$\frac{k_0^2}{b\rho} = \frac{k_0^2 a}{a\rho b} \gg 1. \quad (63)$$

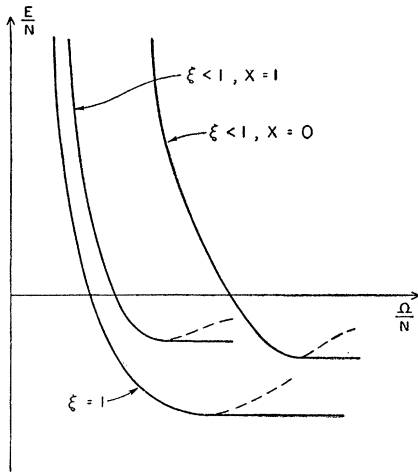


FIG. 8. Qualitative plot of some perturbed energy levels of the system, as a function of available volume per particle. The quantum numbers ξ , x refer to the unperturbed state from which the perturbed state arises, as the interaction is adiabatically turned on. ξ is the fraction of particles in the level $\mathbf{k}=0$. x is the fraction of excited particles in the levels \mathbf{k} , with $0 < |\mathbf{k}| < k_0$.

For $\xi \cong 1$ (very few particles excited), let $\xi = 1 - \Delta$. It is easily verified, keeping (63) in mind, that

$$\epsilon_{\xi, x}(\rho) - \epsilon_1(\rho) = \left\{ k_0(k_0^2 + 16\pi a\rho)^{\frac{1}{2}}(1-x) + \frac{2}{5}k_0^2 x + 4\pi a \left[\frac{b}{a} - \frac{64}{5} \left(\frac{\rho a^3}{\pi} \right)^{\frac{1}{2}} \right] \right\} \Delta > 0.$$

For $0 < \xi < 1$ the formulas become more complicated, but these conclusions are maintained. We illustrate the qualitative behavior of the energy levels of the system by the graph of Fig. 8.

4. Higher-Order Calculations

We now come to an important part of the calculation, important not because the results here will alter any of the formulas used previously; but because they show that the opposite is true. The main result of this section is a verification of the formulas (25), (52), and (54).

The following calculation is to be carried out: Take into account the term V in the Hamiltonian (38), and calculate the corrections to energy levels in the neighborhood of the ground state (i.e., for $\xi \cong 1$). V is defined by (39). In terms of free-particle states, every term of V describes a scattering between two particles. If the momentum transfer in the scattering is greater than k_0 the matrix element is of order a ; and if less than k_0 , of order b . Let us for convenience denote by a capital boldface Latin letter \mathbf{K} a momentum of magnitude greater than k_0 , and by a lower case boldface Greek

letter $\boldsymbol{\lambda}$ a momentum of magnitude greater than 0 but less than k_0 :

$$\begin{aligned} \mathbf{K}: |\mathbf{K}| > k_0, \\ \boldsymbol{\lambda}: 0 < |\boldsymbol{\lambda}| < k_0. \end{aligned} \quad (64)$$

A matrix element of V may be specified by giving all four of the initial and final momenta involved in the scattering process described. The sum of these momenta must be zero. If we use the conditions (25), it is straightforward to show that to calculate the energies to the next order, it is sufficient to take into account the following types of matrix elements:

- (1) $\mathbf{K}_1, \mathbf{K}_2, \mathbf{K}_3, 0$,
- (2) $\mathbf{K}_1, \mathbf{K}_2, \mathbf{K}_3, \mathbf{K}_4$,
- (3) $\mathbf{K}_1, \mathbf{K}_2, \boldsymbol{\lambda}, 0$,
- (4) $\mathbf{K}_1, \mathbf{K}_2, \boldsymbol{\lambda}_1, \boldsymbol{\lambda}_2$,
- (5) $\boldsymbol{\lambda}_1, \boldsymbol{\lambda}_2, 0, 0$.

All other give contributions to a still higher order, by virtue of $b/a \ll 1$ or $k_0 a \ll 1$. Among the matrix elements described by (65), types 1 and 2 contribute to the ground-state energy, and to the excitation spectrum for $k > k_0$. In both cases their treatment is, except for trivial modifications, identical with the higher-order corrections to the hard-sphere Bose gas, as discussed in reference 2. It is shown there that they give rise to corrections in higher powers of $(\rho a^3)^{\frac{1}{2}}$, and hence can be neglected. We shall not repeat these discussions here.

It is sufficient, therefore, to consider matrix elements of the types 3, 4, and 5 of (65). They may be characterized by the fact that they all describe scattering processes in which two momenta are smaller than k_0 , and two greater. They cannot be treated in ordinary perturbation theory by calculating to any finite order; but one must again in essence perform infinite sums, just as in the calculations of the previous sections.

If we retain in V only those matrix elements of types 3, 4, and 5 of (65), it is easily shown that we may neglect V_0' and V_1' altogether, while V_2 , V_3 may be replaced, respectively, by

$$\begin{aligned} \tilde{V}_2 = 8\pi a \Omega^{-1} N^{\frac{1}{2}} \sum_{\mathbf{K}} \sum_{\mathbf{P}, \boldsymbol{\lambda}} [\delta(\mathbf{P} + \mathbf{K} - \boldsymbol{\lambda}) a_{\mathbf{P}}^\dagger a_{\mathbf{K}}^\dagger a_{\boldsymbol{\lambda}} \\ + \delta(\mathbf{P} - \mathbf{K} - \boldsymbol{\lambda}) a_{\mathbf{P}}^\dagger a_{\mathbf{K}} a_{\boldsymbol{\lambda}}] + \text{H.C.}, \end{aligned} \quad (66)$$

and

$$\tilde{V}_3 = 4\pi a \Omega^{-1} \sum_{\mathbf{K}} \sum_{\boldsymbol{\lambda}} (a_{\mathbf{K}}^\dagger a_{-\mathbf{K}}^\dagger a_{\boldsymbol{\lambda}} a_{-\boldsymbol{\lambda}} + a_{\mathbf{K}} a_{-\mathbf{K}} a_{\boldsymbol{\lambda}}^\dagger a_{-\boldsymbol{\lambda}}^\dagger). \quad (67)$$

In the above, the convention (64) is adhered to. The δ functions in \tilde{V}_2 are Kronecker symbols. The Hamil-

tonian to be diagonalized is now

$$\begin{aligned}
 H = & -4\pi b\rho N + \sum_{\mathbf{K}}' [(K^2 + 8\pi a\rho)n_{\mathbf{K}} \\
 & + 4\pi a\rho(a_{\mathbf{K}}^\dagger a_{-\mathbf{K}}^\dagger + a_{\mathbf{K}} a_{-\mathbf{K}})] + \sum_{\lambda} \{[\lambda^2 - 8\pi b\rho \\
 & - 4\pi a\Omega^{-1} \sum_{\mathbf{K}}' (a_{\mathbf{K}}^\dagger a_{-\mathbf{K}}^\dagger + a_{\mathbf{K}} a_{-\mathbf{K}})]n_{\lambda} \\
 & - 4\pi b\rho(a_{\lambda}^\dagger a_{-\lambda}^\dagger + a_{\lambda} a_{-\lambda})\} + \tilde{V}_2 + \tilde{V}_3. \quad (68)
 \end{aligned}$$

We had earlier diagonalized H , when V was completely neglected. Let us transform H into that representation. It is simplest to express this transformation as a linear transformation⁶ of $a_{\mathbf{K}}$. With the substitution

$$\begin{aligned}
 a_{\mathbf{K}} &= (1 - \alpha_{\mathbf{K}})^{-\frac{1}{2}} [b_{\mathbf{K}} - \alpha_{\mathbf{K}} b_{-\mathbf{K}}^\dagger], \\
 a_{\mathbf{K}}^\dagger &= (1 - \alpha_{\mathbf{K}})^{-\frac{1}{2}} [b_{\mathbf{K}}^\dagger - \alpha_{\mathbf{K}} b_{-\mathbf{K}}], \quad (69)
 \end{aligned}$$

where

$$\begin{aligned}
 \alpha_{\mathbf{K}} &= (2y_{\mathbf{K}})^{-1} [1 - (1 - 4y_{\mathbf{K}}^2)^{\frac{1}{2}}], \\
 y_{\mathbf{K}} &= 4\pi a\rho(K^2 + 8\pi a\rho)^{-1}, \quad (70)
 \end{aligned}$$

we thus transform to the new operators $b_{\mathbf{K}}$, $b_{\mathbf{K}}^\dagger$, which again satisfy the commutation rules

$$[b_{\mathbf{K}}, b_{\mathbf{P}}^\dagger] = \delta_{\mathbf{K}\mathbf{P}}. \quad (71)$$

The transformation is therefore a canonical one, provided $\alpha_{\mathbf{K}} < 1$, which is obviously true. We shall refer to this new representation as the b -representation. In this representation

$$\begin{aligned}
 H = & E_0 + \sum_{\mathbf{K}} K(K^2 + 16\pi a\rho)^{\frac{1}{2}} b_{\mathbf{K}}^\dagger b_{\mathbf{K}} + \tilde{V}_2 + \tilde{V}_3 \\
 & + \sum_{\lambda} \{[\lambda^2 - 8\pi b\rho - 4\pi a\Omega^{-1} \sum_{\mathbf{K}} (a_{\mathbf{K}}^\dagger a_{-\mathbf{K}}^\dagger + a_{\mathbf{K}} a_{-\mathbf{K}})]n_{\lambda} \\
 & - 4\pi b\rho(a_{\lambda}^\dagger a_{-\lambda}^\dagger + a_{\lambda} a_{-\lambda})\}, \quad (72)
 \end{aligned}$$

where E_0 is defined in (41) and one must identify: $b_{\mathbf{K}}^\dagger b_{\mathbf{K}} = m_{\mathbf{K}}$. Formula (72) is strictly correct only if all $m_{\mathbf{K}} = 0$ (i.e., $\xi = 1$). But we can still use it in the neighborhood of $\xi = 1$. In particular the excitation spectrum can be obtained from (72) with errors of order N^{-1} . It immediately gives $K(K^2 + 16\pi a\rho)^{\frac{1}{2}}$ for the energy of a phonon of momentum larger than k_0 . The corrections to this spectrum are of higher order in $(\rho a^3)^{\frac{1}{2}}$ and have been neglected from the beginning. \tilde{V}_2 and \tilde{V}_3 contribute to the excitation spectrum only for momenta below k_0 . This contribution we calculate, because it represents the lowest nonvanishing order.

We must now transform \tilde{V}_2 and \tilde{V}_3 , given by (66) and (67), into the b -representation. This transformation affects only $a_{\mathbf{K}}$ and $a_{\mathbf{K}}^\dagger$. The operators a_{λ} , a_{λ}^\dagger , since they commute with the former, may be looked upon as c -numbers during this transformation. In the b -representation \tilde{V}_2 has no diagonal matrix elements. It will be diagonalized by second-order perturbation theory. \tilde{V}_3 has diagonal matrix elements and that is

⁶ N. N. Bogoliubov, J. Phys. U.S.S.R. 2, 23 (1947).

all we shall retain. It is easily shown that further diagonalization of \tilde{V}_2 and \tilde{V}_3 in the b -representation yields only higher order terms that should be neglected.

A state $|m_{\mathbf{K}}\rangle$ of the system in the b -representation is specified by the occupation numbers $b_{\mathbf{K}}^\dagger b_{\mathbf{K}} \equiv m_{\mathbf{K}}$ of independent phonons whose energy is

$$\omega_{\mathbf{K}} = K(K^2 + 16\pi a\rho)^{\frac{1}{2}}. \quad (73)$$

We have, by virtue of (71),

$$\begin{aligned}
 b_{\mathbf{K}}^\dagger b_{\mathbf{K}} |m_{\mathbf{K}}\rangle &= m_{\mathbf{K}} |m_{\mathbf{K}}\rangle, \\
 b_{\mathbf{K}}^\dagger |m_{\mathbf{K}}\rangle &= (m_{\mathbf{K}} + 1)^{\frac{1}{2}} |m_{\mathbf{K}} + 1\rangle, \\
 b_{\mathbf{K}} |m_{\mathbf{K}}\rangle &= m_{\mathbf{K}}^{\frac{1}{2}} |m_{\mathbf{K}} - 1\rangle. \quad (74)
 \end{aligned}$$

We are interested in the energy contributions of \tilde{V}_2 and \tilde{V}_3 in the state $|0\rangle$ (i.e., all $m_{\mathbf{K}} = 0$). We have for the contribution of \tilde{V}_3

$$\langle 0 | \tilde{V}_3 | 0 \rangle = \frac{4\pi a}{\Omega} \left[-\sum_{\mathbf{K}}' \frac{\alpha}{1 - \alpha^2} \right] \sum_{\lambda} (a_{\lambda}^\dagger a_{-\lambda}^\dagger + a_{\lambda} a_{-\lambda}), \quad (75)$$

where we let α stand for $\alpha_{\mathbf{K}}$. The contribution of \tilde{V}_2 is, apart from a term of the form $(\text{const})N(a\rho)(k_0 a)^2 [k_0/(\rho a)^{\frac{1}{2}}]$, which we drop, the following:

$$\begin{aligned}
 \sum_m \frac{|\langle m | \tilde{V}_2 | 0 \rangle|^2}{E_0 - E_m} &= N \left(\frac{8\pi a}{\Omega} \right)^2 \sum_{\lambda} \left\{ \left[-\sum_{\mathbf{K}}' \frac{1 + \alpha^2}{(1 + \alpha)^2} \frac{1}{\omega} \right] a_{\lambda}^\dagger a_{\lambda} \right. \\
 & \left. + \left[\sum_{\mathbf{K}}' \frac{\alpha}{(1 + \alpha)^2} \frac{1}{\omega} \right] (a_{\lambda}^\dagger a_{-\lambda}^\dagger + a_{\lambda} a_{-\lambda}) \right\}, \quad (76)
 \end{aligned}$$

where ω stands for $\omega_{\mathbf{K}}$. Substituting (75) and (76) into (72), we obtain

$$\begin{aligned}
 \langle 0 | H | 0 \rangle &= E_0 + \sum_{\lambda} \{ (\lambda^2 + 8\pi a\rho X - 8\pi b\rho) a_{\lambda}^\dagger a_{\lambda} \\
 & + (4\pi a\rho X - 4\pi b\rho) (a_{\lambda}^\dagger a_{-\lambda}^\dagger + a_{\lambda} a_{-\lambda}) \}, \quad (77)
 \end{aligned}$$

where

$$X \equiv -\frac{4\pi a\rho}{N} \sum_{\mathbf{K}}' \left(\frac{1 - \alpha}{1 + \alpha} \right)^2 \frac{1}{\omega}.$$

After taking into account the subtraction procedure required by \sum' , as explained by (13), and performing some elementary integrals, we find

$$\begin{aligned}
 X = & 16(\rho a^3/\pi)^{\frac{1}{2}} \left[(1 + \nu^2)^{\frac{1}{2}} + (1 + \nu^2)^{-\frac{1}{2}} \right], \\
 & \nu \equiv k_0/(16\pi a\rho)^{\frac{1}{2}}. \quad (78)
 \end{aligned}$$

Now $\langle 0 | H | 0 \rangle$ still has to be diagonalized with respect to a_{λ} , a_{λ}^\dagger . This task is trivial, since the mathematical problem is identical with that solved by the transformations (69). We obtain immediately

$$\langle 0 | H | 0 \rangle = E_0 + \sum_{\lambda} \lambda(\lambda^2 + 16\pi a'\rho)^{\frac{1}{2}} m_{\lambda}, \quad (79)$$

apart from a correction to E_0 of the form $(\text{const})N(a\rho) \times (k_0 a)^2 [k_0/(\rho a)^{\frac{1}{2}}]$, which we drop. In (79), a' is exactly that given by (50). This verifies the formula (52), and

the sound velocity (49) computed from the compressibility of the system. Furthermore, this derivation shows that for small λ *there are no other excitations*. If one is familiar with the results of reference 2 the following statements are now obvious:

1. The conditions (25) are correct.
2. The wave function of the system is the same as that for the hard-sphere gas, except that in all Fourier components with $k < k_0$ we replace a by a' . This justifies the formulas (54).

Perhaps, to make statement 2 more explicit, we should write down the ground-state wave function of the system. Let the ground-state wave function Ψ_0 be expanded in terms of free-particle wave functions. The only free-particle wave functions Φ that enter into this expansion are those in which particles are excited in pairs of total momentum zero. That is, if l_k is the occupation number of the level \mathbf{k} , then $l_{\mathbf{k}} = l_{-\mathbf{k}}$:

$$\Psi_0 = \sum_{l_1=0}^{\infty} \sum_{l_2=0}^{\infty} \cdots [C_{l_1}(\mathbf{k}_1) C_{l_2}(\mathbf{k}_2) \cdots] \Phi(l_1, l_2, \cdots); \quad (80)$$

and up to a normalization constant,

$$C_l(\mathbf{k}) = \begin{cases} (\alpha_K)^l & \text{if } |\mathbf{k}| > k_0 \\ (\alpha_K')^l & \text{if } |\mathbf{k}| < k_0, \end{cases} \quad (81)$$

where α_K is defined by (70), and α_K' is formally the same as (70) except that a' replaces a everywhere. The wave function for a state with one phonon is, up to a normalization constant,

$$\Psi_{\mathbf{k}} = \sum_{j=1}^N e^{i\mathbf{k} \cdot \mathbf{r}_j} \Psi_0, \quad (82)$$

which is the form of the wave function that leads to Feynman's formula (53).

V. DISCUSSIONS

The mathematical method employed in the present investigation is similar to those used in reference 2. The discussions there concerning the validity of the mathematical methods and the application to liquid He^4 also apply to the present case. In this section we discuss only those questions which are particular to the present model.

By showing the consistency of the conditions (25), the calculations in the last section verify the consistency of the assumption that if a level is macroscopically occupied, this fact is not changed by the interactions. This assumption leads to an expansion of the energy in powers of $(\rho a^3)^{\frac{1}{2}}$. It may be formulated physically by saying that a macroscopically occupied level represents a "sea" of inexhaustible particles, which have complete order in momentum space. This order is not destroyed by the interactions. But consistency does not necessarily guarantee correctness. The correctness of this assumption has not been proved,

either in the case of the hard-sphere Bose gas or in the present model. While in the former case one may on physical grounds believe it to be correct, one might not accept it so readily in the present case. An argument in favor of its correctness in the present case, even if only a physical one, is called for.

The mathematical expression of the assumption mentioned above is the exclusion from our consideration states of the system outside the subspace S spanned by states defined by (22). This exclusion is motivated by the fact that it takes of the order of N interactions to take a state in S outside of it. As N approaches infinity the probability for this to happen is very small. The calculation, under this assumption, shows that the smallness of this probability is measured by $(\rho a^3)^{\frac{1}{2}}$. However, by this assumption we have obviously failed to obtain, from direct calculation, states like that represented by point P of Fig. 4. Rather, at that density we obtain the state P' , and the existence of P is deduced by an argument. We would like to give physical explanations as to

- (i) why we failed to obtain the state P by direct calculation,
- (ii) why we can still believe the results for $\rho \geq \rho_0$, and
- (iii) what meaning can be attached to the state P' .

The notation above refers to Fig. 4.

In answer to (i), it is obvious why we failed to obtain P directly. The state P , as the discussion earlier shows, is a state in which the system does not occupy the whole volume Ω . It is therefore possible for the system there to break up into *two* or more macroscopic clusters of particles, each having their own surfaces. Now the unperturbed free-particle state uniformly fills the entire volume. In order to break it up into clusters, each containing of the order of N particles, it is clearly necessary for the interaction to act of the order of N times. Since we have "shut off" such channels of interaction, our failure is not surprising. As long as we restrict ourselves to subspace S , we should not be able to calculate these clustering states, even if we could solve the restricted problem exactly.

If we believe in the validity of conclusions indicated by theories of condensation, we would believe that these macroscopic clusters come into existence abruptly at $\rho = \rho_0$, and therefore they are ignorable for all densities $\rho > \rho_0$. A knowledge of the system for densities $\rho > \rho_0$ is, according to this view, sufficient to determine the energy for all lower densities. The states outside of the subspace S that we have excluded, if taken into account, would of course give us more information. They would also yield the combinatorial information of how the system may break up into clusters of varying sizes. But in the latter we are not interested. This answers (ii).

What significance can we attach to the states like P' of Fig. 4, which is obtained by analytic continuation of the function $E(\rho)$ to $\rho < \rho_0$? It seems plausible that they represent true states of the system if the channels

leading to the formation of macroscopic clusters were artificially "shut off"; but that they must be unstable when these channels are "open." In the absence of surface effects, these states would decay into cluster states in the order of a collision time of the system; but with surface effects, they could be metastable. This is the answer to (iii).

Let us now turn to another physical discussion, concerning what might be expected of the thermodynamic properties of the present model. It is to be emphasized that the value of the following discussion is purely heuristic.

Let us first recall the thermodynamic properties of the hard-sphere Bose gas, as discussed by reference 3. It is there shown that even in the presence of interparticle interaction, the Bose-Einstein condensation remains. The system may exist in two phases, the gas phase and the degenerate phase. In the latter phase the important states of the system are those in which $\xi > 0$, that is, those in which a "sea" of particles exist, whereas in the gas phase only the set of states with $\xi = 0$ is important. The transition from the gas to the degenerate phase is a transition from states that have no momentum-space order, to ones that have. It is clearly the analog of the Bose-Einstein condensation of the ideal gas.

In the present model, there are states possessing a "sea" of particles ($\xi > 0, x = 0$). This "sea" represents a complete order in momentum space, and has a direct counterpart in the hard-sphere case. There are also states that possess no order in momentum space, namely those labeled by $\xi = 0, x = 0$. However, we have a new parameter x , which is a macroscopic parameter. The states for which $x > 0, \xi \neq 1$ represent states in which a finite fraction of the particles are partially ordered in momentum space, their momenta differing from one another by not more than $2k_0$. This means that in ordinary space they should have a correlation over distances of the order of r_0 , the range of the attractive potential. It is plausible that the states with $x > 0, \xi \neq 1$ form new phases, which might be called "liquid" phases, the difference between these new phases being $\xi = 0$, or $\xi \neq 0$. They might be called respectively an "ordinary liquid" and a "degenerate liquid." The transition between them, if it exists, would be the

analog of the Bose-Einstein condensation of the ideal gas. In addition to these, of course, we would still have the gas phase, in which the states $\xi = 0, x = 0$ are important.

It is probable that the above discussion is oversimplifying; but it might be qualitatively correct. The present model therefore offers hope that the qualitative thermodynamic properties of liquid He⁴, in particular the existence of liquids I and II, might be reproducible in a relatively simple way.

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APPENDIX

We shall briefly indicate how the simplified forms for C and γ_k , given by (27) and (28), are arrived at. The exact formula for γ_k , given in (28), may be rewritten as follows

$$\gamma_k = 8\pi a \rho (1 - \xi) \left(1 + \frac{b}{a} \right) x - \frac{8\pi b}{\Omega} \sum_{0 < p < k_0} m_{p+k}. \quad (\text{A1})$$

The sum $\sum m_{p+k}$ in the last term, as a function of \mathbf{k} , is bounded between $N(1 - \xi)x$ and zero. If we use the assumptions (55) about $\{m_k\}$, it is easily seen that this sum becomes equal to the negligible value $(\Omega k_0^3 / 6\pi^2) m_k$ for $|\mathbf{k}| > 2k_0$ and is equal to $N(1 - \xi)x$ for $k = 0$. Between $\mathbf{k} = 0$ and $|\mathbf{k}| = 2k_0$ it is between these values. Since the assumption about $\{m_k\}$ is only a qualitative one, it is in the spirit of this assumption to take the sum $\sum m_{p+k}$ to be a step function:

$$\sum_{0 < p < k_0} m_{p+k} = \begin{cases} N(1 - \xi)x & \text{if } |\mathbf{k}| < k_0 \\ 0 & \text{if } |\mathbf{k}| > k_0. \end{cases} \quad (\text{A2})$$

Substituting this into (A1) yields the expression given in (56) for γ_k .

To evaluate C , we neglect terms of the form $\sum m_k^2$ as compared to $(\sum m_k)^2$. This is in accordance with the basic assumption that no level other than $\mathbf{k} = 0$ is macroscopically occupied. Having made this neglect, we make use of (A2) to obtain the formula (56) for C .