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Phonons and the Properties of a Bose System*

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In this paper we suggest a new ground-state wave fuction and low-temperature density matrix for a strongly interacting system of bosons. Our basic assumption is that the system can support long-wavelength phonons and that these can propagate independently of any other mode of motion. We therefore write the ground-state function as the product of two factors. One factor arises from the zero-point motion of the phonons, and we show that it has the form $\prod_{i<j} f(r_{ij})$, where $\ln f(r)$ has an infinite range. The other factor is assumed to have this same form but with $\ln f(r)$ of finite range; it takes into account the short-range correlations arising from the strong repulsive part of the interparticle potential. The function we have chosen to represent the short-range correlations is not new; functions of this kind were first introduced by Bijl and later by Jastrow. At finite temperatures we use a density matrix for an ensemble of excited phonon states. We find that for small wave vectors k, the structure factor $S(k)$ is equal to $\hbar k/2mc$, a result that was first derived by Feynman. At a finite temperature T, $S(k)$ tends to the constant value k_BT/mc^2, where m is the mass of the particles and c the velocity of propagation of the phonons. The momentum distribution n_k has a k^{-1} singularity at absolute zero and a stronger, k^{-2} singularity at finite temperatures. The small-k behavior of both $S(k)$ and n_k is completely controlled by the correlations introduced by the phonons. Both the ground-state function and the density matrix imply that there is a finite fraction of particles in the zero-momentum state in three dimensions; this fraction does not seem to be appreciably affected by the infinite-range correlations introduced by the phonons. We find, however, that these correlations imply that a one-dimensional Bose system does not exhibit Bose-Einstein condensation at any temperature, while a two-dimensional system exhibits Bose-Einstein condensation only at absolute zero.

I. INTRODUCTION

In this paper we suggest a new approximate ground-state wave function and low-temperature density matrix for a system of interacting bosons.[1] The wave function and density matrix are constructed to take into account both the short-range correlations arising from the strong repulsive interactions between the particles and the infinite-range correlations which we show must be present if the system can support low-lying phonon modes. The physical properties we deduce on the basis of this wave function and density matrix are in excellent agreement with our expectations. Moreover, we are able to show that the infinite-range correlations introduced by the phonon modes are decisive in determining whether or not the system exhibits Bose-Einstein condensation into the zero-momentum state in one, two, and three dimensions.

The importance of the low-lying phonon modes in Bose systems—in particular in superfluid helium—was first emphasized by Landau.[2] Feynman[3] carried these ideas a stage farther by constructing an explicit approximate form for the low-lying phonon states. Both Landau and Feynman argued that the long-wavelength phonon modes should propagate independently of any other modes of motion and of each other. This will be our basic assumption in this paper. It has been confirmed by detailed model calculations[4] and by perturbation analysis.[5] It seems that at the present time there are no experiments which bear directly on this assumption. What we need to know is whether the condition $\omega_k\tau_k \gg 1$ is satisfied for very-long-wavelength phonons at low temperatures. The recent inelastic-neutron experiments of Woods[6] suggest that our assumption is indeed correct. They do not, however, go to small enough wave vectors or low enough temperatures to directly confirm it. Feynman showed that if one assumes that the zero-point motion of the phonons dominates the behavior of the zero-temperature structure factor $S(k)$ at small wave numbers k, then it must behave like $\hbar k/2mc$ for small k. Here c is the velocity of propagation of the phonons and m the mass of the atoms. This behavior of $S(k)$ for small k is different from that of $S(k)$ for a classical fluid. The long-wavelength phonons must therefore introduce correlations into the ground-state wave function which are not present in a classical fluid. We shall show that this, in fact, is the case.

It is, however, quite clear that the long-wavelength phonon modes cannot tell us anything at all about the short-range correlations due to the strong repulsive part of the interparticle potential. These are presumably operative over two or three interparticle spacings and are therefore of a much shorter-length scale than the wavelength of a long-wavelength phonon, whose wavelength should—by definition—be many interparticle distances at least. An approximate wave function that takes these short-range correlations into account was

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[2] L. D. Landau, J. Phys. USSR **5**, 71 (1941).

[3] R. P. Feynman, Phys. Rev. **94**, 262 (1954); R. P. Feynman and M. Cohen, *ibid.* **102**, 1189 (1956).

[4] I. M. Khalatnikov, *Introduction to the Theory of Superfluidity*, (W. A. Benjamin Inc., New York, 1965), Chap. 22.

[5] J. Gavoret and P. Nozières, Ann. Phys. (N. Y.) **28**, 349 (1964).

[6] A. D. B. Woods, Phys. Rev. Letters **14**, 355 (1965).

first suggested by Bijl[7] and later by Jastrow.[8] It has recently been used in variational calculations of properties of liquid He^4 by McMillan[9] and by Levesque *et al.*[10] This wave function has the form of a product of pair functions, $f(r_{ij})$:

$$\psi=\prod_{i<j}^{1,\cdots,N} f(r_{ij}), \quad r_{ij}\equiv|\mathbf{r}_i-\mathbf{r}_j|. \tag{1.1}$$

The function $f(r)$ is real, and the short-range correlations are introduced by taking $f(r)$ to be a function that tends rapidly to zero as $r\rightarrow 0$, and rapidly to unity as $r\rightarrow\infty$. In the variational calculations we have referred to, $f(r)$ was chosen to have the form $\exp[-u(r)]$ where $u(r)$ had the asymptotic form $r^{-(3+\alpha)}$ for large r; $\alpha>0$. We shall call such a pair function $f(r)$ a "finite-range" function. With this kind of function the variational calculations for liquid helium were successful in reproducing the experimental binding energy, and the structure factor $S(k)$ for those values of k for which it has been measured ($0.6\leq k\leq 6$ Å^{-1}).

The structure factor $S(k)$ which follows from a wave function of the form (1.1), with a finite-range pair function, is formally equal to the structure function of a classical fluid at a nonzero temperature. [The interaction potential $\varphi(r)$ and effective temperature T_{eff} of this equivalent classical fluid are related to $f(r)$ by the equation $(2k_BT_{\mathrm{eff}})^{-1}\varphi(r)=-\ln f(r)$]. $S(k)$ will therefore have the same qualitative behavior as the structure factor for a classical fluid. In particular the Ornstein-Zernike theory[11] assures us that $S(0)\neq 0$ and hence $S(k)$ cannot behave for small k in the way suggested by Feynman. A similar difficulty arises with the momentum distribution of the particles n_k. On the basis of perturbation calculations,[5] we expect that at absolute zero n_k will behave like k^{-1} for small k; this is again a result that comes from the zero-point motion of the long-wavelength phonons. [The singular behavior of n_k as $k\rightarrow 0$ should not be confused with the actual value of n_k at $k=0$. This is the number of particles on the zero-momentum state, and, with a finite range $f(r)$, this is known to be finite fraction of the total.[12]] It is quite easy to show that a finite-range pair function $f(r)$ leads to a distribution n_k which tends to a constant value as $k\rightarrow 0$. We therefore see that although the wave function (1.1) can give an excellent description of some of the physical properties of liquid helium, it does not give what we believe to be the correct limiting form for either $S(k)$ or n_k for small k. This strongly suggests that this wave function does not correctly describe the zero-point motion of the long-wavelength phonons.

The aim of this paper is to present a ground-state function and at finite temperatures a density matrix that take into account the short-range correlations that are present in (1.1), and at the same time correctly represent the correlations due to the long-wavelength phonons. In this way we cannot expect to obtain any new information about $S(k)$ or n_k for small k. The behavior of these functions for small k follows quite directly from our basic assumptions without constructing an explicit form for the wave function and density matrix. However, the construction of an approximate ground-state function and density matrix is the only method known to us by which one can take into account both the long-wavelength phonons and short-range correlations. In particular it enables us to compute $S(k)$ and n_k for all k. It is of course not an entirely trivial matter to show that the approximate wave function proposed will lead to the correct small-k behavior for these functions. Sections III and V are devoted to showing that our wave function does indeed lead to the behavior we expect.

As we have already stated, our basic assumption is that at sufficiently low temperatures the system can support long-wavelength phonons that propagate independently of each other and of any other mode of motion. We shall discuss the assumption in more detail in Sec. II. If it is correct, the Hamiltonian for the system can be written as the sum of a harmonic term for the phonons and another term which represents the other modes of motion, and there should be negligible coupling between these two terms. It follows that the ground state function must have the form

$$\psi_0=\psi_R\psi_{\mathrm{ph}}, \tag{1.2}$$

where ψ_{ph} is the ground-state function for the phonon modes, and ψ_R is the ground state for the rest of the Hamiltonian. It is easy to construct ψ_{ph} explicitly and to show that it can be written as a product of pair functions $f(r_{ij})$ *but that the pair function f has an infinite range.* These infinite-range correlations in the ground state control the behavior of $S(k)$ and n_k for small k, and these same correlations make the Ornstein-Zernike theory inapplicable to the ground state. The function ψ_R represents the other modes of motion, and we see no reason to believe that it will have any infinite-range correlations in it. For purposes of calculation we shall choose it to be of the form (1.1) with $f(r)$ of finite range. We believe that (1.2) represents a very plausible approximation to the ground state of a boson system, irrespective of the strength of the coupling or the density of the system; indeed, it may give a good description of liquid He^4. A crucial test of this function will be to calculate the ground-state energy of the system with it and see if the presence of the phonon factor lowers the energy (or at least does not raise it).

The low-lying excited states ψ_{ex} follow at once from our assumption; we simply replace ψ_{ph} in (1.2) by the

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[9] W. L. McMillan, Phys. Rev. 138, A442 (1965).

[10] D. Levesque, D. Schiff, Tu Khiet, and L. Verlet, (unpublished).

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[12] O. Penrose and L. Onsager, Phys. Rev. 104, 576 (1956).

appropriate excited-phonon state,

$$\psi_{\rm ex}=\psi_R\psi_{\rm ph}{}^{(\rm ex)}. \tag{1.3}$$

Now, for a single phonon, $\psi_{\rm ph}{}^{(\rm ex)}$ will have (see Sec. II) exactly the form proposed by Feynman,

$$\psi_{\rm ph}{}^{\rm ex}=(2mc/N\hbar k)^{1/2}\rho_k\psi_{\rm ph}, \tag{1.4}$$

where ρ_k is the Fourier transform of the density $\rho(r)$. Of course (1.3) is only correct for the excited-phonon states; if there are any other lower states, then they cannot be represented by (1.3). However, if there *are* any such states, the phonons could presumably decay into them, and would *not* propagate independently of them. This contradicts our basic hypothesis. Following Penrose,[13] we can construct the density matrix for an ensemble of such states. The most important feature of this density matrix is that its diagonal elements do not this density matrix is that its diagonal elements do not contain any infinite-range correlations. The behavior of $S(k)$ for small k is now quite different and we find that $S(0)=(m\beta c^2)^{-1}$, where $\beta=(k_BT)^{-1}$. This is in complete agreement with what we expect on the basis of the Ornstein-Zernike theory, and is exactly the result obtained by Feynman.[3] The momentum distribution n_k has a k^{-1} singularity at absolute zero; with this density matrix we find a stronger k^{-2} singularity at finite temperatures.

The wave function and density matrix we have constructed lead to qualitatively different properties for a Bose system in one, two, and three dimensions. In three dimensions, we find that there is a condensate; that is, a finite fraction of particles in the zero-momentum state, both at absolute zero and at finite temperatures. In one dimension we do not find a condensate at any temperature, and in two dimensions there is a condensate at absolute zero but not at any finite temperature. These results are entirely controlled by the low-lying phonon modes; for example, if we were to use a finite-range pair function, then there would be a condensate at absolute zero in one, two, and three dimensions. This suggests that low-lying collective modes may be decisive in determining whether or not a Bose system is superfluid.

The plan of the paper is as follows: In Sec. II we state our basic hypothesis in mathematical form and construct the ground-state function and low-temperature density matrix. In this section we also discuss the validity of our basic assumption. Section III is devoted to the calculation of the structure factor at absolute zero and at finite temperatures. In Sec. IV we compute n_0, the fraction of particles in the zero-momentum state, and in Sec. V we discuss the behavior of n_k for small wave numbers. In Sec. VI we examine the influence of the phonon modes on the occurrence of Bose-Einstein condensation in one and two dimensions. Finally, in Sec. VII, we mention some of the physical properties we plan to calculate with our wave function and density matrix, and state some mathematical problems that arise from the infinite-range correlations.

II. WAVE FUNCTION AND DENSITY MATRIX

We write the Hamiltonian of the system of N Bose particles in a volume V in the form

$$H=H_{\rm ph}+H'. \tag{2.1}$$

Here $H_{\rm ph}$ is the harmonic contribution from the long-wavelength phonon modes which can be written[14,15]

$$H_{\rm ph}=\tfrac{1}{2}\sum_{\substack{\mathbf{k}\\ k<k_c}} m_k[\dot\rho_{\mathbf{k}}\dot\rho_{\mathbf{k}}^*+\omega_k^2\rho_{\mathbf{k}}\rho_{\mathbf{k}}^*], \tag{2.2}$$

where $m_k=m/Nk^2$, $\omega_k=ck$, and

$$\rho_{\mathbf{k}}=\sum_{j=1}^{N} e^{i\mathbf{k}\cdot\mathbf{r}_j}. \tag{2.3}$$

The cutoff wavelength $\lambda_c=2\pi/k_c$ must be chosen large compared with the interparticle spacing, so that the Fourier component $\rho_{\mathbf{k}}$ of the density field are the appropriate variables. H' can be written

$$H'=H_R+H_{R,\rm ph}+H_{\rm an},$$

where H_R describes the other modes of motion, $H_{R,\rm ph}$ the interaction between these and the phonons, and $H_{\rm an}$ is the anharmonic interaction between the phonons.

Our basic assumption that the long-wavelength phonon modes propagate independently of any other modes of motion and of each other implies that at sufficiently low temperatures we can neglect $H_{R,\rm ph}$ and $H_{\rm an}$ and write

$$H=H_R+H_{\rm ph}. \tag{2.4}$$

At this point it is worthwhile to make some comments on this assumption. At absolute zero, perturbation analysis[5] shows that for small wave numbers k there is no damping of the phonons to order k^2. At low temperatures, calculations by Khalatnikov[4] show that $\omega_k\tau_k\gg1$, where τ_k is the lifetime of a phonon of wave number k. Both these calculations therefore support our assumption. It follows from Eq. (2.4) that the normalized ground-state wave function ψ_0 can be written as

$$\psi_0(\mathbf{r}_1\cdots\mathbf{r}_N)=Q_N{}^{-1/2}\psi_R(\mathbf{r}_1\cdots\mathbf{r}_N)\psi_{\rm ph}(\mathbf{r}_1\cdots\mathbf{r}_N), \tag{2.5}$$

where Q_N is the normalization constant, ψ_R is the ground state of H_R, and $\psi_{\rm ph}$ is the ground state of $H_{\rm ph}$. This is equal to the product of the ground-state wave functions of the harmonic oscillators described by (2.2); we can write therefore

$$\psi_{\rm ph}(\mathbf{r}_1\cdots\mathbf{r}_N)=\exp\left[-\sum_{\mathbf{k}}\frac{m_k\omega_k}{2\hbar}\rho_{\mathbf{k}}\rho_{\mathbf{k}}^*G(k,k_c)\right], \tag{2.6}$$

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[13] O. Penrose, in *Proceedings of the International Conference on Low Temperature Physics*, edited by J. R. Dillinger (University of Wisconsin Press, Madison, Wisconsin, 1958), p. 117.

[14] R. Kronig and A. Thellung, Physica **18**, 749 (1952).

[15] G. V. Chester, in *Liquid Helium*, edited by G. Careri (Academic Press Inc., New York, 1963), p. 51.

where $G(k,k_c)$ is a function which cuts off the sum over k for large values of k at a characteristic wave vector k_c. Using the expression (2.3) for ρ_k, (2.6) can be written, neglecting an unessential constant, as

$$\psi_{\mathrm{ph}}(\mathbf{r}_1\cdots\mathbf{r}_N)=\exp\Big[-\tfrac{1}{2}\sum_{i<j}^{1\cdots N}\chi(|\mathbf{r}_i-\mathbf{r}_j|)\Big], \quad (2.7)$$

where

$$\chi(r)=\frac{1}{N}\sum_{\mathbf{k}}\frac{2mc}{\hbar k}G(k,k_c)e^{i\mathbf{k}\cdot\mathbf{r}}. \quad (2.8)$$

If for example $G(k,k_c)=\exp(-k/k_c)$, then in the infinite-volume limit, N, $V\rightarrow\infty$, $N/V=n$, $\chi(r)$ is given by

$$\chi(r)=\frac{cm}{\pi^2 n\hbar}[r^2+k_c^{-2}]^{-1}. \quad (2.9)$$

We note that the asymptotic behavior of $\chi(r)$ for large r, $\chi(r)\propto r^{-2}$, is independent of the particular form of the function $G(k,k_c)$. Bogoliubov and Zubarev[16] showed that the ground-state wave function of a weakly coupled Bose gas has the same kind of infinite-range correlations.

As we discussed in the introduction, an excited state with a single phonon of wave vector $\mathbf{k}$ can be represented by a function of the Feynman form (1.4). Penrose[13] has shown how to construct an ensemble of such states: A state which contains, for each $\mathbf{k}$, $N_{\mathbf{k}}$ phonons can be written as

$$\psi_{\mathrm{ex}}=\Big\{\prod_{\mathbf{k}}{}' e^{F_{\mathbf{k}}F_{-\mathbf{k}}}\Big(\frac{\partial}{\partial F_{-\mathbf{k}}}\Big)^{N_{\mathbf{k}}}\Big(\frac{\partial}{\partial F_{\mathbf{k}}}\Big)^{N-\mathbf{k}}e^{-F_{\mathbf{k}}F_{-\mathbf{k}}}\Big\}\psi_0, \quad (2.10)$$

where $F_{\mathbf{k}}=(2mc/N\hbar k)^{1/2}\rho_{\mathbf{k}}$, and $\prod'$ means a product where each pair $(\mathbf{k},-\mathbf{k})$ is included once only. If we weight each state with $\exp(-E/k_BT)$, $E=\sum_{\mathbf{k}}N_{\mathbf{k}}\hbar ck$, the N-particle density matrix at temperature T in the coordinate representation, $\langle R'|\sigma|R''\rangle_T$, is then given by

$$\begin{aligned}\langle R'|\sigma|R''\rangle_T=&\,Q_N^{-1/2}(T)\psi_0(R')\psi_0(R'')\\ &\times\exp\Big\{-\frac{1}{2}\sum_{i,j}^{1\cdots N}[h_1(\mathbf{r}_i'-\mathbf{r}_j')\\ &+h_1(\mathbf{r}_i''-\mathbf{r}_j'')+h_2(\mathbf{r}_i'-\mathbf{r}_j'')]\Big\}, \quad (2.11)\end{aligned}$$

where

$$h_1(r)=N^{-1}\sum_{\mathbf{k}}\frac{2mc}{\hbar k}(e^{2\hbar\beta kc}-1)^{-1}G(k,k_c)e^{i\mathbf{k}\cdot\mathbf{r}}, \quad (2.12)$$

$$h_2(r)=-N^{-1}\sum_{k}\frac{2mc}{\hbar k}\operatorname{csch}(\hbar\beta kc)G(k,k_c)e^{i\mathbf{k}\cdot\mathbf{r}}, \quad (2.13)$$

$\beta=1/k_BT$, and R stands for all the coordinates $\mathbf{r}_1\cdots\mathbf{r}_N$. $Q_N(T)$ is the appropriate normalization constant determined by

$$\int dR\langle R|\sigma|R\rangle_T=1. \quad (2.14)$$

In (2.12) and (2.13), the cutoff function $G(k,k_c)$ has been introduced; the temperature must be such that only phonons with wave vectors less than k_c are excited; this implies T must be such that $\hbar ck_c\gg k_BT$. From (2.11) we can see that the phonon part of the diagonal element of the density matrix, $\langle R|\sigma|R\rangle_T$, is a product of pair functions. The diagonal element is given by the equation

$$\begin{aligned}\langle R|\sigma|R\rangle_T=&\,Q_N^{-1/2}(T)\psi_R(R)\psi_R(R)\\ &\times\exp\Big\{-\sum_{i<j}^{1\cdots N}\chi_T(|\mathbf{r}_i-\mathbf{r}_j|)\Big\}, \quad (2.15)\end{aligned}$$

where

$$\chi_T(r)=N^{-1}\sum_{\mathbf{k}}\frac{2mc}{\hbar k}\tanh(\tfrac{1}{2}\hbar\beta kc)G(k,k_c)e^{i\mathbf{k}\cdot\mathbf{r}}. \quad (2.16)$$

This is a finite-range function; it is easy to show that

$$\chi_T(r)=\frac{m}{\pi n\hbar^2\beta}\frac{1}{r}\operatorname{csch}(\pi r/\hbar\beta c)+O(1/\beta\hbar ck_c).$$

At a finite temperature the infinite-range correlations created by the zero-point motion of the phonons are no longer present. However, there are finite but very long-range correlations present; for example at $T=0.1$°K. If we take for c and m the values appropriate for liquid He^4, then χ_T has a range of about 100 Å.

To compute the physical quantities in which we are interested, we have to specify ψ_R. In the calculations that follow, we assume that it is a product of finite-range pair functions. However, the results we obtain hold also if ψ_R contains correlations between more than two particles, provided these correlations are between a finite number of particles and are of finite range.

III. THE STRUCTURE FACTOR

In this section we study in the infinite-volume limit, the radial distribution function $g(r)$, and the structure factor $S(k)$ for our wave function and density matrix. The radial distribution function at temperature T is defined as

$$g(\mathbf{r}-\mathbf{r}')=\frac{1}{n^2}\Big\langle\sum_{i\neq j}^{1\cdots N}\delta(\mathbf{r}_i-\mathbf{r})\delta(\mathbf{r}_j-\mathbf{r}')\Big\rangle_T, \quad (3.1)$$

where the bracket $\langle\cdots\rangle_T$ indicates an average with the weight function $\langle R|\sigma|R\rangle_T$ given by (2.15). The structure factor is defined in terms of $g(r)$ by the usual relation

$$S(\mathbf{k})=1+n\int d\mathbf{r}[g(\mathbf{r})-1]e^{i\mathbf{k}\cdot\mathbf{r}}. \quad (3.2)$$

At zero temperature, the weight function is simply $\psi_0^2(R)$. We reported in Sec. I that if the wave function has the form of a product of pair functions, then $\psi^2(R)$ is formally equal to the configurational probability distribution for a classical fluid at temperature T_{eff}

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[16] N. N. Bogoliubov and D. N. Zubarev, Zh. Eksperim. i Teor. Fiz. **20**, 1064 (1955) [English transl.: Soviet Physics—JETP **1**, 83 (1955)].

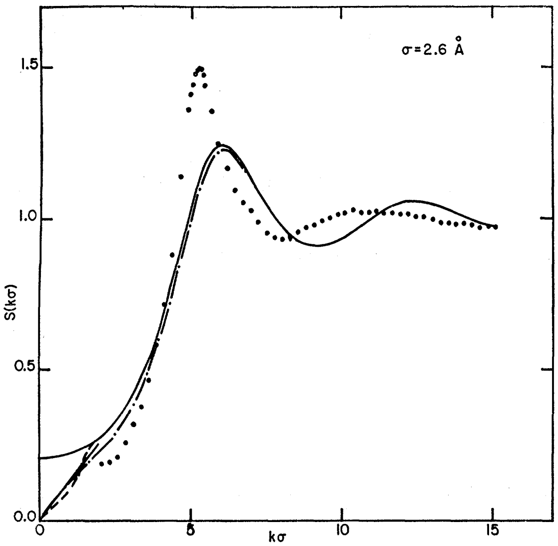

FIG. 1. Structure factor $S(k)$. The full line represents $S_{\mathrm{HS}}(k)$, the solution of the Percus-Yevick equation for hard spheres for $\sigma=2.6$ Å [packing fraction, $\eta=(\pi/6)n\sigma^3$, equal to 0.2004], the dashed and dash-dotted lines represent Eq. (3.6) when $G(k,k_c)=\exp[-(k/k_c)^4]$ and $G(k,k_c)=\exp(-k/k_c)$, respectively, $k_c=0.5$ Å^{-1}, and $S_{\mathrm{SR}}(k)$ is $S_{\mathrm{HS}}(k)$ in this figure. The line through the origin represents (3.8). The points represent the experimental diffraction data [D. G. Henshaw, Phys. Rev. **119**, 9 (1960)] for liquid He^4 at 1.06°K.

interacting with a two-body potential $\varphi(r)$ given by: $-\ln[f(r)]=(2k_BT_{\mathrm{eff}})^{-1}\varphi(r)$. In Sec. II we showed that the zero-point motion of the phonons implies that $\varphi(r)$ has a part of infinite range. Therefore the equivalent classical fluid does not have a thermodynamic limit. The existence of $g(r)$ in the infinite-volume limit has been rigorously proved[17] only for potentials $\varphi(r)$ for which $\int d\mathbf{r}[\exp(-\varphi(r)/k_BT)-1]$ exists. We shall assume that $g(r)$ exists in the infinite-volume limit even though $\varphi(r)$ has an infinite range. It would be interesting to see if this assumption can be rigorously justified. However, if we have infinite-range correlations, then we cannot expect that the asymptotic form of $g(r)$ for large r will be correctly given by the Ornstein-Zernike[11] theory. In other words, $S(0)$ will not be equal to $n\kappa_{T_{\mathrm{eff}}}k_BT_{\mathrm{eff}}$, where $\kappa_{T_{\mathrm{eff}}}$ is the isothermal compressibility of the equivalent classical fluid. Indeed this relation is based on the assumption of the existence of a thermodynamic limit for the system.

In $\ln[f(r)]$ there is a finite-range part $u(r)$ and an infinite-range part, $\chi(r)$. The different character of these functions allows us to separate their effects on the behavior of $S(k)$ and $g(r)$ for small k and large r, respectively. A similar problem has been considered in the case of classical fluid with short- and long (but finite)-range forces.[18–20] The method we use differs from those used before, and it will be particularly useful in the calculation of the momentum distribution n_k (Sec. IV). Let $Q_N[v(r)]$ be the normalization constant when there is an "external potential" $v(r)$:

$$Q_N[v(r)]=\int d\mathbf{r}_1\cdots d\mathbf{r}_N \times\exp\{-\sum_{i<j}^{1\cdots N}(u_{ij}+\chi_{ij})-\sum_{j=1}^{N}v_j\}. \tag{3.3}$$

Here the subscripts i and j indicate the coordinates $\mathbf{r}_i$ and $\mathbf{r}_j$ in the arguments of the functions. The radial distribution function can be expressed in terms of the second functional derivative of the normalization constant (3.3)[21]:

$$g(\mathbf{r}-\mathbf{r}')-1+\frac{1}{n}\delta(\mathbf{r}-\mathbf{r}')=n^{-2}\left\{\frac{\delta^2\ln Q_N[v]}{\delta v(\mathbf{r})\delta v(\mathbf{r}')}\right\}_{v=0}. \tag{3.4}$$

We show in Appendix I that the contribution from the factors containing χ_{ij} in Eq. (3.3) can be expressed in terms of a functional integral.[22,23] The problem of calculating $Q_N[v]$ is then reduced to the calculation of a functional integral with respect to $\phi(\mathbf{r})$ of a functional whose most important term is of the form

$$\langle\exp\{i\sum_{j=1}^{N}[\phi_j+iv_j]\}\rangle_{\mathrm{SR}}. \tag{3.5}$$

Here $\langle\cdots\rangle_{\mathrm{SR}}$ means an average with weight $\psi_R{}^2=\exp[-\sum_{i<j}^{1\cdots N}u_{ij}]$. To evaluate the average in (3.5) we use a cumulant expansion.[24] We show in Appendix I that because of the different range of the functions $\chi(r)$ and $u(r)$, it is good approximation to retain only the two first terms in the cumulant expansion (Gaussian approximation). In this approximation, the structure factor is given by

$$S(k)=S_{\mathrm{SR}}(k)\big/1+n\chi(k)S_{\mathrm{SR}}(k), \tag{3.6}$$

where $S_{\mathrm{SR}}(k)$ is the structure factor corresponding to the short-range function ψ_R and $\chi(k)$ is the Fourier transform of $\chi(r)$:

$$\chi(k)=(2mc/n\hbar k)G(k,k_c). \tag{3.7}$$

From (3.6) and (3.7) we see that, because $S_{\mathrm{SR}}(0)\neq0$,

$$S(k)=\hbar k/2mc \quad\text{as}\quad k\to0, \tag{3.8}$$

which is what we expect on the basis of Feynman's work.[3] If $S(k)$ has the limiting form given by Eq. (3.8),

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[23] A somewhat similar method to that outlined in Appendix A has been used by J. Zittartz, Kölner dissertation, 1964 (unpublished).

[24] R. Kubo, J. Phys. Soc. Japan **17**, 1100 (1962).

then $g(r)-1\sim-\hbar/2\pi^2nmcr^4$ for large r. Enderby *et al.*[25] showed that this asymptotic form for $g(r)$ could arise from a wave function of the form (1.1) provided $\ln[f(r)]$ behaved like r^{-2} for large r. To illustrate the behavior of $S(k)$, Fig. 1 and Fig. 2 show $S(k)$ calculated on the basis of (3.6) when $k_c=0.5$ Å^{-1} and for two different forms of the cutoff function $G(k,k_c)$. For the short-range part $S_{\mathrm{SR}}(k)$, the analytic solution[26] of the Percus-Yevick equation[27] for hard spheres has been used: $S_{\mathrm{HS}}(k)$. This corresponds to a short-range ψ_R with the following $u(r)$: $u(r)=0$ for $r>\sigma$, and $u(r)=\infty$ for $r<\sigma$. We shall call this short-range wave function the "hard-sphere" function. The values $\sigma=2.6$ and 2.9 Å have been assumed. Miller, Pines, and Nozières[28] have suggested that $S(k)$ may have a local maximum at $k\sim0.6$ Å^{-1}. However, the detailed form of $S(k)$ in this region depends on k_c, the shape of the cutoff function $G(k,k_c)$, and the choice of $S_{\mathrm{SR}}(k)$. We therefore cannot at the moment compare our calculations with the form they suggest.

It follows from our basic assumptions that $S(k)$ is equal to $\hbar k/2mc$ for all $k<k_c$, provided $G(k,k_c)=1$ in this range. However, Eq. (3.6) provides an approximate expression for $S(k)$ which is only valid for very small k, and we therefore cannot expect to find from it that $S(k)$ is linear in k for $k\leqslant k_c$. In the intermediate region, between the part dominated by the $\chi(r)$ function and the part dominated by the short-range function $u(r)$, there are probably sizeable corrections to expression (3.6). We hope to present a study of these corrections in a later paper.

At finite temperature, the infinite-range correlations are no longer present. However, the function $\chi_T(r)$ which appears in the density matrix has a much longer range than the typical range of the short-range function $u(r)$ (this range can be estimated from the results of variational calculations).[9,10] We can therefore use the same Gaussian approximation as we used at absolute zero, and we find that $S(k)$ is given by an expression of the same form as Eq. (3.6) but with $\chi(k)$ replaced by $\chi_T(k)$, where

$$\chi_T(k)=\frac{2mc}{n\hbar k}\tanh(\tfrac{1}{2}\hbar\beta kc)G(k,k_c). \tag{3.9}$$

We find that $S(0)$ is equal to $(m\beta c^2)^{-1}$ up to terms of order $[m\beta c^2S_{\mathrm{SR}}(0)]^{-1}$ which are negligible in our temperature range. We note that because we have to satisfy the inequality $\beta\hbar ck_c\gg1$, $S(k)$ will depart from its limiting value for quite small values of k.

IV. BOSE-EINSTEIN CONDENSATION

It is generally recognized that the superfluid properties of He^4 are connected with the existence of a macroscopically populated momentum state in the system—Bose-Einstein condensation. We shall call the fraction of particles in the zero-momentum state n_0 the "condensate." It is therefore of interest to examine the momentum distribution n_k for our system. Penrose and Onsager[12] showed that if in the wave function the correlations decrease fast enough at large separation, an interacting Bose system has Bose-Einstein condensation at zero temperature. However, it is not known how fast these correlations must die away for their analysis to be valid. It is therefore not possible to immediately apply their methods to our ground-state function with infinite-range correlations; for this function we have no rigorous proof that a condensate exists. An argument in favor of the existence of a condensate in the presence of these correlations comes from the weakly interacting Bose system. In this system, these correlations are present, and it is known that a condensate exists.[16] We are only able to give a proof of the existence of a condensate on the basis of a cumulant expansion of the appropriate quantities.

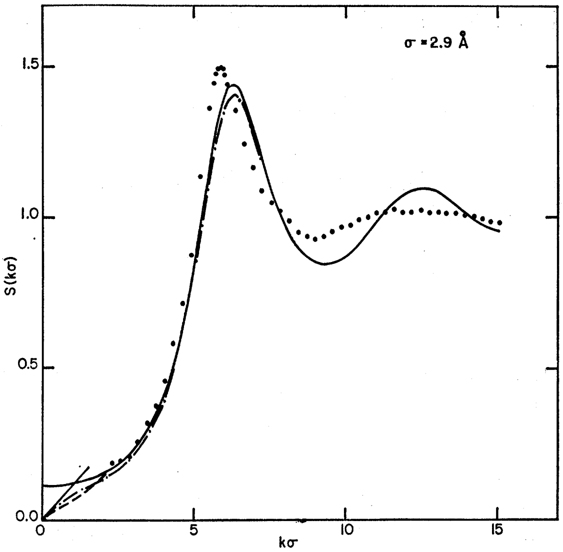

FIG. 2. The same as Fig. 1 for $\sigma=2.9$ Å (packing fraction $\eta=0.278$).

The existence of a condensate is directly related to the presence of off-diagonal long-range order[12] in the one particle density matrix $\langle\mathbf{r}|\sigma_1|\mathbf{r}'\rangle_T$. In fact, if $n_0(T)$ is the density of particle in the zero-momentum state (we are considering a system at rest) we have

$$n_0(T)=\lim_{|\mathbf{r}-\mathbf{r}'|\to\infty}\langle\mathbf{r}|\sigma_1|\mathbf{r}'\rangle_T. \tag{4.1}$$

At zero temperature the density matrix is given by

$$\langle\mathbf{r}|\sigma_1|\mathbf{r}'\rangle_0=N\int d\mathbf{r}_2\cdots d\mathbf{r}_N\psi_0(\mathbf{r},\mathbf{r}_2,\cdots\mathbf{r}_N)\,\psi_0(\mathbf{r}',\mathbf{r}_2,\cdots\mathbf{r}_N). \tag{4.2}$$

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[25] J. E. Enderby, T. Gaskell, and N. H. March, Proc. Phys. Soc. (London) **85**, 217 (1965).

[26] M. S. Wertheim, Phys. Rev. Letters **10**, 321 (1963); E. Thiele, J. Chem. Phys. **39**, 474 (1963).

[27] J. K. Percus and G. J. Yevick, Phys. Rev. **110**, 1 (1958).

[28] A. Miller, D. Pines, and P. Nozières, Phys. Rev. **127**, 1452 (1962).

The condensate n_0 is equal to the infinite volume limit of A_N, where

$$A_N=\frac{1}{V^2}\int d\mathbf{r}d\mathbf{r}'\langle\mathbf{r}|\sigma_1|\mathbf{r}'\rangle_0=\frac{n}{V}\frac{\mathcal{Q}_{N+1}}{Q_N}. \tag{4.3}$$

In (4.3), Q_N is the normalization constant of ψ_0 and $\mathcal{Q}_{N+1}$ is defined as

$$\mathcal{Q}_{N+1}=Q_{N+1}\int d\mathbf{r}d\mathbf{r}'d\mathbf{r}_2\cdots d\mathbf{r}_N\psi_0(\mathbf{r},\mathbf{r}_2\cdots\mathbf{r}_N)\times\psi_0(\mathbf{r}',\mathbf{r}_2\cdots\mathbf{r}_N). \tag{4.4}$$

If the wave function is the "hard-sphere function," then

$$\mathcal{Q}_{N+1}=Q_{N+1}(1+O(1/N)),$$

and from (4.1) and (4.3) we see that $n_0=n^2/z$,[12] where z is the activity of the equivalent classical fluid which is defined as $z=(N+1)Q_N/Q_{N+1}$. In general, if the wave function contains only finite-range functions $u(r)\geqslant 0$, it is easy to see that $\mathcal{Q}_{N+1}\geqslant Q_{N+1}$ and therefore $n_0\geqslant n^2/z$. Unfortunately the infinite-range correlations introduced by the function $\chi(r)$ in ψ_0 render this inequality useless, because the "thermodynamic limit" no longer exists, and the activity of the equivalent classical fluid tends to infinity in the infinite-volume limit.

A_N can be written in the following form

$$A_N=A_N(\mathrm{SR})B_N, \tag{4.5}$$

where $A_N(\mathrm{SR})$ is equal to expression (4.3) when ψ_0 is replaced by ψ_R. A useful way of writing B_N is given in (B5) in the second Appendix. The averages which appear in that expression can be evaluated using the cumulant expansion, and this leads to Eqs. (B5)–(B7) of Appendix B for A_N. We show in Appendix B that A_N is finite in the infinite-volume limit, so we conclude that there is a condensate for our wave function. This is true if the cumulant expansions we used are convergent, an argument for this is presented in the appendix.

If the short-range part of the wave function is a "hard-sphere" function (HS), the expression for n_0 simplifies, and

$$n_0=n_0(\mathrm{HS})\exp(\Delta), \tag{4.6}$$

where

$$\Delta=-\frac{n}{2(2\pi)^3}\int d\mathbf{k}\chi^2(k)S_{\mathrm{HS}}(k)\times[1+n\chi(k)S_{\mathrm{HS}}(k)]^{-1}+\tfrac{1}{2}n\int d\mathbf{r}g(r)\chi^2(r)+\frac{n^2}{2}\int d\mathbf{r}d\mathbf{r}'\chi(r)\chi(r')g(r)g(r')\times[g(|\mathbf{r}+\mathbf{r}'|)-1]. \tag{4.7}$$

Here $n_0(\mathrm{HS})$ is the condensate for the wave function ψ_R, $g(r)$ is the radial distribution function for ψ_0, and $S_{\mathrm{HS}}(k)$ is the structure factor for ψ_R. We have calculated Δ using for $g(r)$ the expression given by Eqs. (3.6) and (3.2). The short-range structure function $S_{\mathrm{HS}}(k)$ was again approximated by the Percus-Yevick solution of the hard-sphere problem[26]; for the physical parameters, the values appropriate for He^4 were used. We find that with $G(k,k_c)=\exp(-k/k_c)$, $\Delta=-0.11$ when $k_c=0.5$ Å^{-1}; with $G(k,k_c)=\exp[-(k/k_c)^4]$, $\Delta=0.04$ with $k_c=0.5$ Å^{-1}. In both cases the hard-sphere diameter was chosen to be 2.6 Å. When $k_c=0.25$ Å^{-1}, $|\Delta|$ becomes of the order of 10^{-3}, irrespective of the form of the cutoff function. We notice that Δ is always small and its value depends on the way the cutoff is introduced. This dependence has no physical meaning because if we change the phonon factor in ψ_0, the short-range factor ψ_R will presumbaly change as well. The corrections to expression (4.7) which come from higher-order cumulants have been estimated and give negligible contributions. From these calculations it appears that the phonon factor in the wave function does not greatly affect the value of the condensate.

At finite temperatures with the density matrix (2.11), it is easy to show that

$$n_0(T)=\lim_{N,V\to\infty}\frac{n}{V}\frac{\mathcal{Q}_{N+1}(T)}{Q_N(T)}e^{h_2(0)/2}=\lim_{N,V\to\infty}A_N(T)e^{h_2(0)/2}, \tag{4.8}$$

where $A_N(T)$ is defined in (4.8), and $Q_N(T)$ and $\mathcal{Q}_{N+1}(T)$ are the same quantities as we defined at zero temperature except that $\chi(r)$ is replaced by $\chi_T(r)$; $h_2(0)$ is the value of function (2.13) at zero distance. Neglecting terms of order, $(\beta\hbar c k_c)^{-1}$, $h_2(0)$ is independent of the form of $G(k,k_c)$; $h_2(0)=-m/4n\hbar^3\beta^2c$. At finite temperature only finite-range functions appear in (4.8); if $u(r)>0$ and if we chose $G(k,k_c)$ so that $\chi_T(r)\geqslant 0$, then the inequality $n_0\geqslant n^2/z$ applies and we are rigorously able to conclude that the system has a condensate. If $\chi_T(r)$ is not always positive we have to resort to the same cumulant expansion as before, and from this we again conclude that there is a condensate at any temperature for which our density matrix is valid. If the short-range part ψ_R is a "hard-sphere" function, (4.6) holds when Δ is replaced by $\tilde{\Delta}(T)=\Delta(T)+\frac{1}{2}h_2(0)$ and $\Delta(T)$ is given by (4.7), where the functions are the appropriate ones for temperature T. We have calculated $\tilde{\Delta}(T)$ in a similar way and we find that $n_0(T)$ decreases very slowly with increasing temperature and at $T=1$°K, $n_0(T)$ differs from n_0 by only a few percent.

V. MOMENTUM DISTRIBUTION

The momentum distribution n_k is the Fourier transform of the one-particle density matrix

$$n_k=\int d\mathbf{r}e^{i\mathbf{k}\cdot\mathbf{r}}\{\langle\mathbf{r}|\sigma_1|0\rangle_T-n_0(T)\}. \tag{5.1}$$

Here we have taken into account that $\langle\mathbf{r}|\sigma_1|\mathbf{r}'\rangle$ is a function only of the difference $|\mathbf{r}-\mathbf{r}'|$ (the system is translationally invariant). In our definition of n_k we have subtracted the singular part at $k=0$, due to the condensate. At zero temperature the one-particle density matrix can be written in the form (to terms of order $1/N$)

$$\begin{aligned}\langle\mathbf{r}_1|\sigma_1|\mathbf{r}_2\rangle_0 &= A_N\tilde{g}^{(2)}(\mathbf{r}_1-\mathbf{r}_2)\\ &\quad\times\exp\{\tfrac{1}{4}[\chi(\mathbf{r}_1-\mathbf{r}_2)+u(\mathbf{r}_1-\mathbf{r}_2)]\}\xrightarrow[N,V\to\infty]{} n_0\tilde{g}^{(2)}(\mathbf{r}_1-\mathbf{r}_2)\\ &\quad\times\exp\{\tfrac{1}{4}[\chi(\mathbf{r}_1-\mathbf{r}_2)+u(\mathbf{r}_1-\mathbf{r}_2)]\},\end{aligned}\tag{5.2}$$

where A_N is defined in (4.3) and $\tilde{g}^{(2)}(\mathbf{r}_1-\mathbf{r}_2)$ is given by

$$\tilde{g}^{(2)}(\mathbf{r}_1-\mathbf{r}_2)=\frac{N(N+1)}{n^2}\frac{1}{\tilde{Q}_{N+1}}\int d\mathbf{r}_3\cdots d\mathbf{r}_{N+1}\times\exp\{-\tfrac{1}{2}\sum_{i,j}^{1\cdots N+1}l_{ij}\}.\tag{5.3}$$

Here

$$l_{ij}=\prod_{s=1}^{2}(1-\tfrac{1}{2}\delta_{s,i})(1-\tfrac{1}{2}\delta_{s,j})(\chi_{ij}+u_{ij})\tag{5.4}$$

and

$$\tilde{Q}_{N+1}=\int d\mathbf{r}_1\cdots d\mathbf{r}_{N+1}\exp\{-\tfrac{1}{2}\sum_{i,j}^{1\cdots N+1}l_{ij}\}.\tag{5.5}$$

We now introduce two new correlation functions, $\tilde{g}^{(1)}(r)$ and $\tilde{g}^{(0)}(r)$; they are given by equations similar to (5.3) except that in (5.4) any number between 3 and $N+1$ replaces 1 *or* 2 for $\tilde{g}^{(1)}(r)$ or 1 *and* 2 for $\tilde{g}^{(0)}(r)$ as indices of the Kronecker symbol. Up to terms of order $1/N$ $\tilde{g}^{(0)}(r)$ is equal to $g(r)$ defined in Sec. II. Apart from a constant factor, these three functions are formally equal to the three distinct classical radial distribution functions which can be defined for a mixture of two particles in a bath of $N-1$ particles and with the effective interaction potential given by (5.4).

The method we used in Sec. III to calculate $g(r)$ can be used for $\tilde{g}^{(2)}(r)$. If $\tilde{Q}_{N+1}[v_1,v_2]$ is the normalization constant when an "external potential" $v(r)$ is introduced acting only on the particles 1 and 2, the following relation holds:

$$\frac{1}{N(N+1)}\tilde{g}^{(2)}(\mathbf{r}_1-\mathbf{r}_2)-\frac{2}{(N+1)^2}+\frac{1}{N+1}\frac{1}{n}\delta(\mathbf{r}_1-\mathbf{r}_2)=\frac{1}{n^2}\left\{\frac{\delta^2\ln\tilde{Q}_{N+1}[v_1v_2]}{\delta v_1(r_1)\delta v_2(r_2)}\right\}_{v_1=0,v_2=0}.\tag{5.6}$$

Again the contribution from the χ functions to $\tilde{Q}_{N+1}[v_1v_2]$ can be expressed in terms of a functional integral, and we are left with the same problem we had in the calculation of $g(r)$ except that the average (3.5) is replaced by

$$\langle\langle\exp\{i\sum_{i=3}^{N+1}\phi_j+i\sum_{j=1}^{2}(\phi_j+iv_j)\}\rangle\rangle_{\mathrm{SR}},\tag{5.7}$$

where now $\langle\langle\cdots\rangle\rangle_{\mathrm{SR}}$ means an average with only the short-range part of (5.4). If the cumulant expansion is used to evaluate the average (5.7) and the first two terms are retained, we obtain

$$\tilde{S}^{(2)}(k)=\tilde{S}_{\mathrm{SR}}{}^{(2)}(k)-n\chi(k)\frac{[\tilde{S}_{\mathrm{SR}}{}^{(1)}(k)-\frac{1}{2}]^2}{1+n\chi(k)S_{\mathrm{SR}}(k)},\tag{5.8}$$

where $\tilde{S}^{(2)}(k)$ and $\tilde{S}^{(1)}(k)$ are related to $\tilde{g}^{(2)}(r)$ and $\tilde{g}^{(1)}(r)$ by equations identical in form to (3.2). The subscript SR on a function means that it is calculated using only the short-range function ψ_R.

Equations (5.1), (5.2), and (5.8) allow us to take into account the effect of the phonons on n_k. We now examine the behavior of n_k for small k. From the linear dependence on k of $\tilde{S}^{(2)}(k)$ for small k we can say that $\tilde{g}^{(2)}(r)-1=O(r^{-4})$ for large r. Therefore the only contribution to n_k which is not regular at $k=0$ comes from the factor $n_0\exp[\chi(r)/4]$ in (5.2). Using this result we find that n_k for small k is given by

$$n_k=n_0mc/2nhk.\tag{5.9}$$

This singular behavior comes from the infinite-range correlations in the wave function, for if the wave function contains only finite-range functions, the momentum distribution is regular at $k=0$.[9] Using perturbation analysis, Gavoret and Nozières[5] showed that n_k has the form given by (5.9).

At finite temperature the one-particle density matrix can be written in the form

$$\begin{aligned}\langle\mathbf{r}_1|\sigma_1|\mathbf{r}_2\rangle_T &= A_N(T)\exp\{\tfrac{1}{2}[h_2(0)-h_2(\mathbf{r}_1-\mathbf{r}_2)]\}\\ &\quad\times\exp\{\tfrac{1}{4}[\chi_T(\mathbf{r}_1-\mathbf{r}_2)+u(\mathbf{r}_1-\mathbf{r}_2)]\\ &\quad\times\tilde{g}^{(2)}(\mathbf{r}_1-\mathbf{r}_2,T)\xrightarrow[N,V\to\infty]{} n_0(T)\\ &\quad\times\exp\{-\tfrac{1}{2}h_2(\mathbf{r}_1-\mathbf{r}_2)+\tfrac{1}{4}[\chi_T(\mathbf{r}_1-\mathbf{r}_2)+u(\mathbf{r}_1-\mathbf{r}_2)]\}\\ &\quad\times\tilde{g}^{(2)}(\mathbf{r}_1-\mathbf{r}_2;T),\end{aligned}\tag{5.10}$$

where $A_N(T)$ is defined in (4.8) and $\tilde{g}^{(2)}(r,T)$ is given by (5.3) with $\chi_T(r)$ in place of $\chi(r)$ in $l(r)$. Now the only singular contribution to n_k for $k=0$ comes from the term $\exp[-\frac{1}{2}h_2(r)]$ in (5.10). In fact $h_2(r)$ behaves like r^{-1} for large r; this arises from the k^{-2} singularity which appears in the definition (2.13) of $h_2(r)$. All the other functions which enter expression (5.10) are finite-range functions so that they give regular contributions to n_k. We find that for small k, n_k is given by

$$n_k=n_0(T)m/n\beta h^2k^2.\tag{5.11}$$

It has been shown previously that this kind of singularity in the momentum distribution is present in a dilute hard-sphere Bose gas.[29]

The way in which we have written the one-particle density matrix leads to a relation which may be useful

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[29] T. D. Lee and C. N. Yang, Phys. Rev. **117**, 897 (1960).

in calculating the condensate n_0. From its definition $\langle \mathbf{r}|\sigma_1|\mathbf{r}\rangle_0 = n$, therefore from (5.2) we deduce that

$$\lim_{r\to 0} \tilde{g}^{(2)}(r)\exp\{\tfrac{1}{4}[\chi(r)+u(r)]\} = \frac{n}{n_0}. \qquad (5.12)$$

The function $\tilde{g}^{(2)}(r)$ can be evaluated using one of the well-known approximate integral equations for the radial distribution function for a mixture of fluids. See for example Ref. 30. If one of these equations gives a good approximation to the true $\tilde{g}^{(2)}(r)$ at small distances, relation (5.12) can be used to evaluate the condensate. We note that if the wave function is a "hard-sphere" function, then (5.12) gives the known[31] relation between the activity and the potential of the mean force at zero distance. [Recall the relation between the activity and n_0 and note that $\tilde{g}_{\mathrm{HS}}^{(2)}(r) = g_{\mathrm{HS}}(r)$.] In general for a short-range force the value of the potential of the mean force at zero separation has not been related to any physical quantity.

VI. ONE- AND TWO-DIMENSIONAL SYSTEMS

In this section we shall study the occurrence of Bose-Einstein condensation in one- and two-dimensional systems. If the ground-state wave function for a one-dimensional (1D) or two-dimensional (2D) Bose system is a product of finite-range pair functions, the properties of these systems would be qualitatively the same as those of a three-dimensional (3D) system; in particular both the 1D and 2D systems would have a condensate. However, we know that a 1D system of impenetrable point bosons[32] does not have a condensate.[33] We shall show that if we take into account the presence of the long-wavelength phonons we obtain qualitatively different results for 1D and 2D systems. Our basic assumption is again that these systems can support such modes and that they propagate independently of any other modes of motion. This assumption is supported by the fact that if a condensate exists, then it is possible by perturbation analysis to show that the lowest modes are long-wavelength phonons. On the other hand, the point Bose model in 1D has phonon modes[34] even though it has no condensate.

We start by considering zero temperature. The phonon factor in the wave function in 1D and 2D is of the same form (2.7) and (2.8), except that the k vectors are in one or two dimensions, respectively. In 2D the infinite-volume limit of $\chi(r)$ can be taken and at large r, $\chi(r) \propto r^{-1}$. What we said in Sec. IV about n_0 in 3D can be repeated here, and we conclude that a condensate exists in 2D systems at zero temperature. We merely note that in one of the cumulant expansions the two terms which constitute the second cumulant [they correspond to the two last integrals in expression (4.7)] are divergent; however, their sum is finite. $S(k)$ and n_k for small k continue to behave like (3.8) and (5.9), respectively.

In 1D we cannot take the infinite-length limit of $\chi(r)$ owing to the k^{-1} singularity in expression (2.8) for $\chi(r)$. However, it is possible to perform the summation over the discrete k values in (2.8), and the result is that

$$\chi(r) = -\alpha \ln\left[\sin\left|\frac{\pi r}{L}\right|\right] + \hat{\chi}(r), \qquad (6.1)$$

where $\alpha = 2mc/\pi\hbar n$, L is the length of the system, and $\hat{\chi}(r)$ is a function of finite range whose detailed form depends on the cutoff function $G(k,k_c)$. In what follows, the functions $\hat{\chi}(r_{ij})$ will be included in ψ_R. The ground-state wave function is therefore

$$\psi_0(r_1\cdots r_N) = Q_N^{-1/2}\psi_R(r_1\cdots r_N) \times \prod_{i<j}^{1\cdots N}\left[\sin\frac{\pi|r_i - r_j|}{L}\right]^{\alpha/2}. \qquad (6.2)$$

We see that in 1D the zero-point motion of the long-wavelength phonons gives rise to correlations in the wave function that extend over the entire length of the system.

If $\alpha = 2$, the phonon factor of the wave function is equal to the exact ground state for a system of point impenetrable bosons[32]; as we have already noted this system has no condensate.[33] We believe that the presence of the factor ψ_R does not affect this conclusion. It is interesting to note that in this system the low-lying modes propagate with a velocity[34] $c = \pi\hbar n/m$ so that $\alpha = 2$. Unfortunately the method used by Lenard[33] cannot be extended to other values of α; his method is based on a matrix representation of the product in (6.2). We have not been able to demonstrate for other positive values of α that there is no condensate; however, there are some arguments which support this conclusion. First, the phonon factor in (6.2) is a function extensively studied by Dyson[35]; functions of this kind arise in the statistical theory of nuclear levels. This function is also equal to the configurational probability distribution for a gas on a circle whose particles interact according to the two-dimensional Coulomb law of repulsion. The temperature T of the system is such that $1/k_BT = \alpha/2$. If we neglect ψ_R, the normalization constant in (6.2) is known from Dyson's work to be a continuous function of α. The quantity $\mathcal{Q}_{N+1}$ is very similar to the normalization constant and this suggests that $\mathcal{Q}_{N+1}$ may also be a continuous function of α. Now we know that the limit of (4.3) when $N\to\infty$ is zero if $\alpha = 2$, so we expect that the same is true for

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[30] J. L. Lebowitz, Phys. Rev. **133**, A895 (1964).

[31] W. G. Hoover and J. C. Poirier, J. Chem. Phys. **37**, 1041 (1962).

[32] M. Girardeau, J. Math. Phys. **1**, 516 (1960).

[33] A. Lenard, J. Math. Phys. **5**, 930 (1964).

[34] E. H. Lieb and W. Lininger, Phys. Rev. **130**, 1605 (1963).

[35] F. J. Dyson, J. Math. Phys. **3**, 140 (1962); **3**, 166 (1962); M. L. Mehta and F. J. Dyson, *ibid.* **4**, 713 (1963).

every α. Secondly, the very strong correlations in the wave function (6.2) reflect themselves in the radial distribution function $g(r)$ which also is known for some values of α.[35] Indeed such systems possess what Dyson called "quasicrystalline order." From the work of Penrose and Onsager,[12] it appears that this is the physical reason for the absence of condensation when $\alpha=2$, and this again suggests that the condensation is absent for every finite positive α. Finally, if n_0 were finite, it is possible to show that n_k has a $1/k$ singularity as $k\rightarrow 0$, and therefore n_k would not be integrable in the infinite length limit, whereas we known that the integral of n_k over κ must be equal to the number of particles. From this we again conclude that there is no condensate.

At finite temperature in the diagonal part of the density matrix, $\chi_T(r)$ appears instead of $\chi(r)$, and $\chi_T(r)$ is a finite-range function both in 1D and 2D. Therefore in the decomposition (5.10) of $\langle r_1|\sigma_1|r_2\rangle_T$, the factor

$$\exp\{\tfrac{1}{4}[\chi_T(r_1-r_2)+u(r_1-r_2)]\}\tilde{g}^{(2)}(r_1-r_2;T)$$

behaves in the same way as in three dimensions; when $|r_1-r_2|\rightarrow\infty$ it goes to 1. The function $h_2(r)$ has a k^{-2} singularity as can be seen from (2.13), so we cannot take the infinite-volume limit of this function in either 1D and 2D. However, in (5.10) the combination $h_2(0)-h_2(r_1-r_2)$ appears and this has a finite limit when $N\rightarrow\infty$. Indeed, at large distances

$$\begin{aligned} &h_2(0)-h_2(r)\\ &\quad=-N^{-1}\sum_k \frac{2mc}{\hbar k}\operatorname{csch}(\hbar\beta kc)G(k,k_c)[1-\cos\mathbf{k}\cdot\mathbf{r}]\\ &\qquad\sim-\frac{m}{\pi n\hbar^2\beta}\ln[r/\hbar\beta c]\quad\text{in 2D}\\ &\qquad\sim-\frac{m}{n\hbar^2\beta}r\quad\text{in 1D}, \end{aligned}\tag{6.3}$$

and taking into account (4.1) and (5.10) we conclude that there is no off-diagonal long-range order and $n_0=0$.[36] It is easy to see that the singularity in n_k is also changed—in 1D there is no singularity at all and in 2D n_k behaves like $k^{-2+m/2\pi n\hbar^2\beta}$ for small k.

Note added in proof. We have calculated η_0 in $2D$ for a finite system and find that $\eta_0(T)\propto\eta_0(0)N^{-\epsilon}$ where $\epsilon=m/4\pi\eta\hbar^2\beta$. At $T=0.1$°K and for the mass and density of He^4, $\epsilon=0.009$. This implies that even though there is no condensate, there is a very large number of particles in the zero momentum state in any finite system of realizable size.

The asymptotic form for large r of the single-particle density matrix, Eq. (6.3), is similar to that found by Rice[37] for the two-particle density matrix for neutral superconductors. Rice obtained his results by using the Landau-Ginzburg[38] functional for the local free energy. It has been suggested by Ginzburg and Pitaevski[39] that the same functional form should be applicable to superfluid helium. If this suggestion is correct, then we can immediately apply Rice's method to obtain the results we have outlined in the section. Alternatively we could make the assumption that a neutral superconductor has independent phonon modes in the electronic degrees of freedom (the neutral Anderson modes[40]) and then apply our techniques to a model wave function and density matrix constructed in a similar way to that given in Sec. II. In this manner we recover Rice's results.

VII. CONCLUSIONS

We have shown in the preceding sections that the wave function and density matrix we have proposed lead to results for $S(k)$ and n_k for small k which are in agreement with our expectations. The results we find for one- and two-dimensional Bose systems are closely paralled by these found by Rice[36] for one- and two-dimensional neutral superconductors. This also lends support to our basic ideas. A major task that remains is to test our wave function and density matrix by computing the numerical values of various physical quantities. A variational calculation of the ground-state energy using k_c and the short-range pair function as variational quantities is, at present, under way. We also plan to carry out numerical calculations of $S(k)$, n_k, and n_0 both at absolute zero and at finite temperatures. The calculation of all these quantities can be reduced to problems in some equivalent classical fluid and we then have available to us all the techniques that have been recently developed in that field.[41] These techniques are now sufficiently far advanced that we are confident that they are adequate at liquid-helium densities.

A number of interesting mathematical problems arise in connection with the infinite-range correlations in our ground-state wave function. Because of the presence of these correlations, we do not know rigorously whether the expectation values in which we are interested are well defined in the infinite-volume limit. The first mathematical task that comes to mind is to try to construct a proof (or disproof) of the existence of these expectation values. Another mathematical problem is the proof (or disproof) of the existence of a Bose-

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[36] Dr. J. W. Kane has informed us that he has obtained very similar results by a different method [Ph.D. thesis, University of Illinois (unpublished)].

[37] T. M. Rice, Phys. Rev. **140**, A1889 (1965).

[38] V. L. Ginzburg and L. D. Landau, Zh. Eksperim. i Teor. Fiz. **20**, 1064 (1950).

[39] V. L. Ginzburg and L. P. Pitaevskii, Zh. Eksperim. i Teor. Fiz. **34**, 1240 (1958) [English transl.: Soviet Phys.—JETP **7**, 858 (1958)].

[40] N. N. Bogoliubov, V. V. Tolmachev, and D. V. Shirkov, *A New Method in the Theory of Superconductivity* (Consultants Bureau Enterprises, Inc., New York, 1959); P. W. Anderson, Phys. Rev. **112**, 1900 (1958).

[41] J. S. Rowlinson, Rept. Progr. Phys. **28**, 169 (1965).

Einstein condensation in three dimensions for the wave function ψ_0. In one and two dimensions similar problems arise; in particular it would be interesting to know whether or not the function given by Eq. (6.2) has a condensate for all finite positive α.

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APPENDIX A

We use the following identity to express the square of the phonon part of the wave function:

$$\exp\{-\sum_{i<j}^{1\ldots N}\chi_{ij}\}=\frac{1}{L}\int\delta\phi\,\exp\left\{-\int d\mathbf{r}\,\phi(\mathbf{r})b(\mathbf{r})-\frac{1}{8\pi}\int d\mathbf{r}d\mathbf{s}\,\phi(\mathbf{r})Q(\mathbf{r}-\mathbf{s})\phi(\mathbf{s})\right\},\quad\text{(A1)}$$

where $\int\delta\phi\cdots$ indicates a functional integral,[22]

$$b(\mathbf{r})=-i\sum_{j=1}^{N}\delta(\mathbf{r}-\mathbf{r}_j),\quad\text{(A2)}$$

$$L=e^{-N\chi(0)}\int\delta\phi\times\exp\left\{-\frac{1}{8\pi}\int d\mathbf{r}d\mathbf{s}\,\phi(\mathbf{r})Q(\mathbf{r}-\mathbf{s})\phi(\mathbf{s})\right\},\quad\text{(A3)}$$

and $Q(r)$ is the inverse operator of $\chi(r)$, defined by

$$\int d\mathbf{s}'Q(\mathbf{r}-\mathbf{s}')\chi(\mathbf{s}'-\mathbf{s})=4\pi\delta(\mathbf{r}-\mathbf{s}).\quad\text{(A4)}$$

Using (A1) the normalization constant (3.3) can be written in the following form:

$$Q_N[v(r)]=\frac{Q_N(\mathrm{SR})}{L}\int\delta\phi\,\exp\left\{-\frac{1}{8\pi}\int d\mathbf{r}d\mathbf{s}\,\phi(\mathbf{r})Q(\mathbf{r}-\mathbf{s})\phi(\mathbf{s})\right\}\times\langle\exp\{i\sum_{j=1}^{N}[\phi(\mathbf{r}_j)+iv(\mathbf{r}_j)]\}\rangle_{\mathrm{SR}},\quad\text{(A5)}$$

where $\langle\cdots\rangle_{\mathrm{SR}}$ indicates an average with the short-range function only:

$$\langle\cdots\rangle_{\mathrm{SR}}=Q_N^{-1}(\mathrm{SR})\int d\mathbf{r}_1\cdots d\mathbf{r}_N\times\exp\{-\sum_{i<j}^{1\ldots N}u_{ij}\}\cdots,\quad\text{(A6)}$$

and $Q_N(\mathrm{SR})$ is the normalization constant relative to the short-range function $u(r)$.

The last term in the right-hand side of (A5) can be expressed in terms of a cumulant expansion[24]:

$$\langle\exp\{i\sum_{j=1}^{N}[\phi(\mathbf{r}_j)+iv(\mathbf{r}_j)]\}\rangle_{\mathrm{SR}}=\exp\left\{\sum_{l=1}^{\infty}\frac{1}{l!}M_l[\phi,v]\right\},\quad\text{(A7)}$$

where the first two cumulants have the form

$$M_1[\phi,v]=\langle i\sum_{j=1}^{N}[\phi(\mathbf{r}_j)+iv(\mathbf{r}_j)]\rangle_{\mathrm{SR}}=in\int d\mathbf{r}[\phi(\mathbf{r})+iv(\mathbf{r})],\quad\text{(A8)}$$

$$M_2[\phi,v]=\langle\{i\sum_{j=1}^{N}[\phi(\mathbf{r}_j)+iv(\mathbf{r}_j)]\}^2\rangle_{\mathrm{SR}}-M_1^2[\phi,v]=-n^2\int d\mathbf{r}d\mathbf{s}[\phi(\mathbf{r})+iv(\mathbf{r})]\times S_{\mathrm{SR}}(\mathbf{r}-\mathbf{s})[\phi(\mathbf{s})+iv(\mathbf{s})],\quad\text{(A9)}$$

where

$$S_{\mathrm{SR}}(\mathbf{r})=g_{\mathrm{SR}}(r)-1+(1/n)\delta(\mathbf{r}).\quad\text{(A10)}$$

$Q(\mathbf{r})$ has very large Fourier components for large k as results from its definition (A4); therefore functions $\phi(r)$ which have small k Fourier components only give contributions to the functional integral (A1). Then in (A7) we have an average of slowly varying functions with short-range functions, so that the Gaussian approximation, which corresponds to retain the first two cumulants only, is appropriate.[42] With this approximation the functional integral in (A5) can be performed[22] and the result is

$$\ln Q_N[v]=\frac{n}{2}\int d\mathbf{r}d\mathbf{s}\,v(\mathbf{r})\times\left[S_{\mathrm{SR}}(\mathbf{r}-\mathbf{s})-\frac{n}{2}\int d\mathbf{r}_1d\mathbf{r}_2\,S_{\mathrm{SR}}(\mathbf{r}-\mathbf{r}_1)\times P(\mathbf{r}_1-\mathbf{r}_2)S_{\mathrm{SR}}(\mathbf{r}_2-\mathbf{s})\right]v(\mathbf{s})+D[v],\quad\text{(A11)}$$

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[42] R. Kubo, in *Fluctuation, Relaxation and Resonance in Magnetic Systems*, edited by D. ter Haar (Oliver and Boyd, London, 1962), p. 23.

where $P(\mathbf{r})$ is an operator whose inverse is

$$P^{-1}(\mathbf{r})=\frac{1}{8\pi}Q(\mathbf{r})+\frac{n}{2}S_{\mathrm{SR}}(\mathbf{r}), \tag{A12}$$

and $D[v]$ only contains terms independent of v or linear in v; they give no contribution to $g(r)$ as one can see from (3.4). The second functional derivative of (A11) can be easily performed, and, taking into account (3.2), (3.4), (A4), (A10), and (A12), expression (3.6) for the structure function results.

In the calculation of the condensate n_0, the radial distribution function $g(r;\xi)$ for a partially coupled system enters. By this we mean the system which has one of the particles coupled to the others by $\xi(\chi(r)+u(r))$ rather than $\chi(r)+u(r)$. The radial distribution function $g(r;\xi)$ can be expressed in terms of a second functional derivative, similar to (3.4), of the normalization constant when there is introduced an "external potential" $w(r)$ acting on 1 particle only and an "external potential" $v(r)$ acting on the $N-1$ remaining particles. In this case the phonon part can again be expressed in a form similar to (A1) provided that $b(r)$ is replaced by

$$b(\mathbf{r},\xi)=-i\sum_{j=2}^{N}\delta(\mathbf{r}-\mathbf{r}_j)-i\xi\delta(\mathbf{r}-\mathbf{r}_1). \tag{A13}$$

The function $g(r;\xi)$ can be calculated using the same method as we used to calculate $g(r)$. The corresponding structure factor $S(k;\xi)$ is given by

$$S(k;\xi)=\frac{1+n\chi(k)(1-\xi)}{1+n\chi(k)S_{\mathrm{SR}}(k;\xi)}S_{\mathrm{SR}}(k;\xi), \tag{A14}$$

where $S_{\mathrm{SR}}(k;\xi)$ is the short-range structure function for the partially coupled system.

APPENDIX B

The quantity A_N defined in Eq. (4.3) can be written in the following form:

$$A_N=\left\{\frac{n}{V}\frac{Q_{N+1}}{Q_N}\right\}\langle\exp\{\tfrac{1}{2}\sum_{j=3}^{N+1}(u_{1j}+u_{2j})+\tfrac{3}{4}u_{12}\}\rangle_{\mathrm{SR}}$$
$$\times\langle\langle\exp\{\tfrac{1}{2}\sum_{j=3}^{N+1}(\chi_{1j}+\chi_{2j})+\tfrac{3}{4}\chi_{12}\}\rangle\rangle\langle\langle\exp\{-\sum_{i<j}^{1\cdots N+1}\chi_{ij}\}\rangle\rangle_{\mathrm{SR}}[\langle\exp\{-\sum_{i<j}^{1\cdots N+1}\chi_{ij}\}\rangle_{\mathrm{SR}}]^{-1}, \tag{B1}$$

where $\langle\cdots\rangle_{\mathrm{SR}}$ is defined in Sec. III, $\langle\langle\cdots\rangle\rangle_{\mathrm{SR}}$ is defined in Sec. V, and $\langle\langle\cdots\rangle\rangle$ indicates an average with weight

$$\exp\{-\tfrac{1}{2}\sum_{i,j}^{1\cdots N+1}(\chi_{ij}+m_{ij})\},\quad\text{where}\quad m_{ij}=\prod_{s=1}^{2}(1-\tfrac{1}{2}\delta_{s,i})(1-\tfrac{1}{2}\delta_{s,j})u_{ij}. \tag{B2}$$

Taking into account the formal identity between the first term in the right-hand side of (B1) and n^2/z, where z is the activity of the "equivalent fluid," this term can be written[43]

$$\frac{n}{V}\frac{Q_{N+1}}{Q_N}=n\exp\left\{-n\int_0^1 d\xi\int d\mathbf{r}\,[u(r)+\chi(r)]g(r;\xi)\right\}=\left\{\frac{n}{V}\frac{Q_{N+1}(\mathrm{SR})}{Q_N(\mathrm{SR})}\right\}R_N, \tag{B3}$$

where $g(r;\xi)$ is the radial distribution function for the partially coupled system defined in Appendix A and R_N is given by

$$R_N=\exp\left\{-n\int_0^1 d\xi\int d\mathbf{r}[\chi(r)g(r;\xi)+u(r)(g(r;\xi)-g_{\mathrm{SR}}(r;\xi))]\right\}. \tag{B4}$$

The first factor in the last expression in (B3) multiplied by the second term in (B1) is equal to $A_N(\mathrm{SR})$; therefore A_N can be written in the form (4.5), where B_N is given by

$$B_N=R_N\langle\langle\exp\{\tfrac{1}{2}\sum_{j=3}^{N+1}(\chi_{1j}+\chi_{2j})+\tfrac{3}{4}\chi_{12}\}\rangle\rangle\langle\langle\exp\{-\sum_{i<j}^{1\cdots N+1}\chi_{ij}\}\rangle\rangle_{\mathrm{SR}}[\langle\exp\{-\sum_{i<j}^{1\cdots N+1}\chi_{ij}\}\rangle_{\mathrm{SR}}]^{-1}. \tag{B5}$$

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[43] T. L. Hill, *Statistical Mechanics* (McGraw-Hill Book Company, Inc., New York, 1956), p. 192.

The averages which appear in (B5) can be evaluated using a cumulant expansion[24]; we have, therefore (neglecting the term $\frac{3}{4}\chi_{12}$ in the first average of B5 which gives a contribution of order $1/N$),

$$\langle\langle\exp\{\tfrac{1}{2}\sum_{j=3}^{N+1}(\chi_{1j}+\chi_{2j})\}\rangle\rangle=\exp\left\{\sum_{m=1}^{\infty}\frac{1}{m!}\langle\langle[\tfrac{1}{2}\sum_{j=3}^{N+1}(\chi_{1j}+\chi_{2j})]^m\rangle\rangle^{(c)}\right\}$$

$$=\exp\left\{n\int d\mathbf{r}\,\chi(r)\hat{g}^{(1)}(r)+\frac{n}{2}\int d\mathbf{r}\,\chi^2(r)\hat{g}^{(1)}(r)+\frac{n^2}{2}\int d\mathbf{r}d\mathbf{s}\,\chi(r)\hat{g}^{(1)}(r)\chi(\mathbf{s})\hat{g}^{(1)}(\mathbf{s})[g(\mathbf{r}+\mathbf{s})-1]+\cdots\right\}\quad\text{(B6)}$$

and

$$\langle\langle\exp\{-\sum_{i<j}^{1\cdots N+1}\chi_{ij}\}\rangle\rangle_{\mathrm{SR}}[\langle\exp\{-\sum_{i<j}^{1\cdots N+1}\chi_{ij}\}\rangle_{\mathrm{SR}}]^{-1}=\exp\left\{\sum_{m=1}^{\infty}\frac{(-1)^m}{m!}\langle\langle(\sum_{i<j}^{1\cdots N+1}\chi_{ij})^m\rangle\rangle_{\mathrm{SR}}^{(c)}-\langle(\sum_{i<j}^{1\cdots N+1}\chi_{ij})^m\rangle_{\mathrm{SR}}^{(c)}\right\}$$

$$=\exp\left\{-2n\int d\mathbf{r}\,\chi(r)[\tilde{g}_{\mathrm{SR}}^{(1)}(r)-g_{\mathrm{SR}}(r)+\tfrac{1}{4}\Delta g_{\mathrm{SR}}(r)]+\cdots\right\}.\quad\text{(B7)}$$

Here the superscript (c) to a bracket means a cumulant average, that is,

$$\langle f\rangle^{(c)}=\langle f\rangle;\quad\langle f\varphi\rangle^{(c)}=\langle f\varphi\rangle-\langle f\rangle\langle\varphi\rangle;\ \cdots.\quad\text{(B8)}$$

In (B6) we have written explicitly the first two cumulants only and in (B7) the first cumulant. In Eq. (B6) $\hat{g}^{(1)}(r)$ is the radial distribution function given by an equation similar to (5.3) except that l_{ij} is replaced by $\chi_{ij}+m_{ij}$. In (B7) $\tilde{g}_{\mathrm{SR}}^{(1)}(r)$ is the radial distribution function defined in Sec. V and $\Delta g_{\mathrm{SR}}(r)$ is defined by $\tilde{g}_{\mathrm{SR}}^{(0)}(r)=g_{\mathrm{SR}}(r)+N^{-1}\Delta g_{\mathrm{SR}}(r)$. We note that in the two cumulant expansions (B7) the terms of order N cancel out and only terms independent of N remain. In (B6) the superposition approximation[44] has been used to express the three-particle distribution function in terms of the two-particle distribution functions. It is possible to use a graphical analysis[18] of the different terms which contribute to the cumulants, and in this way it is easy to write higher-order cumulants. It is also possible to use the functional integral method we used to calculate $g(r)$ to evaluate the averages present in (B7). However, we do not pursue this matter further here.

The first term in (B4) and the first term in the last expression of (B6) are divergent in the infinite-volume limit; however, the sum of these two terms is finite in this limit. All the other terms which appear in (B4), (B6), and (B7) are convergent. In fact in (B6) the terms explicitly written or those arising from higher-order cumulants contain in the integrand powers of $\chi(r)$ or $[g(r)-1]$, so that the integrals are convergent in the infinite-volume limit. In (B7) in the integrand there are functions $\tilde{g}_{\mathrm{SR}}^{(1)}(r)-g_{\mathrm{SR}}(r)$ or $\Delta g_{\mathrm{SR}}(r)$ (or similar functions) and these functions go to zero rapidly as $r\to\infty$. We conclude that in the expressions (B4), (B5), (B6), and (B7) for B_N only finite quantities in the infinite volume limit appear; therefore, taking into account (4.5), n_0 is finite in this limit if the cumulant expansions we used are convergent. The cumulant expansions have been used to evaluate averages of slowly varying functions of infinite range, $\chi(r)$, with functions of a shorter characteristic space scale and of finite range: $g(r)-1$ or $g_{\mathrm{SR}}(r)-1$. The cumulant expansion and the Gaussian approximation to it seem appropriate in this case.[42]

If the short-range function $u(r)$ is the "hard-sphere" function (see Sec. III), B_N simplifies. In fact in this case the averages indicated by $\langle\langle\cdots\rangle\rangle$ and $\langle\langle\cdots\rangle\rangle_{\mathrm{SR}}$ are equal to $\langle\cdots\rangle$ and $\langle\cdots\rangle_{\mathrm{SR}}$, respectively; therefore expression (B7) is equal to unity. In (B4) only the region $r<\sigma$ and the infinitesimal region around $\xi=0$ could contribute to the integrals which contain $u(r)$. This is because for $r>\sigma$, or for every finite ξ and $r<\sigma$, $u(r)g(r;\xi)=0$ and $u(r)g_{\mathrm{SR}}(r;\xi)=0$. However, for an infinitesimal ξ the $\chi(r)$ functions give an infinitesimal contribution to $g(r;\xi)$ [this is not true for $u(r)$ which is infinite]; therefore $g(r;\xi)=g_{\mathrm{SR}}(r;\xi)$ and this integral is zero. If we express $g(r;\xi)$ in terms of $S(k;\xi)$, and for this function we use the expression (A14), the condensate can be written in the form given by (4.6) and (4.7), taking into account that $S_{\mathrm{HS}}(k;\xi)=S_{\mathrm{HS}}(k)$ for every finite ξ.

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[44] J. G. Kirkwood, J. Chem. Phys. 3, 300 (1935).