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Energy Spectrum of the Excitations in Liquid Helium*

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A wave function previously used to represent an excitation (phonon or roton) in liquid helium, inserted into a variational principle for the energy, gave an energy-momentum curve having the qualitative shape suggested by Landau; but the value computed for the minimum energy Δ of a roton was 19.1°K, while thermodynamic data require $\Delta = 9.6$°K. A new wave function is proposed here. The new value computed for Δ is 11.5°K. Qualitatively, the wave function suggests that the roton is a kind of quantum-mechanical analog of a microscopic vortex ring, of diameter about equal to the atomic spacing. A forward motion of single atoms through the center of the ring is accompanied by a dipole distribution of returning flow far from the ring.

In the computation both the two-atom and three-atom correlation functions appear. The former is known from x-rays, while for the latter the Kirkwood approximation of a product of three two-atom correlation functions is used. A method is developed to estimate and correct for most of the error caused by this approximation, so that the residual uncertainty due to this source is negligible.

1. INTRODUCTION

LIQUID helium undergoes a thermodynamic transition at 2.19°K. Below this temperature, many of the properties of the liquid are explained by Tisza's phenomonological two-fluid model. Landau realized that the macroscopic properties of the liquid would resemble those of a mixture of two fluids, provided that a certain form is assumed for the energy-momentum curve of the elementary excitations in the liquid. Starting from first principles, one of the authors has recently computed an energy-momentum curve which is based on certain ideas about the nature of the wave functions representing the excitations.[1] The shape of the curve is in qualitative agreement with Landau's, but some serious quantitative discrepancies exist. The ideas of III are pursued further here, and a more complicated wave function is constructed to represent an excitation. The energy-momentum curve computed with this wave function will prove to be in better agreement with Landau's. In addition to the actual

computations, we discuss some approximate methods which may be useful in other work of this sort.

2. LANDAU'S SPECTRUM

The energy momentum curve proposed by Landau[2,3] rises linearly for small p, passes through a maximum, falls to a minimum, and rises steeply for large p. (See Fig. 6.) The excitations in the linear region are quantized sound waves (phonons); their energy, measured relative to the ground-state energy, is

$$E(p) = cp, \tag{1}$$

where c is the velocity of sound (240 m/sec). Near its minimum, the spectrum can be approximated by a parabola,

$$E(p) = \Delta + (p - p_0)^2 / 2\mu. \tag{2}$$

Landau believed that excitations in this region represent some kind of rotation of the fluid, and called them "rotons." In the present paper we are led to the picture of a roton as the closest quantum-mechanical analog of a smoke ring. The remaining portions of the spectrum are not excited at low temperatures. For $T < 2$°K the phonons and rotons are present in sufficiently small

* This paper is based on a Ph.D. dissertation submitted to California Institute of Technology in November, 1955. A preliminary report of this work has appeared [R. P. Feynman and Michael Cohen, Progr. Theoret. Phys. Japan 14, 261 (1955)].

[1] R. P. Feynman, Phys. Rev. 94, 262 (1954), henceforth referred to as III.

[2] L. Landau, J. Phys. (U.S.S.R.) 5, 71 (1941).

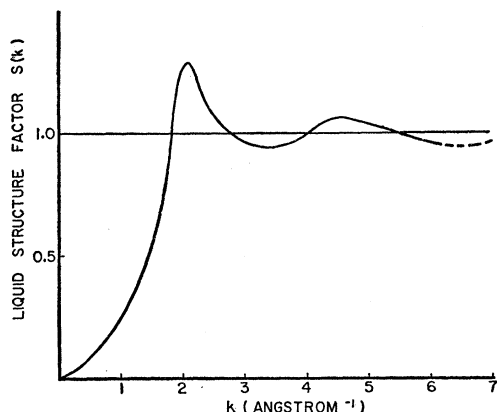[3] L. Landau, J. Phys. (U.S.S.R.) 11, 91 (1947).

FIG. 1. The liquid structure factor $S(k)$, based on the x-ray scattering data of Reekie and Hutchison. The principal maximum corresponds to a wavelength equal to the nearest neighbor distance in helium. Appendix A describes modifications we have made in the data.

numbers to allow them to be treated for thermodynamic purposes as noninteracting. The thermodynamic functions can then be computed; Landau fitted the available (1947) data on specific heat and second-sound velocity with the values

$$\Delta/\kappa = 9.6°K, \quad p_0/\hbar = 1.95 \text{ A}^{-1}, \quad \mu = 0.77 \, m_{\text{He}}. \quad (3)$$

More recent measurements[4] of the velocity of second sound down to $T = 0.015°K$ suggest the values

$$\Delta/\kappa = 9.6°K, \quad p_0/\hbar = 2.30 \text{ A}^{-1}, \quad \mu = 0.40 \, m_{\text{He}}, \quad (4)$$

although the values (3) also fit the data quite well. The value of Δ/κ is quite well determined[5] by the thermodynamic data, since it enters formulas in the form $\exp(-\Delta/\kappa T)$. The differences between (3) and (4) are probably a fair measure of the uncertainty in our knowledge of p_0 and μ.

The reasoning which led Landau to the general form of the spectrum, and his method of deducing the two-fluid picture from the spectrum, will not be reviewed here. He did not attempt to compute the values of Δ, p_0, and μ from first principles.

3. A SIMPLE WAVE FUNCTION FOR THE EXCITATIONS

In III a wave function of the form $\psi = \varphi \sum f(\mathbf{r}_i)$ is proposed to represent an excitation. The physical reasons for this wave function will not be reviewed here. The sum runs over all the atoms in the liquid, and φ is the wave function for the liquid in its ground state. The requirement that ψ be an eigenfunction of the total momentum operator[6] $\mathbf{P} = -i\hbar \sum \nabla_i$ corresponding to

the eigenvalue $\hbar\mathbf{k}$ implies that $f(r) = e^{i\mathbf{k}\cdot\mathbf{r}}$, and thus

$$\psi = \varphi \sum \exp(i\mathbf{k}\cdot\mathbf{r}_i). \quad (5)$$

Substitution of (5) into the variational principle

$$E = \mathcal{E}/\mathcal{I}, \quad (6)$$

where

$$\mathcal{E} = \int \psi^* H \psi \, d^N\mathbf{r} \quad (7)$$

and

$$\mathcal{I} = \int \psi^* \psi \, d^N\mathbf{r}, \quad (8)$$

gives an upper limit[7] for the energy of the lowest excitation of momentum $\hbar\mathbf{k}$. The result is

$$E(k) = \hbar^2 k^2 / 2mS(k), \quad (9)$$

where $S(k)$ is the Fourier transform of the zero-temperature two-atom correlation function $p(r)$,

$$S(k) = \int e^{i\mathbf{k}\cdot\mathbf{r}} p(r) d\mathbf{r}. \quad (10)$$

The data which we have used for $S(k)$ are given in Fig. 1 and are essentially those obtained from x-ray diffraction by Reekie and Hutchison.[8,9] Figure 2 is the corresponding curve for $p(r)$. $S(k)$ exhibits a sharp maximum near $k = 2$ A^{-1}, which corresponds to a wavelength equal to the nearest neighbor distance in the liquid. Accordingly, the spectrum (9) exhibits a minimum at approximately the correct wave number (see curve B of Fig. 6). It is shown in III that the wave function (5) is exact for phonons (small k) and that the limiting form of (9) is $E(k) = \hbar ck$. The occurrence of a minimum at $k = 2$ A^{-1} is in qualitative agreement with Landau's predictions, but the value of Δ/κ computed from (9) is 19.1°K, which is twice the value given by experiment.

4. ARGUMENTS FOR A NEW WAVE FUNCTION

The excitation (5) can be localized in a definite region by the formation of a wave packet. If $h(\mathbf{r})$ is a function, like a Gaussian, which is peaked about some

[4] deKlerk, Hudson, and Pellam, Phys. Rev. **93**, 28 (1954).

[5] Dr. J. R. Pellam (private communication) estimates the uncertainty in Δ/κ to be less than 0.2°.

[6] If the liquid were confined to a box of side L, with fixed walls, then the walls could absorb momentum and the energy eigenstates would not be momentum eigenstates. Instead, we control the density by requiring the wave function to be periodic in all

variables with period L. With this boundary condition, P commutes with H and the energy eigenstates can also be taken as momentum eigenstates.

[7] Eigenfunctions of $\mathbf{P}$ belonging to different eigenvalues $\hbar\mathbf{k}$ are orthogonal. Hence, for different $\mathbf{k}$, the trial functions (5) are orthogonal to each other and also to the true wave functions which minimize (6). The entire spectrum $E(k)$ therefore lies above the true spectrum. In footnote 3 of III it is mentioned that the wave function $\varphi \exp(iN^{-1}\mathbf{k}\cdot\sum \mathbf{r}_i)$, which represents translational motion of the whole liquid, has momentum $\hbar\mathbf{k}$ and energy $\hbar^2 k^2/2mN$, which is certainly lower than any energy we shall compute from (5). The periodic boundary condition, however, rules out such states unless k is as large as $N^{\frac{1}{3}}$.

[8] J. Reekie and T. S. Hutchison, Phys. Rev. **92**, 827 (1953). Their paper contains a curve for $r^2p(r)$, but does not include their data on $S(k)$. We are indebted to Dr. Reekie for sending us the data, which are now generally available in reference 9. Appendix A contains a discussion of some changes which we have made in the data.

[9] L. Goldstein and J. Reekie, Phys. Rev. **98**, 857 (1955).

location in the liquid and falls off smoothly in a distance large compared with $2\pi/k$ but small compared with the size of the box, then the wave function

$$\psi = \sum h(\mathbf{r}_i) \exp(i\mathbf{k}\cdot\mathbf{r}_i)\varphi \qquad (11)$$

represents a localized excitation. The packet will spread in time, and will drift with velocity $\hbar^{-1}\nabla_k E(k)$. The current and density associated with (11) were computed in III. The number density is very close to the average density ρ_0, even in the region of the packet, and the current at a point $\mathbf{a}$ is $\mathbf{j}(\mathbf{a}) = \hbar m^{-1}|h(\mathbf{a})|^2$. The wave function (11) therefore leads to the picture of a total current $\hbar k m^{-1}$ (assume $\int |h(\mathbf{a})|^2 d\mathbf{a} = 1$) distributed over a small region and having everywhere the same direction, with no appreciable change in the number density anywhere. Such a picture clearly cannot represent anything like a stationary state, since in a stationary state the current is divergence-free and there would necessarily be a return flow directed oppositely to $\mathbf{k}$.

One way to incorporate such a backflow into (11) is to multiply the wave function by $\exp[i\sum g(\mathbf{r}_i)]$, obtaining

$$\psi = \varphi \exp[i\sum g(\mathbf{r}_i)]\sum h(\mathbf{r}_i)\exp(i\mathbf{k}\cdot\mathbf{r}_i). \qquad (12)$$

Application of the velocity operator $-i\hbar m^{-1}\nabla_i$ shows that, in addition to whatever velocity it had in (11), the ith atom now has an extra velocity $\hbar m^{-1}\nabla g(\mathbf{r}_i)$. Substitution of (12) into (6) shows that the energy is minimized if $g(r)$ satisfies

$$\nabla\cdot(\mathbf{j} + \hbar\rho_0 m^{-1}\nabla g) = 0, \qquad (13)$$

where $\mathbf{j}$ is the current computed from the old wave function (11). Furthermore, the current arising from (12) is $\mathbf{J} = \mathbf{j} + \hbar\rho_0 m^{-1}\nabla g$, so that (13) states that the best backflow g is that which conserves current. Equation (13), with the physically reasonable boundary condition that $g\to 0$ as $r\to\infty$, completely determines g. At large distances g has the form of the velocity potential for dipole flow, namely $\mathbf{\mu}\cdot\mathbf{r}/r^3$; the dipole moment is

$$\mathbf{\mu} = m(4\pi\hbar\rho_0)^{-1}\int \mathbf{a}[\nabla\cdot\mathbf{j}(\mathbf{a})]d\mathbf{a}$$

$$= -m(4\pi\hbar\rho_0)^{-1}\int \mathbf{j}(\mathbf{a})d\mathbf{a} = -(4\pi\rho_0)^{-1}\mathbf{k}. \qquad (14)$$

The negative sign of $\mathbf{\mu}$ indicates that the direction of the backflow is opposite to that of $\mathbf{k}$, as expected. We shall refer to the value of $\mathbf{\mu}$ given by (14) as the "classical value," since it is derivable from the equation of conservation of current plus the assumption that the momentum density is equal to the current density times the mass. The energy of (12) is only slightly lower than that of (11), the difference being of the order of the reciprocal of the volume of the packet. The important point to be learned from this calculation is that the energy is lowered if the wave function conserves current.

The solution of a somewhat different problem tends to support the same idea. Suppose we want to find the energy of a state in which a foreign atom moves through the liquid with momentum $\hbar k$. The foreign atom is assumed to have the same mass as He atoms, and also to experience the same forces, but it is not subject to Bose statistics. The energy of this situation was computed in III. The simplest trial wave function is

$$\psi = \varphi \exp(i\mathbf{k}\cdot\mathbf{r}_A); \qquad (15)$$

$\mathbf{r}_A$ is the coordinate of the foreign atom, and φ is the wave function for the ground state of the entire system (which is the same as if all the atoms obeyed Bose statistics). With this wave function, Eq. (6) gives $E = \hbar^2 k^2/2m$. A possible way of lowering the energy would be to let the neighbors of the moving atom execute some pattern of flow around it, leaving space in front of it and filling in the hole behind it. Some such pattern is already contained in (15), since the ground-state wave function φ prohibits atoms from overlapping. But in the ground state, readjustments are made by pushing a few immediate neighbors of the foreign atom out of the way; these neighbors are crowded into less than their usual volumes, causing (15) to have a high kinetic energy. If, instead, room could be made for the moving atom by the simultaneous motion of many atoms, each being crowded only slightly, the kinetic energy of the state would be lower. In fact, there is no reason why the crowding cannot be eliminated entirely, since the amount of matter in the system remains constant. Roughly speaking, the requirement of no crowding means that the current is divergence-free, and the no-crowding argument shows physically why it is energetically advantageous to conserve current. The argument is vague, however, and the exact form of the backflow will be determined by more accurate methods.

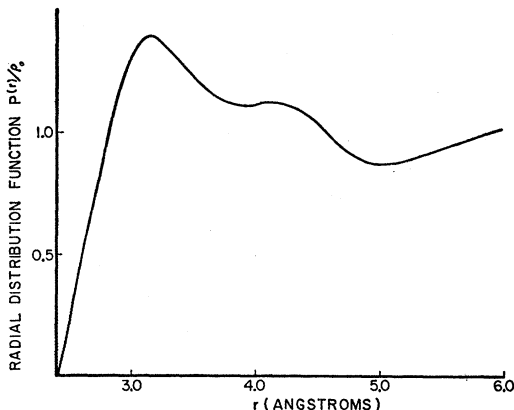A wave function of momentum $\hbar k$ which includes a

FIG. 2. The radial distribution function $p(r)$, based on the data of Reekie and Hutchison.

pattern of backflow around the foreign atom is

$$\psi = \varphi \exp(i\mathbf{k}\cdot\mathbf{r}_A) \exp[i\sum_{i\neq A} g(\mathbf{r}_i-\mathbf{r}_A)]. \qquad (16)$$

When (16) is substituted into the expression (6) for the energy, minimization of E leads to a differential equation which determines $g(\mathbf{r})$. The solution at large r is proportional to $\mathbf{k}\cdot\mathbf{r}/r^3$. Accurate numerical solution is simple, but uncertain because of uncertainty in the values of $p(r)$; since (6) is a variational principle, we may take $g(\mathbf{r})=A\mathbf{k}\cdot\mathbf{r}/r^3$. Substitution of (16) into (6) gives

$$E = (2m)^{-1}\hbar^2 k^2[1 + I_1 A + (I_4 + I_{5a})A^2], \qquad (17)$$

where I_1 and I_4 are integrals defined by Eq. (25) and I_{5a} is an integral defined by (57). The integrals are evaluated further on; only the answer interests us here. Equation (17) becomes

$$E = (2m)^{-1}\hbar^2 k^2(1 + 0.186A + 0.0246A^2), \qquad (18)$$

with A measured in A^3. The energy is minimum when $A = -3.8\ \text{A}^3$; the "classical" value predicted by (14) is $A = -(4\pi\rho_0)^{-1} = -3.6\ \text{A}^3$. The close agreement of the two values seems to indicate that the reduction in energy is due to the physical effects we have mentioned, and is not simply the result of allowing an extra degree of freedom in the wave function. The improved value for the energy is[10]

$$E = 0.648\hbar^2 k^2/2m. \qquad (19)$$

Since the wave function (5) for a phonon or roton is just what would result for symmetrizing (15), one might hope to lower the energy of (5) by adding terms to represent a backflow around each moving atom. The resulting wave function would be the symmetrization of (16), i.e.,

$$\psi = \varphi \sum \exp(i\mathbf{k}\cdot\mathbf{r}_i) \exp[i\sum_{j\neq i} g(\mathbf{r}_{ji})]. \qquad (20)$$

For large k, when this wave function is substituted into the energy and normalization integrals, there is little interference between terms with different i; the energy is therefore given by (19) and is a definite improvement over (9). For small k, (20) cannot lead to a lower energy than (5), because (5) is exact for phonons. At intermediate k, one might thus expect to lower the energy by a factor between 1.00 and 0.65. In fact, we do better than this.

The attempt to find the function $g(\mathbf{r})$ which gives the lowest energy when (20) is substituted into (6)

leads to an intractable equation. We therefore take $g(\mathbf{r})=A\mathbf{k}\cdot\mathbf{r}/r^3$, where A will be chosen to minimize the energy. The difficulty of handling integrals which involve e^{ig} leads one to consider the possibility of replacing $\exp(i\sum g)$ by $1+i\sum g$. The average value of $\sum_{j\neq i} g(\mathbf{r}_{ji})$ is $\int_0^{+\infty} p(r)g(\mathbf{r})d\mathbf{r}$, which is zero because $g(\mathbf{r})$ is an odd function. The mean square value of $\sum_{j\neq i} g(\mathbf{r}_{ji})$ is $k^2 A^2 I_3$, where the integral I_3 is defined and evaluated further on. With the classical value for A (which is close to the optimal value throughout the interesting range of k) the root-mean-square value of $\sum g(\mathbf{r}_{ji})$ turns out to be $0.25k$, where k is measured in inverse angstroms. Even with $k=2\ \text{A}^{-1}$, replacement of $\exp(i\sum g)$ by $1+i\sum g$ is not unreasonable,[11] and we shall work with the wave function

$$\psi = \varphi \sum_i \exp(i\mathbf{k}\cdot\mathbf{r}_i)[1 + i\sum_{j\neq i} g(\mathbf{r}_{ji})], \qquad (21)$$

where $g(\mathbf{r})=A\mathbf{k}\cdot\mathbf{r}/r^3$. This wave function is still an eigenfunction of the total momentum operator $\mathbf{P}$, with eigenvalue $\hbar\mathbf{k}$.

The roton state represented by the function (21) can be described roughly classically as a vortex ring of such small radius that only one atom can pass through the center. Outside the ring there is a slow drift of atoms returning for another passage through the ring. There are at least three ways that the classical picture is modified. (1) The momentum of atoms passing through the center cannot be made smaller because the wave function must return to its original value when, after one moves through, another stands in its old place. The wavelength must be the atomic spacing. (2) The ring does not drift forward as a large smoke ring, because as it is as small as possible there is no force tending to shrink it; such a force in a classical ring is balanced as a consequence of the forward drift. (3) The location of the ring is not definable. In typical quantum-mechanical fashion the lowest energy state corresponds to superposition of amplitude to find the ring anywhere in the liquid. The energy is *less* than the kinetic energy $\hbar^2 k_0^2/2m$ of one atom with momentum $\hbar k_0$ because there is a correlated motion of many atoms moving together so the effective inertia is higher (the energy Δ/κ corresponds to 2.5 atoms moving together at total momentum $\hbar k_0$).

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[10] This is somewhat higher than the value obtained in III, where a rather inaccurate approximation was used for I_4. With the new value for I_4 we find that the effective mass of a He^3 atom moving through He^4 is 5.0 atomic mass units, instead of 5.8. In the calculation it is assumed that the distribution of atoms around the He^3 atom is the same as that around an He^4 atom. The higher zero-point motion of the lighter atom actually pushes its neighbors further away. This effect will increase the mass, but probably by only a small fraction of a mass unit.

[11] Of course, since a trial function is a free choice, it would be mathematically legitimate to insert $1+i\sum g$ into the variational principle (6) even if $\sum g$ were not small, but there would be little physical reason to expect a good answer. If $\exp[i\sum g(\mathbf{r}_i-\mathbf{r}_A)]$ is replaced by $1+i\sum g(\mathbf{r}_i-\mathbf{r}_A)$ in the foreign atom problem, the resulting integrals are among the ones defined and evaluated further on. The energy is given by

$$E = \frac{\hbar^2 k^2}{2m} \frac{1 + 0.186A + (0.0217 + 0.0049k^2)A^2}{1 + 0.0049k^2 A^2}.$$

When $k=2\ \text{A}^{-1}$, the fraction has the minimum value 0.689, which is 6% higher than the value given by (19). The associated value of A is $-3.4\ \text{A}^3$. When $k=2.5\ \text{A}^{-1}$, the fraction is 0.716, corresponding to $A=-3.1\ \text{A}^3$. We conclude that for $k<2\ \text{A}^{-1}$, replacement of $\exp(i\sum g)$ by $1+i\sum g$ does not seriously raise the energy.

5. COMPUTATIONS WITH THE NEW WAVE FUNCTION

(a) Definitions

If the wave function for an excited state is $\psi = F\varphi$, it is easily shown (see III) that

$$\mathcal{E} = \int \psi^* H\psi \, d^N\mathbf{r} = (\hbar^2/2m)\sum_i \int \nabla_i F \cdot \nabla_i F^* \varphi^2 d^N\mathbf{r}. \quad (22)$$

The only memory of the potentials is in the ground-state wave function φ; the information which we need about φ will be taken from experiment, since our main interest here is to test some ideas about the nature of excited states and not to develop a detailed theory of the ground state.[12] Substitution of (21) into (22) and (8) gives $E = \mathcal{E}/\mathcal{I}$ where

$$2m\mathcal{E}/N\hbar^2 = k^2[1 + A(I_1 + I_2) + A^2(k^2 I_3 + I_4 + I_5 + kI_6 + I_7)], \quad (23)$$

$$\mathcal{I}/N = I_8 + AkI_9 + A^2 k^2 I_{10}, \quad (24)$$

and

$$I_1 = -2\mathbf{k}(\rho_0 k)^{-1} \cdot \int \nabla g_1(\mathbf{r}_{21})\rho_2(1,2)d\mathbf{r}_{21},$$

$$I_2 = 2(\rho_0 k)^{-1}\int \exp(i\mathbf{k}\cdot\mathbf{r}_{12})\,\mathbf{k}\cdot\nabla g_1(\mathbf{r}_{12})\rho_2(1,2)d\mathbf{r}_{21},$$

$$I_3 = \rho_0^{-1}\int g_1(\mathbf{r}_{21})g_1(\mathbf{r}_{31})\rho_3(1,2,3)d\mathbf{r}_{21}d\mathbf{r}_{31},$$

$$I_4 = \rho_0^{-1}\int \nabla g_1(\mathbf{r}_{21})\cdot\nabla g_1(\mathbf{r}_{31})\rho_3(1,2,3)d\mathbf{r}_{21}d\mathbf{r}_{31},$$

$$I_5 = \rho_0^{-1}\int \exp(i\mathbf{k}\cdot\mathbf{r}_{23})\nabla g_1(\mathbf{r}_{12}) \cdot \nabla g_1(\mathbf{r}_{13})\rho_3(1,2,3)d\mathbf{r}_{21}d\mathbf{r}_{31}, \quad (25)$$

$$I_6 = 2i(\rho_0 k)^{-1}\int \exp(i\mathbf{k}\cdot\mathbf{r}_{13})g_1(\mathbf{r}_{21})\mathbf{k} \cdot \nabla g_1(\mathbf{r}_{13})\rho_3(1,2,3)d\mathbf{r}_{21}d\mathbf{r}_{31},$$

$$I_7 = -2\rho_0^{-1}\int \exp(i\mathbf{k}\cdot\mathbf{r}_{13})\nabla g_1(\mathbf{r}_{21}) \cdot \nabla g_1(\mathbf{r}_{13})\rho_3(1,2,3)d\mathbf{r}_{21}d\mathbf{r}_{31},$$

$$I_8 = \int e^{i\mathbf{k}\cdot\mathbf{r}}p(r)d\mathbf{r} = S(k) \quad [\text{See Eq. (10)}],$$

$$I_9 = -2i\rho_0^{-1}\int \exp(i\mathbf{k}\cdot\mathbf{r}_{12})g_1(\mathbf{r}_{32})\rho_3(1,2,3)d\mathbf{r}_{21}d\mathbf{r}_{31},$$

$$I_{10} = \rho_0^{-1}\int \exp(i\mathbf{k}\cdot\mathbf{r}_{12})g_1(\mathbf{r}_{31})g_1(\mathbf{r}_{42}) \times \rho_4(1,2,3,4)d\mathbf{r}_{21}d\mathbf{r}_{31}d\mathbf{r}_{41}. \quad (25)$$

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[12] R. M. Mazo and J. G. Kirkwood [Proc. Natl. Acad. Sci. **41**, 204 (1955)] have computed $p(r)$ theoretically by solving an approximate integral equation.

We have written $g(\mathbf{r}) = Akg_1(\mathbf{r})$. The mean density of atoms is $\rho_0 = N/V$. The probability in the ground state that atoms are located at $\mathbf{r}_1$ and $\mathbf{r}_2$ is $\rho_2(\mathbf{r}_1,\mathbf{r}_2)d\mathbf{r}_1 d\mathbf{r}_2$. Except in the negligible region near the surface of the liquid, we have $\rho_2(\mathbf{r}_1,\mathbf{r}_2) = \rho_0 p(r_{12})$. In writing (25) we have made use of the fact that certain integrals like $\int g(\mathbf{r}_{12})\rho_2(\mathbf{r}_1,\mathbf{r}_2)d\mathbf{r}_1 d\mathbf{r}_2$ vanish because g is odd. A term $\rho_0\delta(\mathbf{r}_{12})$ is contained in $\rho_2(\mathbf{r}_1,\mathbf{r}_2)$, and hence $p(r)$ contains a δ-function at the origin. We define p_1 and p_2 by

$$p(r) = \delta(\mathbf{r}) + p_1(r), \quad (26)$$

$$p_1(r) = \rho_0[1 + p_2(r)]; \quad (27)$$

these functions have no singularities and $p_2(r) \to 0$ as $r \to \infty$. Strictly speaking, in the definition of I_1 we should replace $\rho_2(\mathbf{r}_1,\mathbf{r}_2)$ by $\rho_2(\mathbf{r}_1,\mathbf{r}_2) - \rho_0\delta(\mathbf{r}_{12})$ since g is always a function of the relative coordinates of two *distinct* atoms. To avoid unnecessary confusion, however, it is easier to think of $g(\mathbf{r})$ as becoming zero for sufficiently small r. Similar remarks apply to ρ_3 and ρ_4 when they occur in $I_2, \cdots, I_{10}$. If one does not wish to think of $g(\mathbf{r})$ as being modified near the origin, then the ρ's should be understood as containing delta functions of all coordinate differences except those which appear as arguments of g in the same integral. The probability in the ground state that atoms are at $\mathbf{r}_1$, $\mathbf{r}_2$, and $\mathbf{r}_3$ is $\rho_3(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3)d\mathbf{r}_1 d\mathbf{r}_2 d\mathbf{r}_3$. The nonsingular part of ρ_3, which we call ρ_3', is defined by

$$\rho_3(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3) = \rho_3'(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3) + \rho_0 p_1(r_{12})\delta(\mathbf{r}_{23}) + \rho_0 p_1(r_{13})\delta(\mathbf{r}_{12}) + \rho_0 p_1(r_{23})\delta(\mathbf{r}_{13}) + \rho_0\delta(\mathbf{r}_{12})\delta(\mathbf{r}_{23}). \quad (28)$$

No experimental data for ρ_3' are available. If any of the mutual distances, say r_{12}, is large, then

$$\rho_3'(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3) = \rho_0 p_1(r_{13})p_1(r_{23}).$$

If any of the interatomic distances becomes less than 2.4 A, then $\rho_3' = 0$. The approximation[13]

$$\rho_3'(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3) \simeq p_1(r_{12})p_1(r_{13})p_1(r_{23}) \quad (29)$$

has these correct limiting features. Much has been written about the validity of this approximation; for some, but not all purposes (29) is quite sufficient. We shall see that our answer is only slightly sensitive to the difference between the right and left sides of (29). Furthermore, we shall be able to estimate the magnitude and sign of the errors due to (29).

I_1, I_3, and I_4 are independent of k. In the other integrals it will prove possible to extract most of the k-dependence rather simply in the roton region, the remaining complicated terms being very small. This means that the computation of the entire roton spectrum will not be much more difficult than the computation of one point on it. We now discuss the evaluation of the various integrals.

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[13] This is sometimes called the Kirkwood approximation or the superposition approximation.

(b) Evaluation of I_1, I_2, and I_4

I_1 can be done exactly. We integrate by parts over a volume bounded by two concentric surfaces, one lying inside the radius where $p(r)=0$ and the other very far from the origin. The inner surface contributes nothing, but the integrand $g_1(\mathbf{r})p_1(r)$ falls off only as r^{-2}, with the result that the outer surface makes a finite contribution, which is easily computed to be $-(8\pi\rho_0/3)$. We eliminate this contribution by redefining $g(\mathbf{r})$ to have a decay factor, say $e^{-\epsilon r}$, with very small ϵ, which makes surface terms vanish at infinity. This procedure is mathematically legitimate, since we are free to use any wave function we want in the variational principle, and is in accord with the physical idea that all the momentum of the backflow should be contained in a finite volume. It will generally not be necessary to represent ϵ explicitly; the convergence factor will be used only to justify certain operations. After the integration by parts, there remains

$$I_1 = (2\mathbf{k}/k) \cdot \int g_1(\mathbf{r})\nabla p_1(r)d\mathbf{r}$$

$$= (8\pi/3)\int_0^\infty [dp_1(r)/dr]dr = 8\pi\rho_0/3. \quad (30)$$

In the last integral, the integrand should really be $e^{-\epsilon r}(dp_1/dr)$, but if ϵ is small enough the convergence factor will be unity out to radii where dp_1/dr becomes negligible.

After performing the angular integrations in I_2, we find

$$I_2 = 16\pi\rho_0 \int_{r_0}^\infty r^{-1}j_2(kr)[1+p_2(r)]dr$$

$$= 16\pi\rho_0[(kr_0)^{-1}j_1(kr_0)+F(k)] = 16\pi\rho_0 I_{2a}, \quad (31)$$

where r_0 is any radius inside the region where $p_1(r)=0$ [we take $r_0=2.4$ A, the radius where $p_1(r)$ first becomes positive] and

$$F(k) = \int_{r_0}^\infty r^{-1}j_2(kr)p_2(r)dr. \quad (32)$$

In order to do integrals like I_4 and I_5, we need to know the value of $I_{2a}(k)$ for all k. Using tabulated values for the spherical Bessel function j_2, $F(k)$ was evaluated by numerical integration for 23 values of k between 0 and 7 A^{-1}. Figure 3 gives the results for $I_{2a}(k)$. For $k<1.5$ A^{-1}, $F(k)$ is negligible compared with $(kr_0)^{-1} \times j_1(kr_0)$.

One might expect from (25) that $I_2 \to -I_1$ as $k \to 0$. As k approaches zero, $F(k)$ approaches zero and $j_1(kr_0)/kr_0$ approaches $\frac{1}{3}$. Comparison of (30) and (31) thus shows that I_2 approaches $2I_1$ instead of $-I_1$. The reason for the discrepancy is that (31) is wrong when k is very small, of the same order of magnitude as ϵ; in this case we must take account of the term $e^{-\epsilon r}$ in g,

and there will be a correction term which will cause I_2 to change from $16\pi\rho_0/3$ to $-8\pi\rho_0/3$ as k decreases from ϵ to 0.

I_2 can also be evaluated in momentum space, using data for $S(k)$ rather than $p(r)$. In momentum space the integrals converge best for small k rather than large k. The results are not very important because (31) is useful down to $k=0$; but they do provide a check of our numerical work and also of the consistency of the data for $p(r)$ with that for $S(k)$. $S(k)$ was defined by (10) as the Fourier transform of $p(r)$, where $p(r)$ includes a delta function at the origin and a constant term ρ_0 at infinity. Therefore $S(k) \to 1$ as $k \to \infty$ and $S(k)$ includes a term $(2\pi)^3\rho_0\delta(\mathbf{k})$. We define

$$S_1(k) = S(k) - 1 - (2\pi)^3\rho_0\delta(k). \quad (33)$$

It follows that

$$\rho_0 p_2(r) = (2\pi)^{-3} \int e^{i\mathbf{k}\cdot\mathbf{r}}S_1(k)d\mathbf{k}. \quad (34)$$

Taking the Fourier transform of $\nabla g_1(\mathbf{r})$, we obtain after the angular integrations

$$I_2 = 16\pi\rho_0/3 + (2/\pi)\int_0^\infty S_1(k_1)k_1^2 b(k_1/k)dk_1, \quad (35)$$

where

$$b(x) = \frac{5}{6} - \frac{x^2}{2} - \frac{1}{4x}(1-x^2)^2 \log\left|\frac{1-x}{1+x}\right|.$$

The numerical integral in (35) was evaluated for $k=0.5$, 1.0, 1.5, 2.0 A^{-1}. Convergence is good, and the values are accurate to within a few percent. Nevertheless, (35) does not give accurate values of I_2 when $k>1.5$ A^{-1}, because for large k the cancellation between the two terms of (35) is almost complete (as it must be because $I_2 \to 0$ as $k \to \infty$), and hence a 3% error in the numerical integral may cause a 30% error in I_2. We take the volume per atom of liquid helium
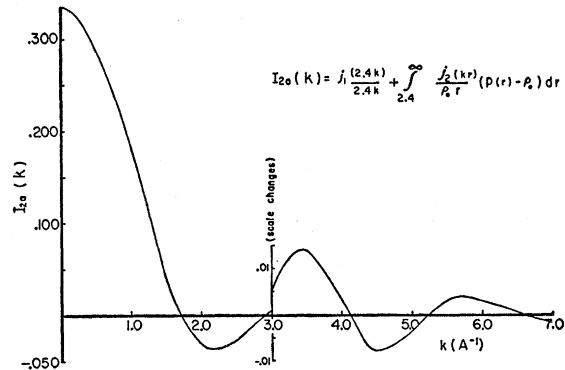
Fig. 3. $I_{2a}(k)$ is the Fourier transform of $p(r)$ times the velocity distribution in the pattern of backflow around a moving atom. In the most important region ($k<1.5$ A^{-1}), $I_{2a}(k)$ would be unchanged if we took $p(r)=0$ for $r<2.4$ A and $p(r)=\rho_0$ for $r>2.4$ A.

as 45 A^3.[14] The following table compares the values of $I_2(k)$ obtained from (31) with those obtained from (35).

$k(A^{-1})$	0	0.5	1.0	1.5	2.0	∞
$I_2(k)$ (A^{-3}) from (31)	0.372	0.322	0.194	0.054	-0.036	0
from (35)	0.372	0.326	0.200	0.050	-0.060	0

The discrepancy at $k=2$ A^{-1} is not serious, for the reasons just mentioned, and the agreement elsewhere is sufficiently close for our purposes. The values derived from (31) are used throughout our work.

I_4 presents no problem if $I_{2a}(k)$ is known for all k. Using (28) and the approximation (29) for ρ_3', and Fourier analyzing $p_2(r_{23})$ with (34) we obtain

$$I_4 = \int p_1(r)[\nabla g_1(\mathbf{r})]^2 d\mathbf{r} + \left[\int p_1(r)\nabla g_1(\mathbf{r})d\mathbf{r}\right]^2$$

$$+ (2\pi)^{-3}(\rho_0)^{-1}\int d\mathbf{k}_1 S_1(\mathbf{k}_1)\left[\int \exp(i\mathbf{k}_1\cdot\mathbf{r})\right.$$

$$\left. \times p_1(r)\nabla g_1(\mathbf{r})d\mathbf{r}\right]^2. \quad (36)$$

The integral in square brackets is a generalization of I_2 to the case where the $\mathbf{k}$ in the exponential has a different direction from the $\mathbf{k}$ in g_1. The angular integrations are easily performed, yielding

$$I_4 = 8\pi\rho_0 \int_{r_0}^{\infty}[1+p_2(r)]r^{-4}dr + (4\pi\rho_0/3)^2$$

$$+ 16\rho_0\int_0^{\infty}k_1{}^2 S_1(k_1)[I_{2a}(k_1)]^2 dk_1$$

$$= 0.01190 + 0.00867 - 0.00790 = 0.01267 A^{-6}. \quad (37)$$

The value obtained for I_4 may be in error because of uncertainties in the values of $p(r)$ and $S(k)$, and also because the approximation (29) is not exact. Discussion of the error due to (29) is postponed until the evaluation of I_3. The uncertainty in $p_2(r)$ is unimportant because the magnitude of $\int_{r_0}^{\infty} p_2(r)r^{-4}dr$ is only 1/10 that of $\int_{r_0}^{\infty} r^{-4}dr$. Similarly, 90% of the contribution to $\int_0^{\infty} k_1{}^2 S_1(k_1)[I_{2a}(k_1)]^2 dk_1$ comes from the region $k_1 < 1.2$ A^{-1}. In this region $I_{2a}(k_1)$ is the same as would result if we took $p_1(r)=0$ for $r<2.4$ A and $p_1(r)=\rho_0$ for $r>2.4$ A, and $S_1(k_1)$ is largely determined by its value and slope at the origin, both of which are known theoretically. The important point to be learned from this discussion is that the values of I_4, and of the other integrals which contribute significantly to the coefficient of A^2 in (23), depend mainly on the gross

[14] The atomic volume of liquid He under its own saturated vapor pressure at 0°K is 46 A^3, but 45 A^3 is closer to the value at 2.06°K, where the structure factor data was taken. Internal inconsistencies would develop if ρ_0 and $S(k)$ were taken at different temperatures. One might ask where the theory takes account of the external pressure. The pressure determines the values of ρ_0 and, more important, $S(k)$. An increase in pressure is expected to sharpen the maxima and minima of $p(r)$ and $S(k)$.

features of $p(r)$ (i.e., its delta function at the origin, vanishing for $r<2.4$ A, and its quick approach to the asymptotic value ρ_0) and not on the details of its behavior. The coefficients of A are more sensitive to the detailed behavior of $p(r)$; it is the detailed behavior which determines the location of the minimum in the energy spectrum. The insensitivity of the quadratic coefficients to the exact form of $p(r)$ can be similarly verified in the computations which follow, and will not be pointed out explicitly.

(c) Approximate Methods

The value of I_4 and the size of the various terms which contribute to it can be understood fairly well in terms of some simple approximations for integrals involving the coordinates of three atoms. With the help of these approximations we can understand the sizes of all the remaining integrals; if we know that an integral is small, it will not be necessary to waste time in evaluating it very accurately.

Suppose we want to do an integral of the form

$$\int f(\mathbf{r}_{21})f(\mathbf{r}_{31})\rho_3(1,2,3)d\mathbf{r}_2 d\mathbf{r}_3$$

(in this integral we shall understand ρ_3 to include a delta function on coordinates 2 and 3, but not on any other pairs). If the positions of 1 and 2 are fixed and 3 is not too close to 2, then $\rho_3(1,2,3)$ can be approximated very closely by $\rho_0 p_1(r_{21})p_1(r_{31})$. We write

$$\rho_3(1,2,3)\simeq\rho_0 p_1(r_{21})p_1(r_{31}). \quad (38)$$

When 3 approaches 2, this is wrong because ρ_3 goes to zero but $p_1(r_{21})p_1(r_{31})$ keeps a finite value (assuming, of course, that $r_{21}>2.4$ A; otherwise both expressions are zero). When 2 and 3 coincide, however, ρ_3 exhibits a delta function and far exceeds $\rho_0 p_1(r_{21})p_1(r_{31})$. The strength of the delta function is such that if we integrate the difference between the two sides of (38) over the positions of 3, the result is exactly zero, i.e.,

$$\int [\rho_3(1,2,3)-\rho_0 p_1(r_{21})p_1(r_{31})]d\mathbf{r}_3=0. \quad (39)$$

We believe this equation not to be a relation among distribution functions in general, but to hold for the distribution functions for the liquid at absolute zero. We do not have a rigorous proof, but shall discuss our reasons for believing it in Appendix B.

If $f(\mathbf{r})$ is a slow-varying function, i.e., $f(\mathbf{r})$ does not change much when $\mathbf{r}$ changes by 2.4 A, then for a fixed value of $\mathbf{r}_{12}$ the value of $f(\mathbf{r}_{31})$ is almost constant over the region where the two sides of (38) differ appreciably. Using (39), we see that the integral

$$\int f(\mathbf{r}_{31})[\rho_3(1,2,3)-\rho_0 p_1(r_{21})p_1(r_{31})]d\mathbf{r}_3$$

is very close to zero. We therefore find

$$\int f(\mathbf{r}_{31})\rho_3(1,2,3)d\mathbf{r}_3 \simeq \rho_0 p_1(r_{21}) \int f(\mathbf{r}_{31})p_1(r_{31})d\mathbf{r}_3,$$

and finally,

$$\int f(\mathbf{r}_{21})f(\mathbf{r}_{31})\rho_3(1,2,3)d\mathbf{r}_2 d\mathbf{r}_3 \simeq \rho_0 \left[\int f(\mathbf{r})p_1(r)d\mathbf{r} \right]^2. \quad (40)$$

Similarly, if f or g is slowly varying,

$$\int f(\mathbf{r}_{21})g(\mathbf{r}_{31})\rho_3(1,2,3)d\mathbf{r}_2 d\mathbf{r}_3$$

$$\simeq \rho_0 \left(\int f(\mathbf{r})p_1(r)d\mathbf{r} \right) \left(\int g(\mathbf{r})p_1(r)d\mathbf{r} \right). \quad (41)$$

Actually, our criterion for a slowly varying function is too stringent. The behavior of $f(\mathbf{r})$ for $r < 2.4$ A is of no importance, since $p_1(r)$ is zero in that range; hence f may be singular at the origin. The important question is, how much does $f(\mathbf{r}_1+\mathbf{r}_2)$ differ from $f(\mathbf{r}_1)$ when $\mathbf{r}_1$ and $\mathbf{r}_2$ are any two vectors of length 2.4 A? And even if the difference is large compared with $f(\mathbf{r}_1)$, (40) is still good if $f(\mathbf{r})$ is such that the major contribution to $\int f(\mathbf{r})p_1(r)d\mathbf{r}$ comes from $r > 3$ or 4 A.

Another type of integral which interests us is

$$\int f(\mathbf{r}_{21})g(\mathbf{r}_{31})h(\mathbf{r}_{23})\rho_3(1,2,3)d\mathbf{r}_2 d\mathbf{r}_3,$$

where f and g are smooth and $h(\mathbf{r})$ oscillates so rapidly that it produces almost complete cancellation when integrated against $p_1(r)$. ρ_3 is still understood to contain a delta function on 2 and 3, and on no other pair. In this case, if 1 and 2 are held fixed and 3 is allowed to vary, the oscillation in $h(\mathbf{r}_{23})$ make the contribution to the integral small. The major contribution comes when 3 and 2 are tied together by the delta function and we find

$$\int f(\mathbf{r}_{21})g(\mathbf{r}_{31})h(\mathbf{r}_{23})\rho_3(1,2,3)d\mathbf{r}_2 d\mathbf{r}_3$$

$$\simeq \rho_0 h(0) \int f(\mathbf{r})g(\mathbf{r})p_1(r)d\mathbf{r}. \quad (42)$$

If $\nabla g_1(\mathbf{r})$ is sufficiently smooth, (40) can be used to estimate I_4. The answer thus obtained is $(4\pi\rho_0/3)^2 = 0.00867$ A^{-6}, which is the middle term of (37); if ∇g_1 were very smooth, the first and third terms would cancel completely. The first term (0.01190 A^{-6}) is larger than the third term (-0.00790 A^{-6}) because $\nabla g_1(\mathbf{r})$ is proportional to r^{-3} and therefore quite strongly peaked for small r; hence the delta function more than compensates for the "hole" in ρ_3. The answer given by (40) is $\frac{2}{3}$ the correct answer.

With the aid of (40)–(42) we can discuss the remain-

ing integrals more intelligently. If Landau's energy spectrum is even qualitatively correct, then the most important points to compute are those in the neighborhood of the roton minimum. The phonon spectrum is guaranteed to be correct; and when the temperature is high enought to excite the portion of the spectrum lying appreciably above the roton minimum, then the picture of the liquid as a gas of independent excitations has broken down. Thus, even if we knew the exact form of the high part of the spectrum, we would not know how to do the thermodynamics. Furthermore, the high-momentum end of the spectrum computed with (20) or (21) is certainly wrong, since the slope dE/dp exceeds the velocity of sound when $k \geq 2.2$ A^{-1}; whenever $|dE(p)/dp| > c$, there obviously exist states with two excitations, one of which is a phonon, which have total momentum p but energy less than $E(p)$. We shall therefore compute the energy at several points in the region 1.6 A$^{-1} \leq k \leq 2.4$ A^{-1}, and also at $k = 1.2$ A^{-1} in order to estimate the height of the hump between the phonon and roton regions.

(d) Evaluation of I_3 and Correction to the Kirkwood Approximation

Since g_1 is smoother than ∇g_1, I_3 is a good candidate for the approximation (40), which predicts $I_3 = 0$ because $\int p_1(r)g_1(\mathbf{r})d\mathbf{r} = 0$. We infer that I_3 is small; but it is important to know *how* small, because the factor k^2 which multiplies I_3 in (23) is fairly large. The exact value of I_3 [i.e., no approximations beyond (29)] can be computed by the method used for I_4. The result is

$$I_3 = I_{3a} + I_{3b}$$

$$= \int [g_1(\mathbf{r})]^2 p_1(r)d\mathbf{r} + \int g_1(\mathbf{r}_{21})g_1(\mathbf{r}_{31})p_1(r_{21})$$

$$\times p_1(r_{31})p_2(r_{23})d\mathbf{r}_{21}d\mathbf{r}_{31}$$

$$= \rho_0 \left\{ (4\pi/3) \int_0^\infty [1+p_2(r)]r^{-2}dr \right.$$

$$\left. + (8/3) \int_0^\infty S_1(k)[I_{9a}(k)]^2 dk \right\}$$

$$= (1/45)(1.707 - 1.470) = 0.0053 \text{A}^{-4}.$$

The integral $I_{9a}(k)$ is defined by Eq. (49). The approximation (40) is based on the idea that I_{3a} and I_{3b} should cancel each other. Since $I_{3a} - I_{3b}$ is only 14% of I_{3a}, the idea behond (40) is good, but (40) tells us nothing about the size of I_3 because $\int g_1(\mathbf{r})p_1(r)d\mathbf{r} = 0$.

If $I_3 = 0.0053$ A^{-4}, then in the roton region the term $k^2 I_3$ contributes about half of the total coefficient of A^2 in (23). Any possibility of serious error in I_3 ought therefore to be investigated carefully. The idea that I_3 is almost zero is based on the approximation (40), which in turn is based on the identity (39). Actually,

the approximate form which we have used for ρ_3 does not satisfy (39) exactly. Slight departures from (39) ordinarily would not affect the validity of (40), were it not for the fact that $\int p_1(r)g_1(r)d\mathbf{r}=0$. In this case the question arises; how much of the failure of I_3 to vanish is real, and how much is due to the fact that the approximate ρ_3 does not satisfy (39)? An exact expression for I_3 is

$$I_3=0.0053-\rho_0^{-1}\int g_1(\mathbf{r}_{21})g_1(\mathbf{r}_{31})[p_1(r_{21})p_1(r_{31})p_1(r_{23})$$

$$-\rho_3'(1,2,3)]d\mathbf{r}_{21}d\mathbf{r}_{31}$$

$$=0.0053-I_{3c}. \tag{43}$$

If any one the mutual distances is less than 2.4 A or more than about 4 A, then $p_1(r_{21})p_1(r_{31})p_1(r_{23})-\rho_3'(1,2,3)$ is very close to zero. Consequently, the integrand of I_{3c} is appreciable only if the three atoms are at the corners of a triangle, each of whose legs may vary in length from 2.4 to 4 A. Therefore, if the spatial variation of $g_1(\mathbf{r})$ were slow, the replacement of $g_1(\mathbf{r}_{21})g_1(\mathbf{r}_{31})$ by $[g_1(\mathbf{r}_{31})]^2$ would not greatly alter the value of I_{3c}. The resulting integral is then easily evaluated. We can, however, find an even better approximation to I_{3c} by taking the angular variation of $g_1(\mathbf{r})$ into account. Since I_{3c} is independent of the direction of $\mathbf{k}$, we can average the integrand over the directions of $\mathbf{k}$. The average of $(\mathbf{k}\cdot\mathbf{r}_{12})(\mathbf{k}\cdot\mathbf{r}_{31})$ is $\frac{1}{3}k^2\mathbf{r}_{21}\cdot\mathbf{r}_{31}$, and in the important configurations the three atoms almost form an equilateral triangle; therefore, the average over these configurations of the cosine of the angle between $\mathbf{r}_{21}$ and $\mathbf{r}_{31}$ is very close to $\frac{1}{2}$. Most of the angular dependence of the integrand is therefore correctly accounted for if we replace $\mathbf{r}_{21}\cdot\mathbf{r}_{31}$ by $\frac{1}{2}r_{21}r_{31}$; at this stage we note that the radii r_{21} and r_{31} are almost equal in the important region, and we take r_{21} and r_{31} to be the same in the integrand. This approximation differs from the preceding one through the presence of the factor $\frac{1}{2}$. We obtain
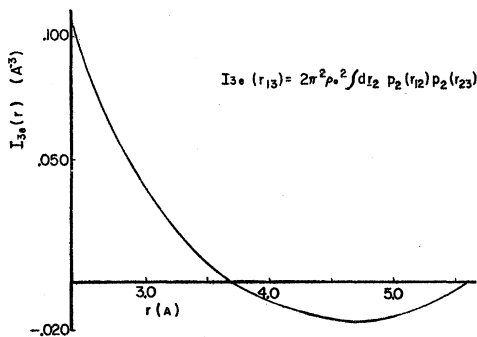
$$I_{3c}\simeq I_{3d},$$

$$I_{3e}(r_{13})=2\pi^2\rho_0^2\int d\mathbf{r}_2\, p_2(r_{12})p_2(r_{23})$$

FIG. 4. $I_{3e}(r)$ measures the error in the Kirkwood approximation, and would vanish for all $r>2.4$ A if the approximation were exact. The rapid decrease of $I_{3e}(r)$ accounts for the high accuracy of the Kirkwood approximation in this computation.

where

$$I_{3d}=(6\rho_0)^{-1}\int r_{31}^{-4}[p_1(r_{21})p_1(r_{31})p_1(r_{23})$$

$$-\rho_3'(1,2,3)]d\mathbf{r}_{21}d\mathbf{r}_{31}.$$

The identities (39) and (70) imply that

$$\int d\mathbf{r}_2[p_1(r_{21})p_1(r_{31})p_1(r_{23})-\rho_3'(1,2,3)]$$

$$=\rho_0^2 p_1(r_{13})\int p_2(r_{23})p_2(r_{12})d\mathbf{r}_2.$$

We find

$$I_{3d}=(3\pi\rho_0)^{-1}\int_{2.4}^{\infty}r^{-2}p_1(r)I_{3e}(r)dr, \tag{44}$$

where

$$I_{3e}(r_{13})=2\pi^2\rho_0^2\int d\mathbf{r}_2\,p_2(r_{12})p_2(r_{23}) \tag{45a}$$

$$=\int_0^{\infty}(kr_{13})^{-1}\sin(kr_{13})[S_1(k)]^2k^2dk. \tag{45b}$$

$I_{3e}(r)$ was computed from (45b) for 19 values of r between 2.4 A and 5.6 A. The numerical integrals converge well, and the results are shown in Fig. 4. Performing the final numerical integration in (44), we find $I_{3d}=0.00040$ A^{-4} and finally

$$I_3=0.0049\ \text{A}^{-4}. \tag{46}$$

The smallness of the correction to I_3 shows that the slight failure of (39) does not cause a significant error in I_3. This fact was not intuitively obvious, however, and needed verification. It should be emphasized that we have gone beyond the Kirkwood approximation. We have written an exact expression I_{3c} for the error due to the Kirkwood approximation, and we have estimated I_{3c} quite accurately by an integral I_{3d} which is easily evaluated. We believe the inaccuracy in the approximation $I_{3c}\simeq I_{3d}$ to be about 25%, and therefore our lack of knowledge of ρ_3 causes a residual uncertainty of 0.0001 A^{-4} in the value of I_3.

By exactly the same method, one can estimate the error in I_4 caused by the Kirkwood approximation. The answer is 0.0001 A^{-6}, which is negligible compared with the value given by (37).

(e) Evaluation of Remaining Integrals

I_9 occurs in (24) as a coefficient of A, rather than A^2, and ought therefore to be treated as accurately as is possible. In I_9, ρ_3 includes delta functions on $\mathbf{r}_{12}$ and $\mathbf{r}_{13}$. Using (29), and noting that several terms are zero because g_1 is odd, we obtain

$$I_9=-2i\int\exp(i\mathbf{k}\cdot\mathbf{r}_{12})g_1(\mathbf{r}_{32})p_2(r_{13})p_1(r_{12})$$

$$\times p_1(r_{23})d\mathbf{r}_{21}d\mathbf{r}_{31}-2i\int\exp(i\mathbf{k}\cdot\mathbf{r}_{12})g_1(r_{12})$$

$$\times p_1(r_{12})d\mathbf{r}_{21}. \tag{47}$$

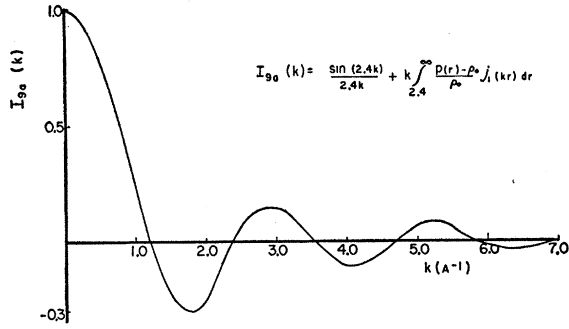$$I_{9a}(k) = \frac{\sin(2.4k)}{2.4k} + k \int_{2.4}^{\infty} \frac{p(r) - p_0}{p_0} j_1(kr) \, dr$$

FIG. 5. $I_{9a}(k)$ is the Fourier transform of $p(r)$ times the velocity potential for the backflow pattern. Like $I_{2a}(k)$ it is determined in in the most important region by the gross features of $p(r)$.

First we consider the second integral, since we must know its value for all $\mathbf{k}$ in order to do the first integral. The integral, like I_2, can be performed in coordinate or momentum space; after the angular integrations are done, the result in coordinate space is

$$\int \exp(i\mathbf{k}_1 \cdot \mathbf{r}) g_1(r) p_1(r) d\mathbf{r} = (\mathbf{k}_1 \cdot k/k_1^2 k) 4\pi\rho_0 i I_{9a}(k_1),$$
(48)

where[15]

$$I_{9a}(k) = (2.4k)^{-1} \sin(2.4k) + k \int_{2.4}^{\infty} p_2(r) j_1(kr) dr. \quad (49)$$

As before, the coordinate space formula proves sufficient over the entire range of k. For small k, when the numerical integral cannot be done accurately, its value is so small as to be unimportant compared with $(2.4k)^{-1} \sin(2.4k)$. Figure 5 gives the values of $I_{9a}(k)$. As in the case of $I_2(k)$, some points were also computed in momentum space, using data for $S(k)$ rather than $p(r)$. The results were in good agreement with the coordinate space computations.

Since $p_1(r_{12}) = \rho_0[1 + p_2(r_{12})]$, the first integral in (47) becomes

$$\rho_0 \int \exp(i\mathbf{k} \cdot \mathbf{r}_{12}) g_1(\mathbf{r}_{32}) p_1(r_{32})[1 + p_2(r_{12})] p_2(r_{13}) d\mathbf{r}_{21} d\mathbf{r}_{31}$$

$$= \rho_0 \int \exp(i\mathbf{k} \cdot \mathbf{r}_{12}) g_1(\mathbf{r}_{32}) p_1(r_{32}) p_2(r_{13}) d\mathbf{r}_{21} d\mathbf{r}_{31}$$

$$+ \rho_0 \int \exp(i\mathbf{k} \cdot \mathbf{r}_{12}) g_1(\mathbf{r}_{32}) p_1(r_{32})$$
$$\times p_2(r_{12}) p_2(r_{13}) d\mathbf{r}_{21} d\mathbf{r}_{31}. \quad (50)$$

The first integral on the right in (50) can be evaluated by writing $\exp(i\mathbf{k} \cdot \mathbf{r}_{12}) = \exp(i\mathbf{k} \cdot \mathbf{r}_{13}) \exp(i\mathbf{k} \cdot \mathbf{r}_{32})$ and using the new integration variables $\mathbf{r}_{31}$ and $\mathbf{r}_{32}$. The result is

$$\int \exp(i\mathbf{k} \cdot \mathbf{r}_{12}) g_1(\mathbf{r}_{32}) p_1(r_{32}) p_2(r_{13}) d\mathbf{r}_{21} d\mathbf{r}_{31}$$
$$= (4\pi i/k) S_1(k) I_{9a}(k). \quad (51)$$

In the second integral on the right in (50) we use the integration variables $\mathbf{r}_{21}$ and $\mathbf{r}_{32}$; Fourier-analyzing $p_2(r_{13})$, we obtain

$$\int \exp(i\mathbf{k} \cdot \mathbf{r}_{12}) g_1(\mathbf{r}_{32}) p_1(r_{23}) p_2(r_{12}) p_2(r_{13}) d\mathbf{r}_{21} d\mathbf{r}_{31}$$

$$= (i\pi\rho_0)^{-1} \int_0^{\infty} \int_0^{\pi} dk_1 d\theta k_1 S_1(k_1) S_1(|\mathbf{k} + \mathbf{k}_1|)$$
$$\times I_{9a}(k_1) \cos\theta \sin\theta, \quad (52)$$

where θ is the angle between $\mathbf{k}$ and $\mathbf{k}_1$. If we let

$$u = |\mathbf{k} + \mathbf{k}_1| = (k^2 + k_1^2 + 2kk_1 \cos\theta)^{\frac{1}{2}}$$

the right side of (52) becomes

$$(2\pi\rho_0 i k^2)^{-1} \int_0^{\infty} dk_1 k_1^{-1} I_{9a}(k_1) S_1(k_1) \int_{|k-k_1|}^{k+k_1}$$
$$\times S_1(u)(u^2 - k^2 - k_1^2) u \, du. \quad (53)$$

Since

$$\int_0^{\infty} dk_1 f(k_1) \int_{|k-k_1|}^{k+k_1} g(u) du = \int_0^{\infty} du g(u) \int_{|k-u|}^{k+u} f(k_1) dk_1,$$

a numerical integral like (53) can be done in several different ways. We look for the way which converges fastest, is least sensitive to information which we do not have [like the value of $S_1(u)$ for large u], and does not involve small differences of big terms. For example, we should avoid dealing with the indefinite integral of $S_1(u)u^3$, since it oscillates badly for large u; hence (53) is not convenient to use as it stands. Probably the best form of (53) is

$$(2\pi\rho_0 i k^2)^{-1} \left[\int_0^{\infty} u S_1(u)(u^2 - k^2) du \right.$$

$$\times \int_{|u-k|}^{u+k} dk_1 I_{9a}(k_1) S_1(k_1)/k_1$$

$$\left. - \int_0^{\infty} u S_1(u) du \int_{|u-k|}^{u+k} dk_1 k_1 I_{9a}(k_1) S_1(k_1) \right]$$

$$= (2\pi\rho_0 i k^2)^{-1} [I_{9b}(k) - I_{9c}(k)]. \quad (54)$$

In this form, the inside integral acts as a convergence factor for the integrand of the outside integral, and the answer is not sensitive to the values of $S_1(u)$ for large u.

[15] Since $\int g_1(\mathbf{r}) p_1(r) d\mathbf{r} = 0$, one might expect the right side of (48) to approach zero as k_1 becomes small. But $I_{9a}(k_1)$ approaches unity for small k_1, and consequently the right side of (48) approaches $\pm\infty$, depending on the angle between $\mathbf{k}$ and $\mathbf{k}_1$. The trouble, as before, is resolved by noting that (48) and (49) are wrong for $k_1 < \epsilon$ (g_1 should really gave a factor $e^{-\epsilon r}$ in it). In the correct version of (49) the term $(2.4k)^{-1} \sin(2.4k)$ is replaced by zero when $k \ll \epsilon$; hence $I_{9a}(k_1)$ goes as k_1^2 when $k_1 \ll \epsilon$, and the right side of (49) approaches zero. The "error" in (48) and (49) has no effect on our computations, but is worth mentioning lest the reader discover it and develop a distrust of the formulas.

The inside integral can be tabulated once and for all as an indefinite integral; thus, the evaluation of (54) involves only a single numerical integration for each value of k.

If (41) were used to estimate $I_9(k)$, the result would be

$$I_9(k) \simeq -2i \int e^{i\mathbf{k}\cdot\mathbf{r}}p_1(r)d\mathbf{r} \int g_1(\mathbf{r})p_1(\mathbf{r})d\mathbf{r} = 0.$$

As in the case of I_3, the question arises: how much of the failure of $I_9(k)$ to vanish is real, and how much is due to the failure of our approximate ρ_3 to satisfy (39)? The analysis proceeds exactly as with I_3, and we find that the quantity

$$I_{9d}(k) = (2/\pi\rho_0) \int_0^\infty p_1(r)j_1(kr)I_{3e}(r)dr \qquad (55)$$

should be subtracted from (47). Combining Eqs. (47)–(55), we obtain

$$I_9(k) = (8\pi\rho_0/k)I_{9a}(k)S(k) \\ + (\pi k^2)^{-1}[I_{9c}(k) - I_{9b}(k)] - I_{9d}(k). \quad (56)$$

Table I gives values of $I_9(k)$, $I_{9b}(k)$, $I_{9c}(k)$, and $I_{9d}(k)$. In the roton region the correction I_{9d} is about one-tenth as large as I_9 (except near $k = 2.4$ A^{-1}, where I_9 is negligible anyway). Since we believe that I_{9d} estimates, within an accuracy of 25%, the error due to the Kirkwood approximation, the residual error in I_9 due to this source is probably only 2 or 3%.

Using (29), we can write I_5 as

$$I_5 = \int_0^\infty p_1(r)[\nabla g_1(\mathbf{r})]^2 d\mathbf{r} + \left[\int_0^\infty e^{i\mathbf{k}\cdot\mathbf{r}}p_1(r)\nabla g_1(\mathbf{r})d\mathbf{r}\right]^2$$

$$+ \int \exp(i\mathbf{k}\cdot\mathbf{r}_{23})\nabla g_1(\mathbf{r}_{21})\cdot\nabla g_1(\mathbf{r}_{31})p_1(r_{21}) \\ \times p_1(r_{31})p_2(r_{23})d\mathbf{r}_{21}d\mathbf{r}_{31}$$

$$= I_{5a} + I_{5b} + I_{5c}. \qquad (57)$$

The oscillatory factor $\exp(i\mathbf{k}\cdot\mathbf{r}_{23})$ makes I_5 a likely candidate for (42), which says[16] $I_5 \simeq I_{5a}$. At the cost of considerable labor we have computed $I_{5b} + I_{5c}$ when $k = 2$ A^{-1} and when $k = 1.2$ A^{-1}, and verified that it could indeed have been neglected.

I_{5a} has been evaluated in connection with I_4. From (31) and (25) we obtain

$$I_{5b}(k) = [8\pi\rho_0 I_{2a}(k)]^2.$$

$I_{5c}(k)$ can be evaluated by the same methods used for I_9. The resulting expression is similar in form to (54), and will not be exhibited here. Laborious computations give

$$I_{5b}(2\text{ A}^{-1}) + I_{5c}(2\text{ A}^{-1}) = -0.0010\text{ A}^{-6}$$

and

$$I_{5b}(1.2\text{ A}^{-1}) + I_{5c}(1.2\text{ A}^{-1}) = 0.0010\text{ A}^{-6}.$$

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[16] Compare (42) with the definition of I_5 in (25).

TABLE I. Values of numerical integrals involved in $I_9(k)$.

k(A^{-1})	$I_{9b}(k)$(A^{-4}) [See (54)]	$I_{9c}(k)$(A^{-4}) [See (54)]	$I_{9d}(k)$(A^{-2}) [See (55)]	$I_9(k)$(A^{-2}) [See (56)]
1.2	−0.019	0.172	0.0076	0.0444
1.6	−0.387	0.089	−0.0002	−0.0054
1.8	−0.406	0.031	−0.0035	−0.0386
2.0	−0.364	−0.017	−0.0047	−0.0518
2.2	−0.086	−0.048	−0.0039	−0.0307
2.4	0.155	−0.054	−0.0020	−0.0044

Since $I_{5a} = 0.0119$ A^{-6}, the complete omission of I_{5b} and I_{5c} would not cause a serious error in the roton spectrum. We shall omit these terms while locating the minimum of the spectrum, and shall reinstate them in the final computation of Δ.

I_6 is estimated by (41) as zero. As in the case of I_3, it is important to find out whether I_6 is really small enough to be neglected. To obtain a more accurate estimate, we write

$$I_6 = I_{6a} + I_{6b},$$

where

$$I_{6a} = (2i/k) \int e^{-i\mathbf{k}\cdot\mathbf{r}}g_1(\mathbf{r})\mathbf{k}\cdot\nabla g_1(\mathbf{r})p_1(r)d\mathbf{r},$$

$$I_{6b} = (2i/k) \int \exp(i\mathbf{k}\cdot\mathbf{r}_{13})g_1(r_{21})\mathbf{k} \\ \cdot\nabla g_1(\mathbf{r}_{13})p_1(r_{31})p_1(r_{21})p_2(r_{23})d\mathbf{r}_{31}d\mathbf{r}_{21}.$$

According to the discussion preceding (41), I_{6a} and I_{6b} will cancel each other almost completely, so I_6 is some fraction (probably about one-fourth) of I_{6a}. Performing the angular integrations in I_{6a}, we obtain

$$I_{6a} = 8\pi\int_0^\infty drr^{-3}p_1(r)[-2(kr)^{-1}\cos(kr) \\ + 8(kr)^{-2}\sin(kr) + 18(kr)^{-3}\cos(kr) \\ - 18(kr)^{-4}\sin(kr)].$$

A rough numerical integration gives

$$I_{6a}(2\text{ A}^{-1}) \simeq -0.003\text{ A}^{-5}.$$

Hence $I_6(2\text{ A}^{-1}) \simeq -0.001$ A^{-5}, and $kI_6 \simeq -0.002$ A^{-6} when $k = 2$ A^{-1}. Since $k^2 I_3 + I_4 + I_5 \simeq 0.040$ A^{-6} near $k = 2$ A^{-1}, we can neglect kI_6 without much error.

Estimation of I_7 by (41) gives

$$I_7 \simeq -2(-4\pi\rho_0/3)8\pi\rho_0 I_{2a}(k) = \tfrac{1}{3}(8\pi\rho_0)^2 I_{2a}(k). \quad (58)$$

Considerations similar to those used in estimating I_6 show that (58) is accurate to better than 0.001 A^{-6}.

When k is in the roton region, the major portion of I_{10} comes from the term $\delta(\mathbf{r}_{12})\rho_3(2,3,4)$, which is contained in $\rho_4(1,2,3,4)$. When $r_{12} \neq 0$, the oscillations of $e^{i\mathbf{k}\cdot\mathbf{r}_{12}}$

make the contribution to the integral very small.[17] If we neglect all of ρ_4 except $\delta(\mathbf{r}_{12})\rho_3(2,3,4)$, we are making essentially the approximation which was used in I_5 and was shown to be very accurate there. We then obtain

$$I_{10} \simeq I_3 \tag{59}$$

and our evaluation of the integrals in (25) is completed.

The oscillation argument which leads to (59) fails when k is very small. For any value of k the requirement that the normalization integral $\mathcal{J}$ have no roots when considered as a polynomial in A leads to the inequality

$$I_{10} > I_9{}^2/4I_8. \tag{60}$$

The failure of (59) for small k is most easily seen by noting that I_3 becomes much smaller than the right side of (60) as $k \to 0$.

For $k \geq 1.2\,\mathrm{A}^{-1}$, the coefficient of A^2 in (23) is

$$\frac{E(k)}{E_1(k)} < \frac{1+A[I_1+I_2]+A^2[k^2I_3+I_4+I_{5a}+\frac{1}{3}(8\pi\rho_0)^2I_{2a}]}{1+A[kI_9/I_8]+A^2[k^2I_3/I_8]}$$

$$= \frac{1+A[0.186+1.117I_{2a}(k)]+A^2[0.0246+0.0049k^2+0.108I_{2a}(k)]}{1+A[kI_9(k)/S(k)]+A^2[0.0049k^2/S(k)]}$$

$$= E_2(k)/E_1(k). \tag{61}$$

$E(k)$ is the true lowest energy of a state having momentum $\hbar\mathbf{k}$; $E_1(k)$ is the energy computed with the wave function (5), i.e., $E_1(k)=\hbar^2k^2/2mS(k)$; $E_2(k)$ is the spectrum we have computed, subject to the omissions and approximations noted above.

For $k=2\,\mathrm{A}^{-1}$, (61) becomes

$$\frac{E_2(k)}{E_1(k)} = \frac{1+0.149A+0.0406\,A^2}{1-0.0822A+0.0156\,A^2}. \tag{62}$$

The first attractive feature of (62) is that the coefficients of A in the numerator and denominator have opposite signs, so that the denominator increases while the numerator decreases. The optimal value of A is -3.5, which is very close to the classical value $A_{cl}=-3.6$. The minimum value of $E_2(2)/E_1(2)$ is 0.659, corresponding to $E_2(2\,\mathrm{A}^{-1})/\kappa=12.6°\mathrm{K}$.

Computation of the coefficients in (61) and minimization of the resulting expressions yield the results given in Table II. We estimate the minimum value of $E_2(k)/\kappa$ as $12.0°\mathrm{K}$, corresponding to $k=1.85\,\mathrm{A}^{-1}$. If

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[17] If the integral

$$J(\mathbf{r}_{12})=(\rho_0)^{-2}\int \rho_4(1,2,3,4)g_1(\mathbf{r}_{31})g_1(\mathbf{r}_{42})d\mathbf{r}_3d\mathbf{r}_4,$$

were to become large compared with $J(0)$ as r_{12} grows large, then the growth of J might offset the oscillations of $\exp(i\mathbf{k}\cdot\mathbf{r}_{12})$ and (58) would be wrong. It is easy to see, however, that as 1 and 2 go farther apart, $J(\mathbf{r}_{12})$ approaches $[\int p_1(r)g_1(\mathbf{r})d\mathbf{r}]^2$, which is zero. Since the factorization of J into a product of two integrals becomes more nearly exact as r_{12} increases, it is very plausible that J decreases with increasing r_{12} and is largest when 1 and 2 coincide. In the latter case, J is equal to I_3.

estimated well by

$$k^2I_3+I_4+I_{5a}+\tfrac{1}{3}(8\pi\rho_0)^2I_{2a}(k).$$

We have omitted I_{5b}, I_{5c}, and kI_6, and have approximated I_7 by (58). I_{5c} and kI_6 have both been shown to be very small, and are both difficult to compute; omission of these terms simplies the computation of the energy spectrum, and does not significantly change the location of the minimum. I_{5b} has been omitted for the sake of consistency, since it is even smaller than I_{5c}. After locating the minimum, we shall reinstate the omitted terms in our final computation of Δ. We estimate I_{10} by (59).

6. THE IMPROVED ENERGY SPECTRUM

With the omissions and approximations mentioned in the preceding paragraph, we obtain

we estimate $I_{5c}(1.85\,\mathrm{A}^{-1})$ and $I_6(1.85\,\mathrm{A}^{-1})$ by the values of the corresponding integrals at $k=2\,\mathrm{A}^{-1}$, we find that the coefficient of A^2 in the numerator of (61) should be diminished by $0.003\,\mathrm{A}^{-6}$ when $k=1.85\,\mathrm{A}^{-1}$. This change lowers the energy by $0.5°\mathrm{K}$ and we obtain the following as the final result of this computation[18]:

$$p_0/\hbar=1.85\,\mathrm{A}^{-1}, \quad \Delta/\kappa=11.5°\mathrm{K}. \tag{63}$$

It is evident from Table II that $E_2(k)/E_1(k)$ passes through a minimum near $k=1.2\,\mathrm{A}^{-1}$. In any correct theory $E_2(k)/E_1(k)$ must approach unity for very small k because we cannot lower the energy of a phonon. By studying the behavior of the integrals in (25) for very small k, we have verified that our spectrum does indeed

TABLE II. The energy spectrum $E_2(k)$ computed from (61).[a]

$k(\mathrm{A}^{-1})$	$A_{opt}(\mathrm{A}^3)$	$E_2(k)/E_1(k)$	$E_2(k)/\kappa(°\mathrm{K})$
1.2	−3.6	0.569	14.08
1.6	−3.7	0.576	13.44
1.8	−3.6	0.594	12.00
2.0	−3.5	0.659	12.59
2.2	−3.0	0.730	16.86
2.4	−2.5	0.791	24.04

[a] $E_2(k)$ is essentially the spectrum computed here. Some further small corrections lower the minimum energy to $11.5°\mathrm{K}$. $E_1(k)$ is the spectrum previously computed with a simpler wave function. A_{opt} is the optimal value of the strength of the return flow in the wave function (21), and is chosen so as to minimize $E_2(k)$. The values of A_{opt} are close to the "classical" value $-3.6\,\mathrm{A}^3$ computed from a current conservation argument.

[18] A similar result has been obtained from perturbation theory by C. G. Kuper, Proc. Roy. Soc. (London) 233, 223 (1955). As he points out, the perturbation theory is not reliable because of the large size of the energy change.

have the correct limiting behavior.[19] A more direct way of seeing the result is to look at (21) [or (20)] when k is very small. The correlation term $g(\mathbf{r}_{ij})$ is significant only when atoms i and j are fairly close. But in this case $\exp(i\mathbf{k}\cdot\mathbf{r}_1)$ and $\exp(i\mathbf{k}\cdot\mathbf{r}_j)$ are almost equal because k is small, and hence the correlation terms cancel almost completely because g is odd. Thus, (21) is almost the same as (5) for small k, and leads to the same energy.

For high k, $E_2(k)/E_1(k)$ approaches unity because the approximation $\exp[i\sum g(\mathbf{r}_{ji})]\simeq1+i\sum g(\mathbf{r}_{ji})$ fails badly. We noted earlier that if we could compute with the wave function (20), the interference between terms with different i would vanish when k is large. If $E_3(k)$ is the energy arising from (20), we should find that for large k,

$$E_3(k)/E_1(k)=0.65,$$

as in the foreign atom problem. It is amusing to conjecture on how much $E_3(k)$ might lie below $E_2(k)$ when $k=1.8\ \text{A}^{-1}$. The accuracy of the approximation $\exp(i\sum g)=1+i\sum g$ in the foreign atom problem (see reference 11) suggests that E_3 may be 0.5° less.

The energy spectrum $E_2(k)$ is shown in Fig. 6 as curve A. We have also plotted B: $E_1(k)=\hbar^2k^2/2mS(k)$; C: de Klerk, Hudson, and Pellam's spectrum [Eq. (4)]; D: spectrum of the form (2), with $\Delta/\kappa=9.6°$, $p_0/\hbar=1.85\ \text{A}^{-1}$ and μ chosen so that $\mu^{\frac{1}{2}}p_0^2$ has the same value as in C. (The specific heat depends on μ and p_0 only through the product $\mu^{\frac{1}{2}}p_0^2$.) From the curvatures of A, C, and D it is clear that our spectrum $E_2(k)$ predicts too small a value of μ. In a computation of this sort, however, it is doubtful that the curvature has much significance.

Curve A brings out the fact that the "hump" between the phonon and roton regions is not nearly so high as one might expect from (1). Consequently, when computing the specific heat or normal fluid density at temperatures high enough to excite rotons, it is probably also necessary to take into account the deviations of the phonon spectrum from linearity (and also the deviations of the roton spectrum from pure parabolic behavior). Qualitatively, it appears that such corrections might improve the agreement between the theoretical spectrum and the specific heat and second sound data.

7. DISCUSSION OF ACCURACY

Initially, the major potential sources of error in this computation were (a) the absence of information about the true form of $\rho_3(1,2,3)$; (b) absence of information about $\rho_4(1,2,3,4)$; (c) uncertainties in the data for $S_1(k)$ at large k (see Appendix A).

The uncertainty caused by (a) has, we think, been minimized by the introduction of a correction to the Kirkwood approximation. The errors remaining in I_3

FIG. 6. The energy spectrum of excitations. Curve A is the spectrum $E_2(k)$ computed from Eq. (61). Curve B is the spectrum $E_1(k)$ computed with the simpler wave function (5). Curve C is the Landau-type spectrum used by de Klerk et al.[4] to fit the second sound and specific heat data. Curve D is a Landau-type spectrum with p_0 taken the same as in A, and μ and Δ chosen to fit the specific heat data. For small k, all curves are asymptotic to the line $E=\hbar ck$.
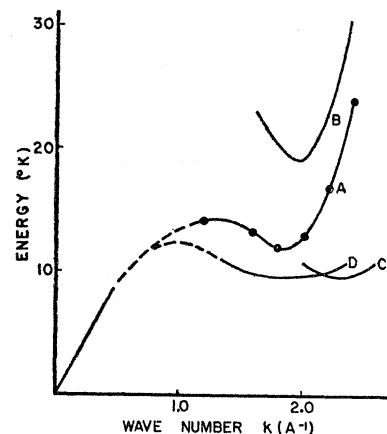
and I_9 after the correction are probably less than three percent; the resultant error in Δ/κ is less than 0.3°.

The approximation (59), which gives rise to the error (b), ought to be about as accurate as the approximation $I_5\simeq I_{5a}$, since both approximations are based on the same oscillation argument. The latter approximation was found accurate to better than 10% in the roton region. A ten percent change in I_{10} would alter the value of Δ/κ by 0.2°; we regard this number as a fair estimate of the error caused by (b).

Considerable pains were taken to arrange the numerical work in such a way that the answers are insensitive to the behavior of $S_1(k)$ for large k. The residual error due to (c) is found mainly in the coefficient of A^2 in the numerator of (61). This coefficient may be in error by 5%, and the resulting error in Δ/κ might be as much as 0.4°.

We consider the value $\Delta/\kappa=11.5°$ to be accurate within 0.6°, i.e., the lowest energy computable with the wave function (21) is between 10.9° and 12.1°.

A wave function which gives a good value of the energy may, of course, be inaccurate for calculation of other properties of the system. On the other hand this function was chosen by a physical argument, and achieved a very considerable increase in the accuracy of the energy, without in fact using any variable parameters. It might be argued that some of this increase should be associated simply with the fact that we have one extra parameter A to vary. But had we used the A determined by the physical argument (-3.6) we would have obtained practically the same energy as if we let it vary.

For this reason we believe that the wave function (20) [or for practical calculations (21)] not only gives the energy well but is a reasonably accurate physical description of the excitations. On the basis of this optimistic hope, (21) is currently being employed in the calculation of other properties of helium.

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[19] If $g(\mathbf{r})$ falls off sharply at large r, the analysis is simple. In our case the analysis is complicated by the slowness with which $\mathbf{k}\cdot\mathbf{r}/r^3$ falls off, but the ultimate result is the desired one.

APPENDIX A. DATA USED FOR $S(k)$ AND $p(r)$

The curve for $S(k)$ given in Fig. 1 is essentially that obtained from x-ray scattering by Reekie and Hutchison.[8,9] The proper normalization of the data can, in principle, be determined from the fact that $S(k) \rightarrow 1$ as $k \rightarrow \infty$. According to Goldstein and Reekie,[9] "limitations inherent in the very low scattering cross section of liquid helium and the experimental technique have prevented effective exploration (of the range $k > 6$ A^{-1})." Since $S(k)$ is still oscillating strongly at $k = 6$ A^{-1}, the normalization of $S(k)$ is uncertain by a few percent. For $k \gtrsim 2.5$ A^{-1}, the percent error in $S(k) - 1$ is large, and our computations would be totally unreliable if the integrals had not been set up in such a way as to be insensitive to the behavior of $S(k) - 1$ for large k. We feel that $S(k)$ ought to oscillate about its asymptotic value, and have therefore taken $S(k) = 1$ at a point whose ordinate is the average of the values of $S(k)$ at the minimum near 3.4 A^{-1} and the maximum near 4.6 A^{-1}. With Reekie's normalization, $S(k)$ is unity at an ordinate much nearer to the minima of the oscillations. Our normalization maximizes the cancellation at large k when we are performing integrals whose integrand contains $S(k) - 1$ as a factor. Since $S(k)$ is the Fourier transform of $p(r)$, we find [see (34)]

$$-2\pi^2 \rho_0 = \int_{0^+}^{\infty} k^2 [S(k) - 1] dk. \quad (64)$$

The relation (64) might serve as a test of the normalization of $S(k)$, were it not for the fact that the numerical integral gives no sign of converging if we cut it off at $k = 6$ A^{-1}. The left side of (64) is equal to -0.43 A^{-3}. With our normalization, integration of the right side out to $k = 6$ A^{-1} gives $+0.44$ A^{-3}, but the integrand is still oscillating wildly and there is a chance of ultimately converging to a correct answer. With Reekie's normalization, integration of the right side out to $k = 6$ A^{-1} gives a positive value much larger than $+0.44$ A^{-3}, and the contribution from $k > 6$ A^{-1} will also be positive unless the successive minima of $S(k)$ cease to be closer and closer to the asymptotic value of unity. At any rate, the consistency of the results which we have obtained by performing the same integral in coordinate and momentum space convinces us that our $S(k)$, which is 0.97 times Reekie's, is sufficiently accurate for the present computations.

Most of the curve in Fig. 1 represents data taken at 2.06°K. According to reference 9, there is very little change in the values of $S(k)$ for $k > 0.9$ A^{-1} as the temperature decreases from 2.5°K to 1.25°K. Therefore, in the range $k > 0.9$ A^{-1}, it is probably safe to represent the zero-temperature structure factor $S(k)$ by the data taken at 2.06°K. For $k < 0.9$ A^{-1}, the temperature dependence of $S(k)$ is more important, and it is necessary to extrapolate $S(k)$ linearly to zero by using (65). We have done this, using a slope about 20% higher than the theoretical value in order to join the experimental data smoothly. The error thus introduced is small.

Reekie and Hutchison[8] have computed $p(r)$ for $r \leq 6$ A by inverting their data for $S(k)$. The curve for $p(r)$ which we have given in Fig. 2 is obtained from one of their graphs[20] and, as has been previously mentioned, seems consistent with our curve for $S(k)$. The numerical inversion of diffraction data is not unambiguous, since the integrand of the relevant numerical integral is not small at the cut-off value $k = 6$ A^{-1}. Furthermore, an arbitrary cutoff procedure must be used to make $p(r)$ vanish for $r < 2.4$ A. More recently, Goldstein and Reekie[9] have employed an IBM 701 calculator to compute $p(r)$ out to 20 A, using the data of Reekie and Hutchison. Their article was not published until after the completion of the present calculation; the authors state that the results out to 6 A "fully confirm" the results of reference 9. Goldstein and Reekie apply the integral test (69) to their curves for $p(r)$ and find satisfactory results. Since the integrands do not become small until $r \gtrsim 13$ A, we found it impossible to apply the test to the curve in Fig. 2.

APPENDIX B. IDENTITIES SATISFIED BY $p(r)$ AND $S(k)$

To understand the behavior of $S(k)$ for small k, we note that as long as we are concerned with disturbances of long wavelength (small k) the liquid can be treated as a continuous compressible medium. If $\rho(r,t)$ is the number density in such a medium and we define the normal coordinates

$$q_k = \int \rho(r,t) e^{ik \cdot r} dr,$$

then the energy is

$$E = \tfrac{1}{2} \sum_k m_k [\dot{q}_k \dot{q}_k^* + \omega_k^2 q_k q_k^*],$$

where $\omega_k = ck$ and $m_k = m/Nk^2$. Quantum mechanically, $\rho(r)$ is replaced by the operator $\sum_i \delta(r - r_i)$ and q_k then goes over into the quantum-mechanical normal coordinate $q_k = \sum \exp(ik \cdot r_i)$. $S(k)$ is just $1/N$ times the expectation value of q_k^2. Since the average values of the potential and kinetic energies are equal for a harmonic oscillator, it follows that $S(k) = \langle E_k \rangle / mc^2$, where $\langle E_k \rangle$ is the average energy of the oscillator representing sound of wave number k. When $T = 0$, all the oscillators are in their ground states, and hence $\langle E_k \rangle = \tfrac{1}{2}\hbar\omega_k = \tfrac{1}{2}\hbar ck$ and

$$S(k) = \hbar k / 2mc \quad \text{(small } k). \quad (65)$$

When $T \neq 0$, the oscillator representing phonons of wave number k is no longer necessarily in its ground

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[20] Figure 2 was obtained by dividing the data of reference 8, Fig. 1, by r^2. There are slight discrepancies between the resultant curve for $p(r)$ and the curve given in reference 9, Fig. 3. Errors of this magnitude in $p(r)$ would have a negligible effect on our results.

state, but may be in its nth excited state with probability proportional to $\exp(-E_n/\kappa T)$. It follows that $(\beta = 1/\kappa T)$

$$S(k) = (\hbar k/2mc)\coth\tfrac{1}{2}\beta\hbar ck \qquad (66)$$

$$= (\beta mc^2)^{-1} + (\beta\hbar^2/12m)k^2 - \cdots. \qquad (66a)$$

From (66) there follows immediately the famous formula

$$\lim_{k\to 0}S(k) = \rho_0\kappa T\chi_T, \qquad (67)$$

where ρ_0 is the number density and χ_T the isothermal compressibility of the liquid. When $\hbar ck$ becomes greater than κT, (66) becomes essentially linear in k. Strictly speaking, however, $S(k)$ starts quadratically from a nonzero value except when $T=0$. The possibility of a linear behavior of $S(k)$ for small k, as predicted by (65) when $T=0$, has been sometimes questioned on the basis of (10). From (10) it follows that

$$S(k) - 1 = 4\pi\int_{0^+}^{\infty}[p(r) - \rho_0](kr)^{-1}\sin(kr)r^2dr. \qquad (68)$$

Since $p(r) - \rho_0$ approaches zero for large r, it is argued that it is legitimate to expand $(kr)^{-1}\sin kr$ as $1 - (kr)^2/6 + \cdots$. Integrating term by term, one finds

$$S(k) - 1 = C_1 + C_2 k^2 + \cdots, \qquad (68a)$$

where

$$C_1 = 4\pi\int_{0^+}^{\infty}[p(r) - \rho_0]r^2dr,$$

$$C_2 = -\tfrac{2}{3}\pi\int_{0^+}^{\infty}[p(r) - \rho_0]r^4dr.$$

Hence it appears that $S(k)$ always starts quadratically in k. The fallacy in the argument lies in the fact that $p(r)$ may not approach its asymptotic value fast enough, and the expansion may be meaningless. For example, if $p(r) - \rho_0$ decreases as r^{-3} for large r, (68) converges perfectly well but C_1 and C_2 are infinite. When $T=0$, $p(r) - \rho_0$ falls off slowly enough to invalidate the expansion, and (65) is correct; at any finite temperature $p(r) - \rho_0$ ultimately falls off exponentially and the expansion (68a) is legitimate. One might think that all the coefficients of (68a) can be determined by comparison with (66a); this is incorrect because (66) is wrong for large k. Using (67) and (68), however, we do obtain the important result

$$1 + 4\pi\int_{0^+}^{\infty}[p(r) - \rho_0]r^2dr = \rho_0\kappa T\chi_T, \qquad (69)$$

and when $T=0$

$$1 + 4\pi\int_{0^+}^{\infty}[p(r) - \rho_0]r^2dr = 0. \qquad (70)$$

The result (69) can also be obtained by rather simple classical arguments. It follows directly from the definition of $p(r)$ that the left side of (69) is $\langle(N - \bar{N})^2\rangle_{Av}/\bar{N}$, where N is the number of atoms in a large subvolume of the liquid, and the bar denotes "average," but statistical mechanics shows that $\langle(N - \bar{N})^2\rangle_{Av}/\bar{N} = \rho_0\kappa T\chi_T$, whence (69) follows.

One might think that (70) is a simple consequence of the definition of $p(r)$. For if an atom is known to be at $\mathbf{r}_1$, the probability that there is an atom at $\mathbf{r}_2$ is $\rho_2(\mathbf{r}_1,\mathbf{r}_2)/\rho_1(\mathbf{r}_1)$. If $\mathbf{r}_1$ is not near the surface of the liquid, then $\rho_1(\mathbf{r}_1) = \rho_0$; if $\mathbf{r}_1$ and $\mathbf{r}_2$ are both far from the surface, then $\rho_2(\mathbf{r}_1,\mathbf{r}_2) = \rho_0 p(r_{12})$. If we integrate $\rho_2(\mathbf{r}_1,\mathbf{r}_2)/\rho_1(\mathbf{r}_1)$ over all locations $\mathbf{r}_2$, excluding the point $\mathbf{r}_1$, the answer must be exactly $N - 1$. But if we integrate $\rho_1(\mathbf{r})$ over all positions of $\mathbf{r}$, the answer is exactly N. Consequently

$$\int_{\mathbf{r}_2\neq\mathbf{r}_1}[\rho_2(\mathbf{r}_1,\mathbf{r}_2)/\rho_1(\mathbf{r}_1) - \rho_1(\mathbf{r}_2)]d\mathbf{r}_2 = -1. \qquad (71)$$

If we take $\mathbf{r}_1$ far from the surface, $\rho_1(\mathbf{r}_1)$ can be replaced by ρ_0. Furthermore, the integrand is appreciable only when $\mathbf{r}_2$ is near $\mathbf{r}_1$, in which case $\rho_2(\mathbf{r}_1,\mathbf{r}_2)/\rho_1(\mathbf{r}_1) - \rho_1(\mathbf{r}_2) = p(r_{12}) - \rho_0$ (there are no complications at the surface of the liquid since the surface corrections to both terms of the integrand are identical). Then (71) reduces exactly to (70).

Something must be wrong with the preceding argument at finite temperatures, since (70) is false if $T\neq 0$. The difficulty lies in the fact that, at finite T, the limiting value of $\rho_2(\mathbf{r}_1,\mathbf{r}_2)/\rho_0$ for large $\mathbf{r}_{12}$ is not ρ_0, but is slightly lower by an amount of order $1/N$. Since $\mathbf{r}_2$ runs over a volume proportional to N, there is a finite negative contribution to (71) from the region of very large r_{12} (i.e., the region where $\rho_2(r_1,r_2)/\rho_0$ has reached its asymptotic value, which is not exactly equal to ρ_0). Since (71) is rigorously true, the integral

$$4\pi\int_{0^+}^{\infty}[p(r) - \rho_0]r^2dr,$$

which represents the contribution to the left side of (71) from the region where r_{12} is not very large, must be greater than -1; thus we arrive at (69) instead of (70).

The slight lowering of the density at infinity when an atom is known to be at the origin is not hard to understand, since the localization of one atom decreases by one the number of atoms eligible to occupy the site at infinity. In the classical perfect gas $\rho_0\kappa T\chi_T = 1$; since the atoms are independent, the localization of one atom simply lowers the mean density by $1/V$ throughout the rest of the volume. In a real liquid, however, $\rho_0\kappa T\chi_T\to 0$ as $T\to 0$. Finally, when $T=0$, (70) implies that no influence propagates to infinity, even in order $1/N$, when an atom is localized at the origin. In this case, a

density excess at the origin is surrounded by a rarefaction slightly further away, so that no change occurs in the density at infinity.

Thus, the simple counting argument used to prove (70) is actually correct when $T=0$, because there is no change in the density far away when we localize an atom at the origin. For the same reason, we believe that any identity based on a counting argument becomes correct when $T=0$. We therefore believe in the truth of the identity

$$\int_{\mathbf{r}_3 \neq \mathbf{r}_2, \mathbf{r}_1} d\mathbf{r}_3 \left[\frac{\rho_3(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3)}{\rho_0 p(r_{12})} - \rho_0 \right] = -2, \qquad (72)$$

although we cannot give a rigorous proof of it. Equations (70) and (72) are easily combined to give Eq. (39), which we have used in our work (one must remember that, in (39), ρ_3 is defined to include a delta function on $\mathbf{r}_{23}$).

Equation (39) is easily understood for small or large values of r_{12}. If $r_{12} < 2.4$ A, both sides of (39) are identically zero for all $\mathbf{r}_3$. If 1 and 2 are far apart, then ρ_3 can be written as

$$\rho_0 p_1(r_{31}) p_1(r_{32}) + \rho_0^2 \delta(\mathbf{r}_{32})$$

and the right side becomes $\rho_0^2 p_1(r_{31})$. If 3 is far from 2, then both sides are equal. Hence the only contribution to the integral comes when 3 is near 2; but then we can set $p_1(r_{31}) = \rho_0$ and we are left with

$$\int d\mathbf{r}_{32} \rho_0^2 [p_1(r_{32}) + \delta(\mathbf{r}_{32}) - \rho_0],$$

which vanishes as a result of (70).

Even if (39) is not rigorously true for intermediate values of r_{12}, it cannot fail badly; for when r_{12} is greater than 2.4 A, but not very large, then for any fixed radius r_{32} the solid angle in which 3 interferes with 1 is small (less than one-quarter of the total solid angle available to $\mathbf{r}_{23}$).