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Atomic Theory of the Two-Fluid Model of Liquid Helium

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It is argued that the wave function representing an excitation in liquid helium should be nearly of the form $\Sigma_i f(\mathbf{r}_i)\phi$, where ϕ is the ground-state wave function, $f(\mathbf{r})$ is some function of position, and the sum is taken over each atom i. In the variational principle this trial function minimizes the energy if $f(\mathbf{r})=\exp(i\mathbf{k}\cdot\mathbf{r})$, the energy value being $E(k)=\hbar^2k^2/2mS(k)$, where $S(k)$ is the structure factor of the liquid for neutron scattering. For small k, E rises linearly (phonons). For larger k, $S(k)$ has a maximum which makes a ring in the diffraction pattern and a minimum in the $E(k)$ *vs* k curve. Near the minimum, $E(k)$ behaves as $\Delta+\hbar^2(k-k_0)^2/2\mu$, which form Landau found agrees with the data on specific heat. The theoretical value of Δ is twice too high, however, indicating need of a better trial function.

Excitations near the minimum are shown to behave in all essential ways like the rotons postulated by Landau. The thermodynamic and hydrodynamic equations of the two-fluid model are discussed from this view. The view is not adequate to deal with the details of the λ transition and with problems of critical flow velocity.

In a dilute solution of He^3 atoms in He^4, the He^3 should move essentially as free particles but of higher effective mass. This mass is calculated, in an appendix, to be about six atomic mass units.

IN a previous paper,[1] II, a physical argument was given to interpret the fact that the excitations which constitute the normal fluid in the two-fluid theory of liquid helium were of two kinds. Those of lowest energy are longitudinal phonons. The main result of that paper was to give the physical reason for the fact that there can be no other excitations of low energy. It was shown that any others must have at least a minimum energy Δ. No quantitative argument was given to obtain this Δ nor to get an idea of the type of motion that such an excitation represents. In this paper we expect to determine Δ and the character of the excitations.

The physical arguments of II are carried a step further here to show that the wave function must be of a certain form. The form contains a function whose exact character is difficult to establish by intuitive arguments. However, the function can be determined, instead, from the variational principle as that function which minimizes the energy integral.

THE WAVE FUNCTION FOR EXCITED STATES

In II the exact character of the lowest excitation was not determined, but various possibilities were suggested. One is the rotation of a small ring of atoms. A second is the excitation of an atom in the local cage formed around it by its neighbors. Still a third is analogous to the motion of a single atom, with wave number k about $2\pi/a$, where a is the atomic spacing, the other atoms moving about to get out of the way in front and to close in behind. It is not clear that they are really distinct possibilities, for they might be merely different ways of describing roughly the same thing.

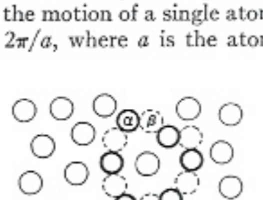

FIG. 1. Typical configuration of the atoms. If an excitation represents rotation of a ring of atoms such as the six in heavy outline the wave function must be plus if they are in the α positions and minus if they are moved to the intermediate β positions.

We shall now try to find the form of the wave function which we would expect under the assumption that one or another of these possibilities is correct. It will turn out that all of the alternatives suggest the same wave function, at least to within a function $f(\mathbf{r})$, of position $\mathbf{r}$, which is determined only vaguely.

First, suppose that the excitation is the rotation of a small ring of atoms. The number of atoms in the ring is determined, according to II, by the condition that it is the smallest ring that can be considered to be able to turn easily as an independent unit in view of the interatomic forces. For illustrative purposes we suppose this means that there are six atoms in the ring.

We can describe the wave function for this excitation by giving the amplitude associated with every configuration of the atoms. Suppose Fig. 1 represents a typical configuration, the six atoms of the ring in question (say ring A) being indicated by heavy outline. We discuss how the amplitude changes as we rotate this ring, leaving the other atoms out of account for a moment. Suppose the wave function is positive, say $+1$, if the atoms are in the position shown by the full circles in Fig. 1, which we arbitrarily call the α position. Suppose all the six atoms move around together, and let the ring turn about 60°. The atoms then appear again in α position, although which is which has been changed, so the wave function, by the Bose statistics, is still $+1$. On the other hand, for a 30° rotation, if the atoms are located as indicated in the figure by dotted circles (β position), the wave function will change to -1 for the first excited state. We need only discuss the real part of the wave function—the imaginary part, if any, can be dealt with in a similar way. (Actually since we deal with an eigenstate of the energy, the real part of

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[1] R. P. Feynman, Phys. Rev. 91, 1291, 1301 (1953), hereafter called I, II, respectively.

the wave function is an eigenfunction also.) For orientations intermediate between α, β the function is correspondingly intermediate between $+1$ and -1, but to simplify the remarks we describe it for just the configurations α, β. The wave function for excitation of this ring we call ψ_A. It is $+1$ if the A ring is at α, and -1 if at β, and does not depend on how other rings of atoms are oriented. We can describe this wave function as follows. Consider a function of position $\mathbf{r}$ in space, $f_A(\mathbf{r})$ which is $+1/6$ if $\mathbf{r}$ is at one of the six positions of the centers of the atoms for the α position of ring A, is $-1/6$ if it is at a β position, and is zero if $\mathbf{r}$ is at any other place in the liquid far from the A ring. Then consider the quantity $\sum_i f_A(\mathbf{r}_i)$ where the sum is taken over all the atoms, i, in the liquid. For a configuration of the liquid for which there are atoms at the six α positions the quantity is $+1$, while if six atoms are at β position, it is -1. This suggests that we can write $\psi_A = \sum_i f_A(\mathbf{r}_i)$.

Actually this is incomplete because it does not correctly describe what happens if atoms in other parts of the liquid move. If ring A is in the α position, we wish the complete wave function to be $+1$ as far as this is concerned, but to drop to zero if two atoms overlap in other parts of the liquid, etc., just as for the ground state. That is, we expect (disregarding normalization)

$$\psi_A = \sum_i f_A(\mathbf{r}_i)\phi, \tag{1}$$

where ϕ is the ground-state wave function, a function of all the coordinates. This takes care of another matter also. What happens if some atoms are on α and some on β? This should be of very small amplitude because we do not wish the atoms to overlap on account of the repulsions. This is not correctly described by $\sum_i f_A(\mathbf{r}_i)$, but the ϕ factor does guarantee such a behavior. It is small for such overlaps. Of course, if the ring contained many atoms it could readjust just a little and the ϕ would not prevent, for example, all those near one side of the ring being α, and those on the opposite side of the ring being β. We are not guaranteed that (1) will describe well the amplitude for such a configuration. In fact, it wouldn't be expected that a function of just one variable could describe the motion of several atoms. However, by the arguments of II the ring is supposed to be small, in fact, so small that one part of the ring cannot move independently of the rest. The ring is so small that if one atom is at α, there cannot be a large amplitude for finding atoms at β because of the interatomic repulsions. This is represented in (1) by the factor ϕ which falls if two atoms approach (see II for a full description of the properties of ϕ).

Not knowing the exact size and shape of the ring we cannot say what the exact function $f_A(\mathbf{r})$ should be. But at least we conclude in this case the excited-state wave function is of the form

$$\psi = \sum_i f(\mathbf{r}_i)\phi, \tag{2}$$

where $f(\mathbf{r})$ is *some* function of position.

We might try to improve (1) by noting that, of course, the energy should be essentially the same if the excited ring were somewhere else in the liquid, say at B. The function

$$\psi_B = \sum_i f_B(\mathbf{r}_i)\phi \tag{3}$$

would describe this if $f_B(\mathbf{r})$ is $+1/6$ for $\mathbf{r}$ at some one of the six α positions of some other ring B, and $-1/6$ for intermediate β positions, and zero elsewhere. Or we could locate the ring at still another position, etc. Any one atom might be thought of as belonging to more than one ring. This produces a kind of interaction between adjacent rings. Because of this interaction, a better wave function than (1) might be some linear combination of these possibilities, say $c_A\psi_A + c_B\psi_B + \cdots$. But we can still conclude that the form of the wave function is given by (2), but now, with the function $f(\mathbf{r}) = c_A f_A(\mathbf{r}) + c_B f_B(\mathbf{r}) + \cdots$, for any linear combination of functions of the form (2) is still of this form.

If the lowest excited state which we seek were something like the excitation of a single atom in a cage formed from its neighbors we would guess the wave function to be of the form (2) also. Because there would be a nodal plane across the cage, and we would take $f(\mathbf{r})$ to be positive if $\mathbf{r}$ is in the cage on one side of the plane, and negative if on the other, and to fall off to zero if $\mathbf{r}$ goes outside the cage. We do not care which atom is in the cage so the sum on i is taken over all atoms. Those which are outside the cage contribute nothing to the sum, because $f(\mathbf{r})$ is zero there. Further, there is no appreciable amplitude for there being more than one atom in the cage, because of the action of the factor ϕ which is very small if the atoms penetrate each other's mutual potential. The ϕ also takes care of the fact that the atoms in remote parts of the liquid behave independently of what the excited atom is doing, and act just as in the ground state. Further, linear combinations, representing the alternatives that the excited cage may be located at different places in the liquid, are still of the form (2).

The third possibility was only crudely described in II. It was noted that if the atoms were considered as roughly confined to cells, then a wave function representing the motion of an atom A could be $\exp(i\mathbf{k}\cdot\mathbf{r}_A)$, where $\mathbf{r}_A$ is the position of A, and it is assumed that as A moves about, the other atoms move around to make way for it so that the density is maintained roughly uniform. This would correspond in the liquid to a wave function

$$\exp(i\mathbf{k}\cdot\mathbf{r}_A)\phi, \tag{4}$$

where ϕ is the ground-state wave functions of all the atoms including A. The factor ϕ does the equivalent of keeping the atoms in cells so that the density is nearly uniform no matter where $\mathbf{r}_A$ is. For small $\mathbf{k}$ this is a possibility only if atom A is different from the others and does not obey the Bose statistics. If the symmetry is taken into account then we must replace this by the symmetrical sum

$$\sum_i \exp(i\mathbf{k}\cdot\mathbf{r}_i)\phi. \tag{5}$$

If ϕ had no large scale density fluctuations this would be no wave function at all, because there would be just as many atoms in the region where $\exp(i\mathbf{k}\cdot\mathbf{r})$ is positive as where it is negative and the sum cancels out.[2] This is in concert with the idea that the wave function cannot depend on where atom A is on a large scale. For if A moves a long distance and the others readjust to keep the density uniform, on a large scale (the scale $1/k$ for small k), the result is just equivalent to the interchange of atoms and the wave function cannot change as a consequence of the Bose symmetry. On the other hand, if while the atom moves from one position to that of its neighbor the wave function changes sign and returns, then (5) may be allowed. That is, something like (5) with k of order $2\pi/a$ may be a possibility. This again is of the form (2), but with $f(\mathbf{r})=\exp(i\mathbf{k}\cdot\mathbf{r})$. The argument just given for this alternative is admittedly not as complete as for the others, mainly because the original idea of what the state is, was based on such a crude model of atoms in cells. Insofar as the idea can be carried over to the case of the true liquid perhaps we can say the form (5), or (2) will represent it.

Since all the examples have led to the same form, we might expect that a more general argument could be made for the validity of (2). This is, in fact, possible starting from the general argument given in II to show why the excited states, other than phonons, can be expected to have an excitation. It was pointed out there that the excited-state function ψ must be orthogonal to the ground state. For some configuration, say α, of the atoms it acquires its maximum positive value. Then it will be negative for some other, say β, which represents some stirring from the α configuration without change of large scale density (to avoid phonon states). But stirring reproduces a configuration nearly like α although with some atoms interchanged. Thus it is hard to get the configuration β to be very far (in configuration space) from α to keep the gradient of ψ small in going from α to β.

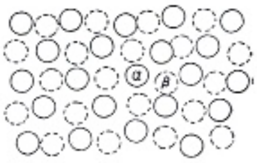

FIG. 2. In general the lowest excitation energy results if the configuration of atoms (solid circles) for which the wave function is most positive is as far as possible from that (dotted circles, β) for which it is most negative. All the β positions must be as far as possible from α positions, therefore.

The lowest state would have the β configuration as far as possible from α. This means that in β as many atoms as possible are moved from sites (call them α positions) occupied by atoms in α. Hence β must be a configuration in which the atoms occupy sites (β positions) which are placed as well as possible between the α positions. (See Fig. 2.) In all these configurations, of course, the gross density must be kept uniform and the atoms should be kept from overlapping, to avoid high potential energy terms. If all atoms are on α positions ψ is maximum positive, and if all on β, maximum negative. The transition is made as smoothly as possible, and the kinetic energy thereby kept down, if for other configurations the amplitude is taken to be just the number of atoms on α positions minus the number on β positions. The number is just $\sum_i f(\mathbf{r}_i)$ where $f(\mathbf{r})$ is a function which is $+1$ if $\mathbf{r}$ is at an α position, and -1 if at a β position (and varies smoothly in between these limits as $\mathbf{r}$ moves about). It is of course a modulation to be taken on ϕ, because we wish to give small amplitude to configurations in which atoms overlap, etc., just as in the ground state. We are led, therefore, to (2). We can add the information that $f(\mathbf{r})$ must vary rapidly from plus to minus in distances of half an atomic spacing. That is, we expect that $f(\mathbf{r})$ will consist predominently of Fourier components of wave number $\mathbf{k}$ of absolute magnitude $k=2\pi/a$.

In the above argument it is not self-evident that in going from the configuration of all atoms at α positions to that of all at β, the amplitude must be just linear in the number on α, N_α minus the number of β, N_β. Perhaps some other smooth function of this number, like $\sin[\pi(N_\alpha-N_\beta)/2N]$ might be better. However, for the majority of possible configurations N_α and N_β are nearly equal; in fact, for almost all, $(N_\alpha-N_\beta)/N$ is of order $\pm N^{-\frac{1}{2}}$. For such a small range of the variable, the function, whatever it is, ought to behave nearly linearly. If the wave function (2) is wrong for a very few special configurations it will not be important as we shall determine the energies by the variational method, and the special configurations will contribute only a small amount to the integrals because of their small share of the volume in configuration space.

THE EXCITATION ENERGY

We have concluded that a function of the form (2) should be a good approximation to the wave function of the excited state.[2a] The function $f(\mathbf{r})$ is known only imperfectly, however. We shall determine this function $f(\mathbf{r})$ by using the variational principle. The Hamiltonian of the system is

$$H=-(\hbar^2/2m)\textstyle\sum_i\nabla^2_i+V-E_0, \tag{6}$$

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[2] We shall see later that (5), for small $\mathbf{k}$, is actually a satisfactory wave function because ϕ does have the long wave density variations of the zero point motion of the sound field. We are trying to get excited states orthogonal to phonon states, and (5) for small $\mathbf{k}$ is not orthogonal. It is, in fact, just the wave function for such a phonon state. This is discussed later.

[2a] Wave functions of this form have been proposed before, for example by A. Bijl, Physica 7, 869 (1940). However, an argument establishing their validity for large $\mathbf{k}$ has been lacking, and it has not been clear that functions of other forms might not give much lower states.

where V is the potential energy of the system, and we measure energies above the ground-state energy E_0, so E_0 is subtracted in (6). Therefore the ground-state wave function satisfies

$$H\phi=0. \tag{7}$$

If we write

$$\psi=F\phi, \tag{8}$$

where F is a function of all the coordinates, then we can verify, using (7), that

$$H\psi=H(F\phi)=-(\hbar^2/2m)\sum_i(\phi\nabla^2{}_iF+2\nabla_i\phi\cdot\nabla_iF)=\phi^{-1}(-\hbar^2/2m)\sum_i\nabla_i\cdot(\rho_N\nabla_iF), \tag{9}$$

where $\rho_N(\mathbf{r}^N)=\phi^2$ is the density function for the ground state, that is, the probability of finding the configuration $\mathbf{r}^N$ (we use $\mathbf{r}^N$ to denote the set of coordinates $\mathbf{r}_i$ of all the atoms, and $\int\cdots d^N\mathbf{r}$ to represent the integral over all of them).

The energy values come from minimizing the integral, (note ϕ is real)

$$\mathcal{E}=\int\psi^*H\psi d^N\mathbf{r}=(\hbar^2/2m)\sum_i\int(\nabla_iF^*)\cdot(\nabla_iF)\rho_Nd^N\mathbf{r}, \tag{10}$$

subject to the condition that the normalization integral,

$$\mathcal{I}=\int\psi^*\psi d^N\mathbf{r}=\int F^*F\rho_Nd^N\mathbf{r}, \tag{11}$$

is fixed. The energy is then $E=\mathcal{E}/\mathcal{I}$.

In these expressions we must substitute

$$F=\sum_if(\mathbf{r}_i). \tag{12}$$

Consider the normalization integral first. It is

$$\mathcal{I}=\sum_i\sum_j\int f^*(\mathbf{r}_j)f(\mathbf{r}_i)\rho_Nd^N\mathbf{r}.$$

For a fixed i and j we can integrate first over all of the other atomic coordinates. This integral on ρ_N gives the probability for finding the ith atom at $\mathbf{r}_i$ and the jth at $\mathbf{r}_j$; therefore

$$\mathcal{I}=\int f^*(\mathbf{r}_1)f(\mathbf{r}_2)\rho_2(\mathbf{r}_1,\mathbf{r}_2)d^3\mathbf{r}_1d^3\mathbf{r}_2, \tag{13}$$

where ρ_2 is the probability of finding an atom at $\mathbf{r}_1$ per cm^3, and at $\mathbf{r}_2$ per cm^3. These density functions can be defined in general by

$$\rho_k(\mathbf{r}_1',\mathbf{r}_2'\cdots\mathbf{r}_k')=\sum_i\sum_j\cdots\sum_n\int\delta(\mathbf{r}_i-\mathbf{r}_1')\times\delta(\mathbf{r}_j-\mathbf{r}_2')\cdots\delta(\mathbf{r}_n-\mathbf{r}_k')\rho_N(\mathbf{r}^N)d^N\mathbf{r}. \tag{14}$$

For example, $\rho_1(\mathbf{r})$ is simply the chance of finding an atom at $\mathbf{r}_1'$, for the liquid in the ground state. This is independent of $\mathbf{r}$ and is the number density ρ_0 in the ground state. In the same way $\rho_2(\mathbf{r}_1,\mathbf{r}_2)$ can be written as $\rho_0p(\mathbf{r}_1-\mathbf{r}_2)$ where p is the probability of finding an atom at $\mathbf{r}_2$ per unit volume if one is known to be at $\mathbf{r}_1$. Except near the liquid surface it is a function of only the distance from $\mathbf{r}_1$ to $\mathbf{r}_2$, so (13) is

$$\mathcal{I}=\rho_0\int f^*(\mathbf{r}_1)f(\mathbf{r}_2)p(\mathbf{r}_1-\mathbf{r}_2)d^3\mathbf{r}_1d^3\mathbf{r}_2. \tag{15}$$

The energy integral (10), with the substitution (12) becomes

$$\mathcal{E}=(\hbar^2/2m)\sum_i\int\nabla_if^*(\mathbf{r}_i)\cdot\nabla_if(\mathbf{r}_i)\rho_Nd^N\mathbf{r}.$$

The integral of ρ_N over all atomic coordinates except $\mathbf{r}_i$ gives a result involving only $\rho_1(\mathbf{r}_i)=\rho_0$. Therefore we have simply

$$\mathcal{E}=\rho_0(\hbar^2/2m)\int\nabla f^*(\mathbf{r})\cdot\nabla f(\mathbf{r})d^3\mathbf{r}. \tag{16}$$

The best choice of f is that which minimizes the ratio of (16) to (15). The variation with respect to f^* gives the equation

$$E\int p(\mathbf{r}_1-\mathbf{r}_2)f(\mathbf{r}_2)d^3\mathbf{r}_2=-(\hbar^2/2m)\nabla^2f(\mathbf{r}_1),$$

where the energy E is $\mathcal{E}/\mathcal{I}$. This has the solution

$$f(\mathbf{r})=\exp i(\mathbf{k}\cdot\mathbf{r}), \tag{17}$$

with the energy value

$$E(\mathbf{k})=\hbar^2k^2/2mS(\mathbf{k}), \tag{18}$$

where $S(\mathbf{k})$ is the Fourier transform of the correlation function,

$$S(\mathbf{k})=\int p(\mathbf{r})\exp(i\mathbf{k}\cdot\mathbf{r})d^3\mathbf{r}. \tag{19}$$

It is a function only of k, the magnitude of $\mathbf{k}$.

It is readily verified that the solution is orthogonal to the ground state if we exclude $\mathbf{k}=0$. In fact, the solutions for different values of $\mathbf{k}$ are orthogonal to each other. This is because they all belong to different eigenvalues, $\hbar\mathbf{k}$, of the total momentum operator

$$\mathbf{P}=(\hbar/i)\sum_i\nabla_i,$$

as is directly verified from (2) with (17), taking $\mathbf{P}\phi=0$ since the ground state has zero total momentum.[3] Since

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[3] The argument is not rigorous because the momentum of the entire liquid can be changed without appreciable energy change by moving the center of gravity. This multiplies the wave function by a factor like $\exp(-i\hbar\mathbf{k}N^{-1}\cdot\sum_i\mathbf{r}_i)$. This function is so different from (2), however, that the orthogonality is probably not destroyed.

this operator commutes with the Hamiltonian, we have in (18) an upper limit to the energy for each value of k. (In fact, we could have obtained (17) from (2) by this argument.) Since we expect that (2) is a good wave function for functions f which vary from plus to minus in a distance of order $a/2$, we expect that (18) is not only an upper limit, but also a good estimate of the energy in a range of k's in the neighborhood of $k=2\pi/a$. In fact, our arguments suggest that $E(\mathbf{k})$ should have a minimum as a function of k in that region. These expectations are verified in the next section.

DISCUSSION OF THE ENERGY SPECTRUM

To find the consequences of (18) we shall have to discuss the behavior of $S(k)$ defined in (19).

The function $p(\mathbf{r}_1-\mathbf{r}_2)$ gives the probability per unit volume that a particle is at $\mathbf{r}_2$ if one is known to be at $\mathbf{r}_1$. If $\mathbf{r}_2$ is close to $\mathbf{r}_1$ it is zero, for the atoms cannot overlap. On the other hand, if $\mathbf{r}_2$ coincides with $\mathbf{r}_1$ there is an atom there, so p contains a delta function $\delta(\mathbf{r}_1-\mathbf{r}_2)$. For large r_2 it approaches ρ_0. Since the structure of the liquid ought to be more or less like that in a classical fluid, as r increases from zero, $p(r)$ probably rises to a maximum at the nearest neighbor spacing, falls, then rises again to a lower and wider maximum for next nearest, and with rapidly decreasing smaller oscillations approaches unity.[4] The integral $\int(p(\mathbf{r})-1)d^3\mathbf{r}$ vanishes since the integral of $\rho_2(\mathbf{r}_1,\mathbf{r}_2)$ with respect to $\mathbf{r}_2$ is exactly ρ_1 times the number of atoms $N=\rho_0 V$.

The Fourier transform function $S(k)$ is just the liquid structure factor which determines the scattering of neutrons (or x-rays, after multiplication by the atomic structure factor) by the liquid at absolute zero. It is therefore a quantity which can be directly determined experimentally. For large k it approaches 1 because of the delta function in $p(\mathbf{r})$. It has a delta function at $\mathbf{k}=0$, but this value of k is not of interest to us in (18), because the wave function ψ must be orthogonal to the ground state. The behavior at small k depends on the variations of $p(r)$ over long distances, that is, on long wavelength density fluctuations. These are the zero point fluctuations of the sound field in the ground state, since for wavelengths longer than the atomic spacing the approximation of a continuous sound field is good. This may be analyzed as follows. The operator representing the density at a point $\mathbf{r}$ is

$$\rho(\mathbf{r})=\sum_i\delta(\mathbf{r}-\mathbf{r}_i). \qquad (20)$$

Its Fourier transform is

$$q_{\mathbf{k}}=\int\rho(\mathbf{r})\exp(i\mathbf{k}\cdot\mathbf{r})d^3\mathbf{r}=\sum_i\exp(i\mathbf{k}\cdot\mathbf{r}_i). \qquad (21)$$

Evidently, the $S(\mathbf{k})$ is the expected value of $|q_{\mathbf{k}}|^2$ in the ground state. For long wave sound $q_{\mathbf{k}}$ is just the coordinate of the normal mode, so its mean square can be easily determined, for example, by noting that the mean potential energy is half of the ground-state energy $\frac{1}{2}\hbar\omega$. In this way one finds $S(\mathbf{k})=\hbar k/2mc$ for small k, where c is the velocity of sound.

The behavior of $S(\mathbf{k})$ for intermediate k is familiar to us from the x-ray studies of classical liquids. The density distribution in the ground state is roughly similar to such a liquid. There is some local structure produced by the tendency of the atoms to stay apart. This quasi-crystalline local order makes a maximum in the $S(k)$ curve for k near $2\pi/a$. There may be smaller subsidiary maxima for near multiples of this k. For helium, because of the large zero point motion, these maxima may be broader and less marked than in other liquids. The main maximum is responsible for the main ring in the x-ray diffraction pattern. It is shown clearly in the preliminary neutron diffraction data reported by Henshaw and Hurst.[5]

To summarize: with rising k, $S(k)$ starts linearly as $\hbar k/2mc$, rises then to a maximum near $k=2\pi/a$, and falls again to approach, with possible minor oscillations, the limit unity. Consequently the quantity $E(k)=\hbar^2k^2/2mS(k)$ should start linearly as $\hbar kc$, but should then show a dip with a minimum at $k=k_0$ say, near $2\pi/a$, finally rising, eventually as $\hbar k^2/2m$. These relations are shown in Fig. 3.

We have argued that (2) should be a good approximation to the wave function for functions that contain wave numbers in the vicinity of $2\pi/a$. Therefore we can expect the energy values (18) to be good in the neighborhood of this wave number. It is gratifying to see that there is a minimum in this region. The minimum value we shall call Δ. Ordinarily the variational method only permits one to interpret the minimum value of E as one varies a parameter such as k. On the other hand, in our case each value of k has significance since these values correspond to different eigenvalues of the momentum operator, as has been remarked. Therefore we can believe the behavior of the curve through a range of k near k_0, where it behaves parabolically, so we can write $E(k)$ in Landau's form $\Delta+\hbar^2(k-k_0)^2/2\mu$ where μ is a constant determining the curvature.

It is at first disconcerting that values of the energy lower than Δ can be obtained by going to very small values of k. But the energy here varies as $\hbar kc$, just that expected for phonon excitation. In fact, a moment's reflection shows that, for small k, the wave function (2) is just that which represents phonon excitation. Excitation of a given phonon means that the harmonic oscillator representing the corresponding normal mode is in the first excited state. The wave function is therefore $q_{\mathbf{k}}\phi$, if $q_{\mathbf{k}}$ is the normal coordinate of the mode excited. This coordinate is the Fourier transform of the density, so (21) shows that (2) with (17) represents a phonon for small k. Since the wave function is correct the energy must be exact, and is therefore $\hbar kc$.

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[4] J. Reekie and T. S. Hutchison, Phys. Rev. **92**, 827 (1953), have determined $p(r)$ by x-ray scattering.

[5] D. G. Henshaw and D.G. Hurst, Phys. Rev. **91**, 1222 (1953).

Although we have made an argument only to show that (2) should be valid for high k, we see now that it is also valid for small k, that is for $f(\mathbf{r})$ which vary slowly. Since the energy curve is valid for the smaller k and for a range about $2\pi/a$, we can accept it as reasonable for all k from zero up to and slightly beyond the minimum.

On the other hand, for still larger k, another state of lower energy exists with the same total momentum. It is the state of double excitation, one of $\mathbf{k}_1$, the other of $\mathbf{k}_2$, such that $\mathbf{k}_1+\mathbf{k}_2=\mathbf{k}$ and still $E(\mathbf{k}_1)+E(\mathbf{k}_2)<E(\mathbf{k})$. This becomes possible for k so high that the slope dE/dk of the energy curve exceeds $\hbar c$, the initial slope. The curve for very large k, therefore, does not have the same validity as that for lower k, but we need not enter into this matter, because at temperatures of a few degrees such high-energy states would not be appreciably excited. Such questions may be of importance in discussing nonequilibrium phenomena. One process by which the number of excitations can change is for an excitation to pick up enough momentum that it can divide spontaneously into two.

It is easy to misinterpret the meaning of the wave function

$$\psi=\sum_i \exp(i\mathbf{k}\cdot\mathbf{r}_i)\phi, \tag{22}$$

so a few remarks might be appropriate here. It looks at first, on inspection of the first factor, that this represents the excitation of a single particle. This is correct at very high $k(ka\gg 2\pi)$ and it is also correct for the ideal gas case for which the atoms do not interact (ϕ is constant then). But our arguments for intermediate k show that this is not the case. Because of the correlations in position implied by the factor ϕ, the motion of one atom implies the motion of others. Thus the factor in front of ϕ selects from that function certain correlated motions, in spite of the fact that each term in the factor depends on just one variable.

We can get a better idea of how this works by taking the extreme case of very low k. Here (22) represents a sound wave but at first sight there is no sign of the density variations that such a wave usually brings to mind. Let us take the real part and consider

$$\sum_i \cos(\mathbf{k}\cdot\mathbf{r}_i)\phi \tag{23}$$

for small k. Now, for most configurations, allowed by ϕ, the atoms are fairly uniformly distributed, so that there are just as many in the regions where the cosine is positive, as where it is negative. Therefore the sum over all the atoms of $\cos(\mathbf{k}\cdot\mathbf{r}_i)$ is zero. The wave function is zero for nearly all configurations. It is only for the rare configurations in which the number in positive regions exceeds that in regions where the cosine is negative that the wave function does not vanish. In this way (23) selects configurations for which the mean density varies as $\cos(\mathbf{k}\cdot\mathbf{r})$. Since such density fluctuations are, according to the behavior of ϕ, most likely produced by small cooperative motions of large numbers of atoms, the state described is very far from the one particle state it would be if the cosine factor appeared alone, not multiplied by ϕ.

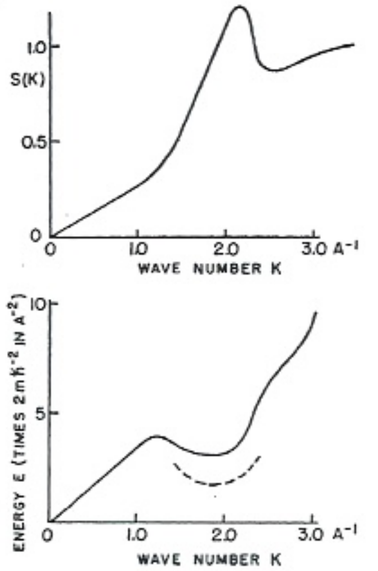

FIG. 3. The upper curve gives the liquid structure factor determined from neutron diffraction (reference 5) and extrapolated to zero k. The lower curve gives the energy spectrum of excitations as a function of wave number (momentum $\cdot\hbar^{-1}$) which results from the formula $E=\hbar^2k^2/2mS(k)$ derived in the text. The initial linear portion represents excitation of phonons while excitations near the minimum of the curve, where it behaves as $\Delta+\hbar^2(k-k_0)^2/2\mu$, correspond to Landau's rotons. However, data on the specific heat indicate that the theoretical curve should lie lower, closer to the dashed curve.

In the region of the energy minimum at k_0 the wave function represents a situation intermediate between the cooperative motion of phonons, and the excitation of a single particle. Several atoms move together because of the correlations implied by ϕ. It is hard to make a clear picture out of this vague idea. There is nothing to indicate that the state carries an intrinsic angular momentum. One must be careful because the state is degenerate, as all directions of k with the same magnitude k_0 give the same energy Δ. Perhaps, if more complicated wave functions were tried, some special linear combination representing a kind of microscopic vortex ring or one with intrinsic angular momentum has in fact a lower energy. States of low k will be called phonons, and states of momentum near k_0 will be called rotons in this paper, in accordance with the terminology of Landau,[6] although we do not necessarily mean to imply that rotons carry intrinsic angular momentum or represent vortex motion.

MULTIPLE EXCITATION

We have obtained the energy spectrum $E(k)$ of what we may call single excitations. They have the form of

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[6] L. Landau, J. Phys. U.S.S.R. **5**, 71 (1941); **8**, 1 (1941). See also R. B. Dingle, Supplement to Phil. Mag. **1**, 112 (1952).

plane waves through the liquid. By taking linear combinations we can make wave packets that are more or less confined to a local region. Unless the region is very small there would be only a negligible energy addition required to do this. The remainder of the liquid is quiet as in the ground state. It is conceivable that another packet could be located somewhere far away and the energy would be close to $E(\mathbf{k}_1)+E(\mathbf{k}_2)$ if $\mathbf{k}_1$ and $\mathbf{k}_2$ are the momenta of the majority of the waves in each packet. Thus we should expect states with several excitations, the energy being the sum of the energies of each packet separately. This neglects a kind of interaction energy between them. It will be valid if the density of excitations is very small, but one cannot expect to apply it to situations in which the number of excitations is any appreciable fraction of the number of atoms in the liquid.

Mathematically, if the function

$$F=\sum_i \exp i\mathbf{k}_1\cdot\mathbf{r}_i$$

gives $E(k_1)$ for the energy, we might expect the wave function for two excitations to correspond to $\psi=F\phi$, with

$$F=[\sum_i \exp(i\mathbf{k}_1\cdot\mathbf{r}_i)][\sum_j \exp(i\mathbf{k}_2\cdot\mathbf{r}_j)]. \qquad (24)$$

It is readily verified, by substitution into the variation integral, that the energy is $E(\mathbf{k}_1)+E(\mathbf{k}_2)$ within correction terms of order $1/V$, where V is the volume of the entire fluid. This is just what one would expect if the excitations behaved like interacting particles, for the relative probability of their being within their range of interaction varies inversely as the volume. The expression (24) is unaltered on reversing the order of the factors, so the state in which the first excitation has momentum $\mathbf{k}_1$ and the second has $\mathbf{k}_2$ is the same as that in which the momenta are reversed. Thus the excitations obey Bose statistics. The expression (24) is not orthogonal to (17) with $\mathbf{k}=\mathbf{k}_1+\mathbf{k}_2$, so there undoubtedly are matrix elements between states of different numbers of excitations, and collisions must be possible which change this number. In summary, the excitations behave much like interacting Bose particles which may be created and destroyed, and whose energy as a function of momentum is given by $E(k)=\hbar^2k^2/2mS(k)$.

THERMODYNAMIC PROPERTIES OF HELIUM II

From this we may determine the thermodynamic behavior of liquid helium at low temperature. At sufficiently low temperatures the number of excitations will be small, so the interactions between them can be neglected. The approximation of independence leads in the usual way to the formula for the Gibbs free energy (taking the ground-state energy as zero),

$$F=kTV\int \ln[1-\exp(-\beta E[\mathbf{k}])]d^3\mathbf{k}(2\pi)^{-3}, \qquad (25)$$

with $\beta=1/kT$. The number of excitations of momentum $\mathbf{k}$ is

$$n_{\mathbf{k}}=[\exp\beta E(\mathbf{k})-1]^{-1}. \qquad (26)$$

We need not enter into further details as this has been thoroughly analyzed by Landau,[6] who first proposed the form of energy spectrum we have deduced here. At low temperatures only the lowest energy excitations can become excited. That is, only the phonons are excited and the specific heat varies as T^3. At higher temperatures some of the states near the minimum of the curve, at k_0 become excited. The specific heat then rises rapidly, controlled predominantly by the $\exp(-\beta\Delta)$ factor, governing the number of rotons excited. For temperatures of a few degrees few rotons are excited and only the phonon part, and the part of the curve near the minimum, are important. Landau[7] has shown that one obtains good agreement with the specific heat (and with the measured values of the velocity of second sound) if one chooses the parameters $\Delta=9.6$°K, $k_0=1.95$ A^{-1}, and $\mu=0.77$. This means the energy curve near the minimum behaves as $2mE/\hbar^2=1.6+1.3(k-1.95)^2$, with k in reciprocal angstroms (one A^{-2} corresponds to a temperature of 6°K). In the phonon region the curve is

$$2mE/\hbar^2=2.6k,$$

in the same units, if the speed of sound is 240 meters/sec. Henshaw and Hurst[5] have published some preliminary data on the neutron scattering by liquid helium at 4.2°K. From it $S(k)$ may be directly determined (see Fig. 3). The curve for $E(k)$ calculated in this way behaves as

$$2mE/\hbar^2=3.0+1.0(k-2.0)^2$$

near the minimum (and is consistent with $2.6k$ for small k). This corresponds to a value of Δ of 18° which is impossibly large. Such a discrepancy may be due to the inaccuracy of the trial function (2), the true energy being lower than that calculated with this trial function. Such a large discrepancy in energy is discouraging, because the physical arguments did seem to indicate that (2) should be a reasonably good first approximation.

The expression (25) should not hold at high temperature because it neglects the interactions among the large number of excitations which (26) demands at such a temperature. Without an estimate of these interactions it is hard to judge the region in which deviations are to be expected. We shall make a very rough preliminary argument here.

To the approximation that the energy in a mode is proportional to an integer n, this mode behaves like a harmonic oscillator. The coordinate of this oscillator $q_{\mathbf{k}}$ has a mean square value $2n+1$ times its value in the ground state. For what size $q_{\mathbf{k}}$ is the harmonic oscillator approximation poor? If we knew this we could put a limit on the ranges of $q_{\mathbf{k}}$ and hence of $n_{\mathbf{k}}$, for which (25) might be expected to be valid. In our case the various $q_{\mathbf{k}}$ from (21) are not independent, because they can all be defined in terms of the same $3N$ variables $\mathbf{r}_i$.

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[7] L. Landau, J. Phys. U.S.S.R. **11**, 91 (1947); Phys. Rev. **75**, 884 (1949).

Thus, for example, if $q_{\mathbf{k}}$ is known for $3N$ values of $\mathbf{k}$, it is known in principle for all others. It is very difficult to see what this interdependence means to (25).

But one can notice that one restriction is

$$\int |q_{\mathbf{k}}|^2 d^3\mathbf{k}(2\pi)^{-3}=N, \tag{27}$$

where the integral is taken over all $\mathbf{k}$. Hence we may guess that we should restrict (25) by the condition that the excess $|q_{\mathbf{k}}|^2$ over that for the ground state, summed on all states, cannot exceed N. This excess for a given mode is $2n_{\mathbf{k}}$ times the ground-state mean value of $|q_{\mathbf{k}}|^2$. This latter is $S(k)=\hbar^2k^2/2mE(k)$, so we obtain the restriction

$$\hbar^2m^{-1}\int (k^2/E(k))n_{\mathbf{k}}d^3\mathbf{k}(2\pi)^{-3}=1. \tag{28}$$

The thermodynamics which would result (by adding a chemical potential μ to $E(k)$ in (25), (26) to allow for (28)) will show a second-order transition.[8] But without a deeper analysis we are in no position to take Eq. (28) literally. We can only use it as a rough criterion for validity of (25). If the integral on the left is much less than 1, then (25) should hold. At 2°K the integral amounts to roughly 0.2, so perhaps we are entitled to trust (25) even to within a few tenths of a degree of the transition temperature.

MOTION OF THE FLUID AS A WHOLE

The existence of such excitations moving as nearly free particles in a background fluid is the central concept of the two-fluid model of Tisza[9] and Landau. The consequences of these ideas for excitations with a spectrum such as (18) have been carefully analyzed in a general manner by Landau and Dingle.[6] There is nothing to add that is new in this direction. However, we shall review briefly how the equations of this model arise, emphasizing the behavior of the wave function.

Beside the states which represent local internal excitation of part of the fluid, there are, of course, states in which the entire body of fluid moves. In general, in these cases the boundaries of the fluid move also. For example, at absolute zero, the entire fluid may move as a body with velocity $\mathbf{v}$. This center-of-gravity motion is described by

$$\psi=\exp(im\mathbf{v}\cdot\textstyle\sum_i\mathbf{r}_i)\phi,$$

if we assume ϕ corresponds to the ground state at rest in the laboratory system.

Suppose we wish to represent a situation in which the velocity $\mathbf{v}(\mathbf{r})$ varies from point to point, but only very gradually on an atomic scale. We might try something like this. The atoms in a region about some point P have their center of gravity moving at velocity $\mathbf{v}_P$ corresponding to this point. They must contribute a phase $m\mathbf{v}_P\cdot\sum_i\mathbf{r}_i$ where the sum is taken only over those near P. Corresponding contributions would come from sums near other points so the total factor ought to be $\exp[im\sum_i\mathbf{v}(\mathbf{r}_i)\cdot\mathbf{r}_i]$. The wave function is, therefore, of the form

$$\psi=\exp[i\textstyle\sum_i s(\mathbf{r}_i)]\phi, \tag{29}$$

where $s(\mathbf{r})$ is some function of position. We have suggested that it is $m\mathbf{v}(\mathbf{r})\cdot\mathbf{r}$. However, as is usual when one has waves whose wavelength varies from point to point, the wave number is not the phase divided by r, but more accurately it is the gradient of the phase. Therefore (29) represents the fluid in motion, the velocity at any point being given by

$$\mathbf{v}(\mathbf{r})=m^{-1}\nabla s. \tag{30}$$

As a consequence of (31), $\nabla\times\mathbf{v}=0$. Velocity fields for which this is not true cannot be represented in such a simple manner, and represent, as we have seen in II, states involving large numbers of excitations. The problem they present is being studied. For regions which are not simply connected, such as a torus, s need not be single-valued. For example, in the torus we could take $s=\phi$, the cylindrical angle. This would represent a permanent circulation[10] even though $\nabla\times\mathbf{v}=0$ locally.

Substitution of (29) into the variational principle to obtain a steady-state solution leads [see (10), (11) with $F=\exp(i\sum_i s(r_i))$] to the energy expression

$$\frac{\rho_0}{2m}\int \nabla s(\mathbf{r})\cdot\nabla s(\mathbf{r})d^3\mathbf{r}, \tag{31}$$

which is the kinetic energy $\rho_0 m v^2/2$ per unit volume. It is minimum for variations in s if $\nabla\cdot(\nabla s)=0$, that is, $\nabla\cdot\mathbf{v}=0$. The flow must be incompressible. We have not allowed, in (29), for variations in density. For a singly connected region this has but one solution $\mathbf{v}=0$, unless the boundaries move. In a multiply connected region, like a ring, circulation of angular momentum in multiples of $N\hbar$ is possible. There are so few of these special states that the statistical mechanics is not affected. The variables, $\mathbf{v}(\mathbf{r})$, representing such motions can be specified as external known variables like pressure and volume.

EXCITATIONS IN A MOVING FLUID

Next we study the motion and energy of an excitation in a moving fluid. The wave function is

$$\psi=\textstyle\sum_i f(\mathbf{r}_i)\exp[i\sum_j s(\mathbf{r}_j)]\phi.$$

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[8] This conclusion is modified if the interaction of the rotons and the hydrodynamic modes is taken into account.

[9] L. Tisza, Phys. Rev. **72**, 838 (1947).

[10] It was suggested in II, reference 9, that to observe this experimentally one might have to avoid letting the liquid have a free surface. But R. Peirels has pointed out (private discussion) that although the atoms evaporating from the moving liquid to the gas carry angular momentum out, only those of the gas which are moving along with the liquid can condense, bringing back angular momentum—so in equilibrium there would be no damping of the motion from this effect. There are other effects, however, such as those which cause resistance to capillary flow at high velocities, which might be expected to damp the motion.

When this is put into the variational principle, one finds directly

$$\mathcal{E}/\mathcal{I}=E(k)+m\int \mathbf{j}(\mathbf{r})\cdot\mathbf{v}_s(\mathbf{r})d^3\mathbf{r} +\tfrac{1}{2}m\int \rho(\mathbf{r})\mathbf{v}_s(\mathbf{r})\cdot\mathbf{v}_s(\mathbf{r})d^3\mathbf{r}, \quad (32)$$

where $E(k)$ is given in (18), $\mathbf{v}_s(\mathbf{r})=m^{-1}\nabla s$, and we have defined

$$\rho(\mathbf{a})=\int \rho_3(\mathbf{a},\mathbf{r}_1,\mathbf{r}_2)f^*(\mathbf{r}_1)f(\mathbf{r}_2)d^3\mathbf{r}_1d^3\mathbf{r}_2/I, \quad (33)$$

$$\mathbf{j}(\mathbf{a})=\hbar\int \rho_2(\mathbf{a},\mathbf{r})[f^*(\mathbf{r})\nabla f(\mathbf{a}) -f(\mathbf{r})\nabla f^*(\mathbf{a})]d^3\mathbf{r}/Imi, \quad (34)$$

with

$$I=\int \rho_2(\mathbf{r}_1,\mathbf{r}_2)f^*(\mathbf{r}_1)f(\mathbf{r}_2)d^3\mathbf{r}_1d^3\mathbf{r}_2. \quad (35)$$

These ρ, $\mathbf{j}$, are the expected values of density and current density that belong to the state representing a single excitation.

We shall analyze this for the case of a single excitation of nearly definite momentum in the form of a large wave packet, large compared with the central wavelength. That is, we take $f(\mathbf{r})=\exp(i\mathbf{k}\cdot\mathbf{r})g(\mathbf{r})$ where $g(\mathbf{r})$ is a smooth amplitude function, such as a Gaussian, with width very large compared to $1/k$, but small compared to the size of the vessel. Such a packet will drift and spread slowly in a way completely determined by $E(k)$ and the principle of superposition. We wish to determine the additional effects of the possibility of general liquid flow.

The current density associated with this excitation is found from (34). We make the approximation that $\nabla f=i\mathbf{k}f$ since g varies so slowly, obtaining,

$$\mathbf{j}(\mathbf{a})=\hbar\mathbf{k}m^{-1}\int \rho_2(\mathbf{a},\mathbf{r})\{g^*(\mathbf{r})g(\mathbf{a})\exp[-i\mathbf{k}\cdot(\mathbf{r}-\mathbf{a})] +g(\mathbf{r})g^*(\mathbf{a})\exp[+i\mathbf{k}\cdot(\mathbf{r}-\mathbf{a})]\}d^3\mathbf{r}/I.$$

Now, because of the variation of the exponentials, contributions to this integral come only from $\mathbf{r}$ within a limited distance from $\mathbf{a}$. Within such a distance $g(\mathbf{r})$ is nearly the same as $g(\mathbf{a})$, so all the g factors can be evaluated at $\mathbf{a}$ and taken outside the integral. The integral on $\mathbf{r}$ is then easy by (19) and one finds

$$\mathbf{j}(\mathbf{a})=\hbar\mathbf{k}\rho_0S(k)|g(\mathbf{a})|^2/mI.$$

The normalization integral may be done in a similar manner. It is

$$I=\int\int g^*(\mathbf{r}_1)g(\mathbf{r}_2)\rho_2(\mathbf{r}_1,\mathbf{r}_2) \times\exp[-i\mathbf{k}\cdot(\mathbf{r}_1-\mathbf{r}_2)]d^3\mathbf{r}_1d^3\mathbf{r}_2.$$

Since $\mathbf{r}_2$ must be near $\mathbf{r}_1$ for a large contribution, we may replace $g(\mathbf{r}_2)$ by $g(\mathbf{r}_1)$, integrate $\mathbf{r}_2$ directly and obtain

$$I=\rho_0S(k)\int |g(\mathbf{r})|^2d^3\mathbf{r}.$$

If we assume $g(\mathbf{r})$ is normalized, $\int|g(\mathbf{r})|^2d^3\mathbf{r}=1$, so that $|g(\mathbf{a})|^2=d(\mathbf{a})$ is the density in the packet at $\mathbf{a}$, or roughly the probability of finding the excitation at $\mathbf{a}$, the current is

$$\mathbf{j}(\mathbf{a})=(\hbar\mathbf{k}/m)d(\mathbf{a}), \quad (36)$$

that is, a total current $\hbar\mathbf{k}/m$ distributed at density $d(\mathbf{a})$.

The particle density at $\mathbf{a}$ is

$$\rho(\mathbf{a})=\int \rho_3(\mathbf{a},\mathbf{r}_1,\mathbf{r}_2)g^*(\mathbf{r}_1)g(\mathbf{r}_2) \times\exp[-i\mathbf{k}\cdot(\mathbf{r}_1-\mathbf{r}_2)]d^3\mathbf{r}_1d^3\mathbf{r}_2/I. \quad (37)$$

The points $\mathbf{r}_1$ and $\mathbf{r}_2$ must be close. If point $\mathbf{a}$ is not close to these points we can use the asymptotic form,

$$\rho_3(\mathbf{a},\mathbf{r}_1,\mathbf{r}_2)=\rho_0\rho_2(\mathbf{r}_1,\mathbf{r}_2), \quad (38)$$

to show directly that $\rho(\mathbf{a})$ is the density ρ_0 of the fluid, far from the packet. It is nearly so, even in the region of the packet, for since its dimensions are large, $\mathbf{a}$ is nearly always far from $\mathbf{r}_1,\mathbf{r}_2$, and further, the integral over all $\mathbf{a}$ of $\rho_3(\mathbf{a},\mathbf{r}_1\mathbf{r}_2)-\rho_0\rho_2(\mathbf{r}_1,\mathbf{r}_2)$ is exactly zero.

It is true that the distance of influence in ρ may not be very small, because of the correlations in the sound field. That is, the excitation produces a small strain in the fluid which makes a field of stress in the vicinity. Such fields provide a mechanism of interaction between excitations (as well as a correction to the energy of one). In a more detailed analysis such effects should be taken into account. Here we proceed to a first approximation and neglect them. To the approximation of neglecting compressibility, then, we find $\rho(\mathbf{a})=\rho_0$; the presence of an excitation does not change the fluid density.

Thus we picture an excitation in the form of a drifting wave packet as carrying a total current $\hbar\mathbf{k}/m$, and drifting (if $\mathbf{v}=0$) at the group velocity $\mathbf{v}_g=\partial E/\partial\mathbf{k}$, but as not appreciably altering the density.

This clearly violates the conservation of matter. For a moment we overlook this difficulty. It is discussed in the section following the next.

If this packet is in a general velocity field $\mathbf{v}_s(\mathbf{r})$ we may determine its energy from (32). In integral $\int\mathbf{j}(\mathbf{r})\cdot\mathbf{v}_s(\mathbf{r})d^3\mathbf{r}$ we shall assume that $\mathbf{v}_s$ does not vary appreciably over a region as small as the packet, and may be taken outside the integral sign. The integral of $\mathbf{j}$ is then $\hbar\mathbf{k}/m=\mathbf{p}/m$, giving the following results:

The energy of an excitation in a moving fluid is

$$E=E(p)+\mathbf{p}\cdot\mathbf{v}_s, \quad (39)$$

where $\mathbf{v}_s$ is the velocity of the fluid where the excitation (considered as a packet) is located. The total momentum associated with the packet is $\mathbf{p}$, and it contributes a current $\mathbf{p}/m$ to the total in the fluid. The energy contributed by the moving fluid has density $\rho_0 m\mathbf{v}_s^2/2$, and it contributes to the current density $\rho_0\mathbf{v}_s$.

The group velocity of the excitation is $\partial E/\partial\mathbf{p}$ so that $\mathbf{v}_g=\mathbf{v}_{g0}+\mathbf{v}_s$ where $\mathbf{v}_{g0}$ is the group velocity in liquid at rest, $\partial E(p)/\partial\mathbf{p}$. Thus the excitation just drifts along with the background fluid motion, of velocity $\mathbf{v}_s$. Equation (39) can be obtained much more simply by a Galilean transformation of coordinates. Indeed, it is in this way that it was obtained by Landau and Dingle.[6]

RELATION TO THE TWO-FLUID MODEL

The two paragraphs at the end of the previous section contain the main relations by which the hydrodynamics and thermodynamics of the two-fluid model is derived. We review here a few of the steps, very briefly, in order to make clear the relation of the excitations to what is called the normal fluid. For further details see reference 6.

Thermodynamic equilibrium results, for a system with Bose statistics, if the excitations are distributed so that the number of those with energy E is

$$n=[\exp(\beta E)-1]^{-1}.$$

This may be obtained, for example, by maximizing the entropy, keeping the total energy constant. Another distribution which is also in equilibrium can be got by maximizing the entropy, keeping both total energy and total momentum constant. It is

$$n=\{\exp[\beta(E-\mathbf{p}\cdot\mathbf{u})]-1\}^{-1}, \tag{40}$$

where $\mathbf{u}$ is a constant.

In our liquid, the density of excitations per unit volume at a point $\mathbf{r}$ in this case would be, substituting (39) into (40),

$$n=\{\exp[\beta(E(\mathbf{p})+\mathbf{p}\cdot\mathbf{v}_s(\mathbf{r})-\mathbf{p}\cdot\mathbf{u})]-1\}^{-1}. \tag{41}$$

In order to interpret $\mathbf{u}$, we study the total current density. Since each excitation contributes a current $\mathbf{p}/m$ the total current density contributed by the excitations is

$$m^{-1}\int\mathbf{p}\{\exp[\beta(E(\mathbf{p})+\mathbf{p}\cdot(\mathbf{v}_s-\mathbf{u}))]-1\}d^3\mathbf{p}(2\pi)^{-3}.$$

At this stage we shall only consider the case of low macroscopic velocities. Expanding to the first order in in $\mathbf{v}_s-\mathbf{u}$ this may be written in the usual way as

$$\rho_n(\mathbf{u}-\mathbf{v}_s),$$

where ρ_n is defined as

$$\rho_n=\frac{\beta}{3m}\int p^2\{\exp[\beta E(p)]-1\}^{-2}d^3\mathbf{p}(2\pi)^{-3}. \tag{42}$$

To this we must add the current of the background $\rho_0\mathbf{v}_s$, so that the total macroscopic current density can be written

$$\mathbf{j}=\rho_n\mathbf{u}+\rho_s\mathbf{v}_s, \tag{43}$$

if we put $\rho_s=\rho_0-\rho_n$.

In view of these separations we can say, artificially, that the liquid behaves as though there were two parts, superfluid at density ρ_s moving at velocity $\mathbf{v}_s$, and normal at density ρ_n and velocity $\mathbf{u}$ (which we write hereafter as $\mathbf{v}_n$). The current is the sum of these two partial currents. In a similar manner the change of the internal energy, at constant entropy, produced by the velocities can be shown to second order to be the sum of the kinetic energies $\frac{1}{2}\rho_s\mathbf{v}_s^2+\frac{1}{2}\rho_n\mathbf{v}_n^2$.

In a vessel with fixed walls in thermal equilibrium, if the liquid background is flowing, its velocity $\mathbf{v}_s$ must have no component normal to the wall. Further, the total current normal to the wall must vanish, so that the normal component of $\mathbf{v}_n$ must also vanish at the walls. But in equilibrium $\mathbf{v}_n$ is constant everywhere and must therefore vanish everywhere. We say the normal fluid is stationary in equilibrium with fixed walls, even though the superfluid moves with the velocity $\mathbf{v}_s$. Incidentally, the superfluid velocity is irrotational, $\nabla\times\mathbf{v}_s=0$.

If the walls move together at constant velocity, then equilibrium results if $\mathbf{v}_n$ is this velocity; the normal fluid moves at the same velocity as the walls.

We extend Eq. (40) to situations slightly out of thermal equilibrium by assuming $\mathbf{v}_n$ is not constant but varies from place to place. The failure of equilibrium will bring in various irreversible processes associated with the normal fluid, such as viscosity. If we leave these out of account, the remainder of the hydrodynamic equations which result can be derived in exactly the manner already given by Dingle.[5] We need enter no further in this direction, as nothing new is gained. The resultant hydrodynamical equations can most easily be interpreted from the model of helium as consisting of two interpenetrating fluids.

Nevertheless, it is difficult to understand these partial fluids from a detailed kinematic point of view. Kinematically we have a general, or background fluid in which excitations move. The velocity of the superfluid, $\mathbf{v}_s$, is the general velocity of this background, but the density of superfluid is not ρ_0. The velocity of the normal fluid, $\mathbf{v}_n$, appears as a parameter in the distribution function. It can be shown to be the average group velocity of the excitations. But the difficulties arise if one tries to interpret the formula (42) for ρ_n from a direct kinematical point of view. It is not the average value of any quantity that can reasonably be ascribed to an individual excitation. It appears to have meaning only for the entire group of excitations in, or near, thermal equilibrium.

The division into a normal fluid and superfluid, although yielding a simple model for understanding

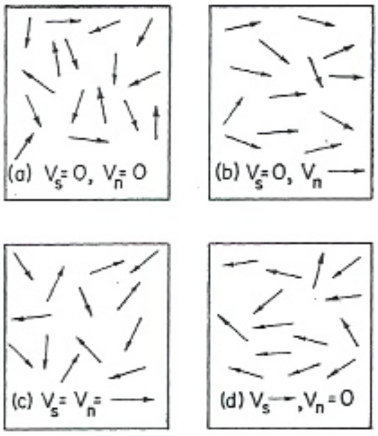

FIG. 4. At intermediate temperatures the main excitations are rotons which carry an intrinsic momentum, indicated by the arrows. If they drift relative to the background fluid, they tend to polarize upstream. This is illustrated for various values of v_s the background fluid velocity, and v_n the absolute drift velocity of the rotons. The total current is $\rho_0 v_s$ plus the polarization current of the rotons. Although mathematically correct, the separation of this current into the two parts, $\rho_s v_s$ and $\rho_n v_n$, characteristic of the two fluid model seems somewhat artificial from the microscopic viewpoint.

the final equations, appears artificial from a microscopic point of view. This opinion is shared by Landau and by Dingle.[5]

It is interesting to look at what is happening on a microscopic scale for various conditions of the velocities $\mathbf{v}_s$, $\mathbf{v}_n$. Consider a temperature not too low so that the predominant excitations are rotons. If the fluid is at rest a roton created with exactly the minimum energy Δ has no group velocity, but it has a momentum, of magnitude p_0 pointing in some direction. We will call it the direction of polarization and represent our roton by an arrow in this direction in Fig. 4. Not all rotons have exactly this energy Δ, but may differ by order kT from it, and have therefore nonzero group velocity. (Incidentally, the group velocity is parallel to or opposite to the polarization.) The rotons therefore may move about in a random manner like the molecules of a gas. Like gas molecules they can also have an average drift velocity relative to the fluid. Now we will assume [as required by (39), (41)] that if the rotons are drifting relative to the fluid in a certain direction, they tend (as a result of collisions among themselves) in equilibrium to polarize themselves in the direction in which they drift (that is, opposite to the velocity of the liquid moving past them). The general drift velocity of the rotons in space we call the normal fluid velocity, v_n. The motion of the fluid as a whole we call the superfluid velocity, v_s. Let us consider some examples.

First, with the fluid at zero velocity ($v_s=0$), and no drift of the rotons ($v_n=0$), they remain unpolarized (Fig. 4 (a)). If they are drifting to the right ($v_n>0$) they will tend to polarize in this direction, lining up to oppose the liquid passing them (Fig. 4 (b)). Now if the liquid is in motion ($v_s=v$), and all the rotons drift with the liquid in the same direction ($v_n=v$), there is no relative motion and no tendency to polarize (Fig. 4 (c)). This situation is not in equilibrium with stationary walls. Collisions of the rotons with the walls will stop their drifting motion and they will remain at rest relative to the walls. However, they will become polarized opposite to the fluid passing them (Fig. 4 (d)).

This interpretation of the velocities of the partial fluids of the two-fluid model is fairly simple and direct. It is otherwise with the current. The natural way to discuss the current (or momentum) from the microscopic view is to split it into two parts. First the current produced by the flow of the moving fluid, $\rho_0 v_s$, and second the current produced by the polarization. It is then easy to see what the current is in each case. In the first two cases, 4a, 4b, we have no general fluid motion so that the current is all due to polarization, zero in case *a*, to the right in case *b*. If the fluid moves, but the rotons remain unpolarized, as in 4c, the current is $\rho_0 v_s$, purely due to liquid motion. When the rotons polarize, as in 4d, to oppose this background motion the total current is reduced. But this natural separation is not the same as that utilized in the two fluid view. It is difficult to identify, for example, what is called the current of the normal fluid. It is not current carried by the rotons as they drift from one place to another (which they do with the velocity v_n) because the roton as such carries no mass but is only a disturbance in the liquid. Certainly the value of ρ_n would be hard to obtain this way because the rotons contribute to the current mainly by their polarization, and not by their drift motion. (Of course in a case such as 4b the polarization is in the direction of the drift so we could say the drift acts *as if* it carries current, because it induces polarization. ρ_n is then the ratio of the polarization current to the drift velocity which produces it.)

On the other hand, it is evident that the entropy flow is produced entirely by the drift motion (and not the polarization) of the rotons. Hence it is easy to see why all the entropy flows with the velocity v_n.

THE CONSERVATION OF CURRENT

In the last section we considered a packet of solutions (2) and found that we could picture an excitation in the form of a packet carrying a total current $\hbar\mathbf{k}/m$, and drifting at a group velocity $\partial E/\partial \mathbf{p}$, but as not appreciably altering the density. But such a picture is inconsistent with the conservation of matter. To take an extreme example, for a roton of the minimum energy Δ the group velocity $\partial E/\partial \mathbf{k}$ is zero, but the current $\hbar k_0/m$ is large. If such a current is distributed over a finite region in such a way that the direction is everywhere the same, we evidently cannot conserve material.

On the other hand, it is well known that one can demonstrate the conservation of matter,

$$\partial\rho(\mathbf{a})/\partial t=\nabla\cdot\mathbf{j}(\mathbf{a}), \tag{44}$$

from the Schrödinger equation. The reason that our wave function does not satisfy (44) is that it is not an exact solution of the wave equation. This shows an inaccuracy in our approximate wave function (17).

One way that suggests itself to resolve it, in the case of rotons with $k=k_0$, is to propose a superposition of two waves with opposite momenta $\mathbf{k}$ and $-\mathbf{k}$, like $g(\mathbf{r})\cos(\mathbf{k}\cdot\mathbf{r})$. In this case the current density is zero, and everything is all right. Furthermore, if the same small momentum $\mathbf{l}$ is given to each, so the momenta become $\mathbf{k}+\mathbf{l}$ and $-\mathbf{k}+\mathbf{l}$ with $k=k_0$, the drift velocity $\partial E/\partial\mathbf{k}$ is the same for each partial wave, so that the packet stays together.

On the other hand, with stronger collisions with walls and phonons perhaps the two momentum components would become separated. Further $g(\mathbf{r})\sin(\mathbf{k}\cdot\mathbf{r})$ is just as good a solution, and it must have almost exactly the same energy even if interactions are taken into account, because the exact position of the nodes in a large packet cannot be important. Therefore, a linear combination must again be a possibility and we are led back to the exponential, and to the difficulty of current conservation. This lack of conservation is a symptom that all is not too well with our wave function. It is true that in the cosine case the symptom is hidden, but the conclusion should stand that the wave function could be improved.

The problem can be resolved by considering more complicated functions representing interaction of the excitation with the flow of fluid in its surroundings. One way the current could be conserved would be to have a general return flow of fluid in the region outside the packet. We therefore try the solution

$$\psi=\sum_i g(\mathbf{r}_i)\exp(i\mathbf{k}\cdot\mathbf{r}_i)\exp[i\textstyle\sum_j s(\mathbf{r}_j)]\phi, \tag{45}$$

with the hope of finding an s which produces a velocity distribution $\mathbf{v}=m^{-1}\nabla s$ which shows such a reverse flow. Let us first consider such a packet in otherwise stationary liquid. Then as a boundary condition s should go to zero as we go far from the packet. Substitution into the variation integral gives (32). For the current and density we use our approximations, that $\mathbf{j}(\mathbf{a})$ is given by (36), and $\rho(\mathbf{a})=\rho_0$. There results

$$\mathcal{E}/\mathcal{I}=E(k)+\int\mathbf{j}(\mathbf{r})\cdot\nabla s(\mathbf{r})d^3\mathbf{r}+\frac{\rho_0}{2m}\int\nabla s\cdot\nabla s d^3\mathbf{r}, \tag{46}$$

where we have put, for the packet energy, $E(k)$, which is nearly correct. Variation of s to find a minimum gives the equation

$$\nabla\cdot(\mathbf{j}+\rho_0\nabla s)=0. \tag{47}$$

This equation determines s if we impose the boundary conditions $s\rightarrow 0$ far from the packet. Call this solution s_0 and the velocity distribution $\mathbf{v}_0=\nabla s_0/m$. It is like the field produced by the charge density $\nabla\cdot\mathbf{j}$, that is, at large distances the field of a dipole. It represents the back flow expected. Furthermore the total current operator has for our function the value

$$\mathbf{J}_0=\mathbf{j}+\rho_0\nabla s_0 \tag{48}$$

so that (47) says that now the total current is conserved.

There is a small shift in energy. Substitution of (47) into (46) gives the extra energy (reduction)

$$-\frac{\rho_0 m}{2}\int\mathbf{v}(\mathbf{r})\cdot\mathbf{v}(\mathbf{r})d^3\mathbf{r}.$$

If the order of the dimensions of the packet are L, the current $\hbar\mathbf{k}/m$ is distributed over a volume L^3, so the velocities are of order $\hbar k/mL^3$ and the kinetic energy $(\rho_0\hbar^2k^2/mL^6)L^3$ varies as $1/L^3$. But to confine the packet to such a dimension wave numbers of order $1/L$ in $g(r)$ must be used, so we find from (18) (for the case $k=k_0$) excess energies of order $1/L^2$ needed to confine the packet. Thus, for large packets, spreading the packet over even larger dimensions will decrease the energy, in spite of the energy of the currents we have just calculated. For extremely small packets our analysis does not hold because of the approximations made.

Here we have just gone far enough to save the theorem of conservation of current. We have only dealt with the background current in a semiclassical way. More complex states consisting of superpositions of expressions like (45) should be considered if a correct calculation of the quantum-mechanical "self-energy" of a roton due to coupling with the general velocity field is to be carried out. Since the "self-energy" is negative, the corrected value of Δ will be nearer the experimental result. This problem is being studied.

A more correct picture of a packet excitation, then, is that of a kind of region of polarization (that is, $\mathbf{j}$) which induces a distribution of velocity field around it, $\rho_0\nabla s_0$. The field is analogous to that produced by electrical polarization, the electric field $\mathbf{E}$ corresponding to the velocity field $\nabla s/m$, and the electric displacement vector $\mathbf{D}$ being analogous to the total current density, since its divergence vanishes. We can use this analogy to determine the behavior of the system directly, as it is easily verified that all the equations correspond. There is, however, one important difference. The signs of interaction are reversed. Thus (39) shows that rotons tend to line up opposed to the external field $\mathbf{v}$, while electric dipoles line up with the field. The analogy must therefore be completed with the remark that the rotons are dipoles of a gravitational type; that is, like poles attract, unlike repel.

The energy of a dipole in an external field is still the moment times the external field, even though the dipole itself creates some field of its own. None of the conclusions of the previous section are changed, therefore.

ROTON INTERACTION VIA THE VELOCITY FIELD

The fact that one roton creates a velocity field in which another may interact produces a kind of interaction between rotons. This is possibly one of the major sources of interaction, especially for not too high roton density. It is interesting to try to see what effect it has. Suppose we consider rotons as small packets all separated from one another and acting as dipoles of strength $\mathbf{p}/m$. Let us suppose there is an average polarization $\mathbf{P}$ per unit volume, and an average background velocity $\mathbf{v}_s$. The mean current density is then

$$\mathbf{J}=\rho_0\mathbf{v}_s+\mathbf{P}. \tag{49}$$

The actual field at any point is not $\mathbf{v}_s$ because of the local variations produced by the individual dipoles. Call the $\mathbf{w}$ velocity that an average dipole feels both from the average effect $\mathbf{v}_s$ and from its neighbors. The latter contribution is proportional to the polarization. In fact, as Lorentz showed for dipoles in random positions, it is $\frac{1}{3}\mathbf{P}/m$, hence

$$\mathbf{w}=\mathbf{v}_s+\alpha\mathbf{P}\rho_0^{-1}, \tag{50}$$

where[11] $\alpha=\frac{1}{3}$. The case $\alpha=0$ is the case previously studied which neglects direct effects between the dipoles.

The energy of a roton in this field is $E(\mathbf{p})+\mathbf{p}\cdot\mathbf{w}$. The statistical mechanics will then be governed by the function,

$$f=kT\int \ln\{1-\exp[-\beta(E(\mathbf{p}) +\mathbf{p}\cdot\mathbf{w}-\mathbf{p}\cdot\mathbf{u})]\}d^3\mathbf{p}/(2\pi)^3. \tag{51}$$

Here $\mathbf{u}$ is zero for equilibrium with fixed walls, and is the normal fluid velocity, $\mathbf{u}=\mathbf{v}_n$. The average polarization then is given by

$$\mathbf{P}=m^{-1}\partial f/\partial\mathbf{w}. \tag{52}$$

The internal energy of the system is

$$U=\tfrac{1}{2}m\rho_0\mathbf{v}_s^2+m\mathbf{P}\cdot\mathbf{w}-(\alpha m/2\rho_0)\mathbf{P}^2+\langle E(\mathbf{p})\rangle, \tag{53}$$

where the average value of $E(\mathbf{p})$ is

$$\begin{aligned}\langle E(\mathbf{p})\rangle=\int E(p)\{\exp[\beta(E(p) &+\mathbf{p}\cdot(\mathbf{w}-\mathbf{u}))]-1\}^{-1}d^3\mathbf{p}/(2\pi)^3\\ &=f+TS-(\mathbf{w}-\mathbf{u})\cdot m\mathbf{P}.\end{aligned}$$

The entropy is $S=-\partial f/\partial T$.

Expanding up to second order in the velocities one finds that the current can still be written as $\rho_s\mathbf{v}_s+\rho_n\mathbf{u}$, and the excess internal energy (at constant entropy and total current) as $\frac{1}{2}\rho_s\mathbf{v}_s^2+\frac{1}{2}\rho_n\mathbf{u}^2$, provided that one writes $\rho_s=\rho_0-\rho_n$ and

$$\rho_n=\rho_n^0(1+\alpha\rho_n^0/\rho_0)^{-1}, \tag{54}$$

where ρ_n^0 is the old expression (42) valid for the case $\alpha=0$. Therefore the expression for the velocity of second sound,

$$c_2=\left(\frac{\rho_n}{\rho_s}\frac{TS^2}{c_v}\right)^{\frac{1}{2}},$$

is unaltered when expressed in terms of ρ_n, etc. Only the theoretical formula for ρ_n is slightly modified. However, the modification is appreciable only when ρ_n^0/ρ_0 is not small, that is, near the transition. At the transition where c_2 goes to zero, ρ_n must equal ρ_0 so that ρ_n^0 given in (42) must equal $1/(1-\alpha)$ or 1.5. Actually ρ_n^0 varies very rapidly in this region so this makes no appreciable change in evaluating Δ and p_0 from the data. Furthermore in this region there may be other interactions which should alter our statistical mechanical analysis anyway. (Actually we cannot even be sure that rotons act as small individual dipoles until we have improved the wave function to include the interaction with the velocity field, as a quantum field.)

With interacting dipoles we would expect the analogue of a transition corresponding to the Curie point for electric dipoles. The analog of the condition for the Curie point comes out to be exactly the criterion that the expression (54) for ρ_n (with ρ_n^0 substituted from (42)) becomes equal to ρ_0. There are a few surprises here, though. Firstly, ordinarily the Curie transition occurs as we lower the temperature, but here it appears on raising the temperature. That is because the Curie point depends markedly on the density. Dipoles polarize if they are cold and dense. In our case at low temperatures they are cold, but not dense enough. As the temperature rises, the density does also, very rapidly, until a point is reached where spontaneous polarization appears even though the temperature has been raised. Another surprise is the fact that there is a transition even if the local field effect is neglected ($\alpha=0$). This difference is a result of the change of sign of the forces. Our dipoles polarize most easily if arranged in a flat region, while for electrical dipoles a needle-like region is preferred. With all the dipoles polarized parallel in the sheet the outside field is zero if the internal field opposed the polarization. But this opposition of polarization and field is just the stable condition for the rotons. In fact, the mutual local field α tends to *de*polarize them and *raises* the transition temperature. (For Onsager's value of α, (54) shows no transition for any temperature.)

One might be tempted to speculate that we could carry the statistical mechanical analysis right up to the transition point and beyond, by simply assuming that the only interaction of importance among rotons is the coupling with the general velocity field. One would just hope that other interactions or limitations to the number of degrees of freedom are not as important as

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[11] Onsager has shown that if one deals with permanent dipoles, mutually impenetrable and roughly spherical, this value of α is in error. If his analysis applies to our case, the value $\alpha=\rho_0(\rho_0+2\rho_s)^{-1}$ results [L. Onsager, J. Am. Chem. Soc. 58, 1486 (1936)].

one would otherwise guess. Aside from the amusing twist that helium I would then be the polarized, organized state, serious difficulties arise. One can analyze these things from the statistical formulas, if the velocities are not considered small and are not expanded. One can, without loss of generality, take states of total current zero, and for simplicity take $\alpha=0$. What happens is this. For any temperature below the transition there are two equilibrium states possible, one unpolarized with $v_s=0$, and the other polarized at finite v_s. Since the latter has higher free energy it is an unstable equilibrium, but the $v_s=0$ is stable (actually only metastable[12]). As we approach the transition point the polarization of the unstable state approaches zero. Above the transition point (more correctly, the point when $\rho_n=\rho_0$) only the $v_s=0$ state is in equilibrium and that is unstable. The instability arises this way. There is a high density of rotons. If a little polarization develops, their energy is reduced. This increases the number of rotons in equilibrium at a fixed temperature as well as the polarization, so that if there is no limit to the number of rotons there is no stable state.

On the other hand, if a limitation of roton number such as (28) is imposed, stable polarized states exist at the higher temperature. But the transition to that state occurs as a first-order transition, and there is another transition at still higher temperatures when the polarization disappears again.

It is therefore evident that we do not correctly describe the region very close to the transition by the usual energy expression (53) (with or without $\alpha=0$). The interactions between rotons is playing a more complicated role than (53) can describe.

In a previous paper an expression was given for the partition function which was presumably reasonably satisfactory right across the transition. However, the analysis was too difficult to carry out. Now that a more detailed picture of the behavior below the transition is available it may be easier to see how that expression can be treated. We still lack a clear picture of what happens in the few tenths of a degree on either side of the λ point.

INTERACTIONS BETWEEN EXCITATIONS

Interactions between the excitations will lead to various irreversible processes, such as viscosity, attenuation of second sound, etc. These questions have been studied by Landau and Khalatnikov.[13] The most important factor in the various mean free paths which are involved is the change in density of the phonons and rotons with temperature. The absolute cross sections depend on the details of the interactions. Interactions between phonons can be thought of as arising from a nonlinear equation of state. An interaction between a phonon and a roton would result if rotons have a different energy for different pressures. According to the theory presented here their energy is $\hbar^2k^2/2mS(k)$. If the liquid is compressed k^2 increases. On the other hand $S(k)$ probably increases even more rapidly from the increase in local order produced by squeezing the nearly impenetrable atoms into a smaller space. Therefore we expect Δ to decrease with pressure. This provides a mechanism for roton-phonon interaction. It also has other effects. The presence of a roton would cause a small increase in density in its neighborhood with the effect falling off inversely as the distance from the roton. This provides a mechanism of long-range interaction between rotons in addition to that due to coupling with the general velocity field. The roton-roton interaction at short distances is a more difficult problem, which probably cannot be adequately solved until a more accurate wave function is available for the roton state.

If the roton energy Δ decreases when the liquid density increases then we would expect that in equilibrium the liquid would shrink if the number of rotons is increased. The volume decrease as the λ point is approached is probably a consequence of this effect. The fall of the λ temperature with rising pressure is thermodynamically related. It may also be seen directly from (42) (supposing the λ point to be $\rho_n=\rho_0$) considering that Δ decreases as the density rises.

SUPERCONDUCTIVITY

It has been suggested that superconductivity is analogous to superfluidity. What can we learn of the former from our study of the latter? It is interesting that if the He atoms were charged (and their net charge canceled by a uniform fixed background charge of opposite sign) the liquid would imitate many of the features of a superconductor. In a magnetic field at absolute zero the London[14] equation, $\mathbf{j}=e\mathbf{A}/mc$, would hold. This is because stirring of atoms is equivalent to interchange so that in the lowest state the wave function cannot vary if atoms are stirred, and the part of the current depending on the wave function gradient vanishes. Other states would take a finite energy to create, there would be states of permanent circulation in multiply connected rings, there would be a second-order transition, etc. How this close analogy is to be interpreted is not clear. The things which, it has been argued here, apply physically to helium cannot be justifiably taken over to the case of Fermi particles, or such particles in interaction with lattice waves, without a complete investigation of their validity in the new environment. For example, at present there is not, in the author's opinion, justification for assuming

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[12] That is, the conventional free-energy expressions for arbitrary v_s are, strictly speaking, not self-consistent. For any temperature there is always some value of v_s for which the free energy is less than its value for $v_s=0$.

[13] L. Landau and I. Khalatnikov, J. Exptl. Theoret. Phys. (U.S.S.R.) **19**, 637, 709 (1949).

[14] F. London, *Superfluids* (John Wiley and Sons, Inc., New York, 1950), Vol. I.

that the form (2) is a reasonable wave function for an assembly of Fermi particles, with ϕ the ground-state function for such particles. In fact, there are definite arguments against it. Possibly the close analogy should only be used to tell us what the problem of superconductivity is. It is, from this point of view, the problem of showing that, in the metal, aside from phonons there are no (or only very few) states of very low energy just above the ground state.

DISCUSSION

We still have left unsolved at least three basic questions. One is to find a clear description of the neighborhood of the transition. A second is to obtain a more perfect roton wave function. The third is to describe states for which the superfluid velocity is not vortex-free. So far we have $\nabla\times\mathbf{v}_s=0$. At high velocities when more energy is available, more complicated motions might be excited. The evidence of high resistance to capillary flow at the higher velocities indicates this. A new element must presumably be added to our picture. We hope to publish some views on this third problem at a later time.

We have limited ourselves to a qualitative analysis of the more curious features of the behavior of liquid helium. The problem of obtaining $S(k)$ or the correlation function for the ground state quantitatively from first principles is beyond the scope of this work.

It has been argued[1] that He^3 atoms in low concentration, in He^4 would act as a gas of free particles, but with an effective mass m'' higher than that of one atom. This mass m'' is calculated in the appendix, where it is found to be about six atomic mass units.

The author has profited from conversations with R. F. Christy and with Michael Cohen.

APPENDIX

According to II an impurity atom of He^3 (at infinite dilution) should behave as an essentially free particle except that its effective mass m'' should exceed the true mass of He^3 due to the inertia of the He^4 atoms which must make way for it as it moves. We shall calculate this excess mass here. First we suppose the impurity atom had the same mass m as the other He^4 atoms (i.e., we neglect the difference in mass of He^3 and He^4).

The wave function for such an atom (coordinates $\mathbf{r}_A$) moving with momentum $\hbar\mathbf{k}$ might be conjectured to be $\exp(i\mathbf{k}\cdot\mathbf{r}_A)\phi$, where ϕ is the ground state of the system (which is the same as if all the atoms were identical). This, as a trial function, gives the variational energy as $\hbar^2k^2/2m$ and shows no mass correction. It does not represent with sufficient accuracy the other atoms moving back when atom A moves forward. This suggests the trial function

$$\psi=\exp(i\mathbf{k}\cdot\mathbf{r}_A)\exp[i\textstyle\sum_i s(\mathbf{r}_i-\mathbf{r}_A)]\phi, \qquad (1\text{–a})$$

where the velocity field $\nabla s(\mathbf{r}_i-\mathbf{r}_A)$ represents a backflow which depends only on the distance from the impurity. To omit the term $i=A$ in the sum we take $s(0)=0$. Substitution into the variational principle gives

$$\begin{aligned}\mathcal{E}=(\hbar^2/2m)\int[k^2-2\mathbf{k}\cdot\textstyle\sum_i\nabla s(\mathbf{r}_i-\mathbf{r}_A)&\\ +\textstyle\sum_i\sum_j\nabla s(\mathbf{r}_i-\mathbf{r}_A)\cdot\nabla s(\mathbf{r}_j-\mathbf{r}_A)&\\ +\textstyle\sum_i\nabla s(\mathbf{r}_i-\mathbf{r}_A)\cdot\nabla s(\mathbf{r}_i-\mathbf{r}_A)]\rho_N d^N\mathbf{r},&\qquad(2\text{-a})\end{aligned}$$

with $\mathcal{I}=1$, as ψ is normalized. We write $\rho_2(\mathbf{r}_i,\mathbf{r}_A)=\rho_0 p(\mathbf{r}_i-\mathbf{r}_A)$, and $\rho_3(\mathbf{r}_i,\mathbf{r}_j,\mathbf{r}_A)=\rho_0 p_3(\mathbf{r}_i-\mathbf{r}_A,\mathbf{r}_j-\mathbf{r}_A)$, and measure all distances from the point $\mathbf{r}_A$, so that (2-a) becomes

$$\begin{aligned}2m\hbar^{-2}\mathcal{E}=k^2-2\mathbf{k}\cdot\int\nabla s(\mathbf{r})p(\mathbf{r})d^3\mathbf{r}&\\ +\int\int\nabla s(\mathbf{r})\cdot\nabla s(\mathbf{r}')p_3(\mathbf{r},\mathbf{r}')d^3\mathbf{r}d^3\mathbf{r}'&\\ +\int\nabla s(\mathbf{r})\cdot\nabla s(\mathbf{r})p(\mathbf{r})d^3\mathbf{r}.&\qquad(3\text{-a})\end{aligned}$$

Then s is to be chosen to minimize this expression.

The function $p_3(\mathbf{r},\mathbf{r}')$ is the probability of finding one atom at $\mathbf{r}$ and another at $\mathbf{r}'$ if there is an atom at the origin ($p(\mathbf{r})$ is just the probability of finding one at $\mathbf{r}$ if one is at the origin). We do not know what this function p_3 is, but in this problem we can approximate it by $p(\mathbf{r})p(\mathbf{r}')$ (except at the origin). A given atom is surrounded by many (eight or ten?) nearest neighbors, and the distribution along one radius r and another r' must be nearly independent except for the relatively small solid angle where the atoms at $\mathbf{r}$ and $\mathbf{r}'$ are close together. Even here, if the functions $s(\mathbf{r})$, $s(\mathbf{r}')$ are smooth enough the average of p_3 over such angles may still give nearly the same result as $p(r)p(r')$. With this substitution our problem is that of minimizing

$$\begin{aligned}2m\hbar^{-2}\mathcal{E}=\left[k-\int\nabla s(\mathbf{r})p(\mathbf{r})d^3\mathbf{r}\right]^2&\\ +\int\nabla s(\mathbf{r})\cdot\nabla s(\mathbf{r})p(\mathbf{r})d^3\mathbf{r}.&\qquad(4\text{-a})\end{aligned}$$

The error made by this approximation is

$$\begin{aligned}\Delta\mathcal{E}=(\hbar^2/2m)\int\int\nabla s(\mathbf{r})\cdot\nabla s(\mathbf{r}')[p_3(\mathbf{r},\mathbf{r}')&\\ -p(\mathbf{r})p(\mathbf{r}')]d^3\mathbf{r}d^3\mathbf{r}'.&\qquad(5\text{-a})\end{aligned}$$

The $s(\mathbf{r})$ which minimizes (4-a) behaves as a dipole field (as $\mathbf{k}\cdot\mathbf{r}/r^3$) at large distances and this produces some convergence difficulties in the first integral in (4-a). They may be easily straightened out as follows. The minimum energy is only very slightly altered if the function $s(\mathbf{r})$ is altered at very large distances in such a way that it falls off eventually more rapidly than $1/r^2$. For such a function the integral may be done by parts, the integrated part vanishing, so we may write

$$2mh^{-2}\mathcal{E}=\left(k+\int s(\mathbf{r})\nabla p(\mathbf{r})d^3\mathbf{r}\right)^2 +\int \nabla s(\mathbf{r})\cdot\nabla s(\mathbf{r})p(\mathbf{r})d^3\mathbf{r}. \qquad (6\text{-a})$$

But in this form all the integrals have a definite limit even if $s(\mathbf{r})$ has no convergence factor (and therefore varies as $1/r^2$). We may therefore use (6-a) and avoid ambiguities from conditionally convergent integrals.

The variational principle shows that s must be a solution of

$$\nabla\cdot[p(\mathbf{r})((1-\beta)\mathbf{k}-\nabla s(\mathbf{r}))]=0, \qquad (7\text{-a})$$

where we have set

$$-\int s(\mathbf{r})\nabla p(\mathbf{r})d^3\mathbf{r}=\beta\mathbf{k}. \qquad (8\text{-a})$$

Multiplication of (7-a) by $s(\mathbf{r})$ and integration, using (8-a), tells us further that

$$\int \nabla s(\mathbf{r})\cdot\nabla s(\mathbf{r})p(\mathbf{r})d^3\mathbf{r}=\beta(1-\beta)k^2,$$

so (6-a) says

$$\mathcal{E}=\frac{h^2k^2}{2m}[(1-\beta)^2+\beta(1-\beta)]=\frac{h^2k^2}{2m}(1-\beta),$$

and the effective mass is $m/(1-\beta)$, an increase over m of

$$\Delta m=\beta m/(1-\beta). \qquad (9\text{-a})$$

If the direction of $\mathbf{k}$ is taken as the z axis, the solution of (7-a) may be written in the form,

$$s(\mathbf{r})=(1-\beta)k(z-zv(r)/r), \qquad (10\text{-a})$$

where $v(r)$ is a function of radius $r=(\mathbf{r}\cdot\mathbf{r})^{\frac{1}{2}}$ only, satisfying

$$\frac{d}{dr}\left(r^2p(r)\frac{dv}{dr}\right)=2pv, \qquad (11\text{-a})$$

and such that v approaches r at large distances. This is easily solved numerically. We used the values of $p(r)$ determined by Reekie and Hutchison.[4] Starting for small r where $p(r)=0$, so that $dv/dr=0$, we chose v at some convenient value and integrated out to radii so large that $p(r)$ was effectively its asymptotic value ρ_0. Asymptotically v has the form $c(r+B/r^2)$ where B, c are constants. Since the equation is homogeneous we may divide the entire solution by c to obtain one with the correct asymptotic form. By substitution of (10-a) into (8-a) one can show, using (11-a), that the expression for (9-a) can be written

$$\Delta m/m=4\pi\rho_0B-1, \qquad (12\text{-a})$$

where we have used the fact that

$$\int_{0+}^{\infty}(\rho_0-p(r))4\pi r^2dr=1 \qquad (13\text{-a})$$

[the origin, where $p(r)$ has a δ function being excluded in this integral]. Actually it is difficult to obtain accuracy with this method because the asymptotic form of v is sensitive to the values of $p(r)$ used. Those of Reekie and Hutchinson[4] extended only up to $r=6\text{A}$ and had to be taken from a graph, so that (13-a) was not accurately satisfied without some small arbitrary readjustments of the values.

On the other hand, the solution showed that $s(\mathbf{r})$ was nearly proportional to z/r^3. Since (6-a) is a variational principle we can therefore obtain a good value of the energy much more simply. We substitute the trial function,

$$s(\mathbf{r})=Az/r^3, \qquad (14\text{-a})$$

directly into (6-a) and determine the parameter A to minimize $\mathcal{E}$. This gives

$$\Delta m/m=\tfrac{1}{2}\left(\frac{4\pi}{3}\rho_0\right)^2\left[\int_{0+}^{\infty}r^{-6}p(r)4\pi r^2dr\right]^{-1}, \qquad (15\text{-a})$$

or, with the data of reference 4, $\Delta m=0.70m$, or 2.8 atomic mass units. (The numerical solution of the differential equation gave the same result within its accuracy of about 10 percent.)

It is difficult to evaluate the small correction arising from the term $\Delta\mathcal{E}$ of (5-a), for p_2 is unknown. If the atoms locally are nearly on a lattice, say face-centered, or body-centered, of cubic symmetry, $\Delta\mathcal{E}$ vanishes with the trial function (14-a).

If the mass of the impurity atom is not four atomic units it is readily shown that Δm is unchanged, provided that the distribution $p(r)$ of atoms around the impurity is assumed to be unchanged. This is also expected physically for the extra mass is due to the motion of the He^4 atoms in the environment of the impurity. Therefore for a He^3 atom the effective mass should be 5.8 atomic mass units. The higher zero-point motion of a lighter atom changes $p(r)$ by pushing the neighbors farther away, thereby raising Δm a little (but this effect must be a fraction of a mass unit because the effective mass is almost certainly less than the 6.8 which it would be if the He^3 had the larger mass of 4 units).

This result is not in good agreement with the determinations which have been made from experiment, as summarized by Daunt.[15] These give values nearer 8 or 9 atomic mass units.

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[15] J. G. Daunt, Advance in Physics (Phil. Mag. Supplement) **6**, 209 (1952), particularly p. 258.