ATOMIC THEORY OF LIQUID HELIUM*

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Liquid helium II is studied from frist principles. We show how the central features of the two fluid model arise.

In previous work[1] the λ-transition was interpreted as the Bose-Einstein condensation of a non-ideal gas. We are concerned here with lower temperatures. The ground state wave function and the types of excited states available at low temperatures are studied.

The wave function Ψ, of the ground state is visualized qualitatively. The helium atoms are nearly hard spheres. The wave function is everywhere real and positive and is symmetric for interchange of the atoms. It is described by giving the amplitude for various configurations of the atoms. If atoms are in contact or overlapping the function vanishes, and it is largest when they are well separated from one another. Thus the atoms tend to stay apart and to produce a kind of local structure similar in density distribution to that of a classical liquid.

An increase of mean density over a large volume represents an energy increase because of the rise of zero-point energy occasioned by the decrease of free volume. Long wave sound can therefore be carried by the liquid, and there are density fluctuations corresponding to the zero-point oscillations of this sound field.

Keeping the mean separations of the atoms fixed, and the mean density fixed, there are still configurations which differ from one another, but just in the sense that one can be "stirred" into the other. Since the structure is fairly open in the liquid, there is no effective barrier to such stirrings, and the lowest state corresponds to equal amplitude for all such configurations.

What are the character and energy of the lowest excited states of the system? First, there are excitations of the long compressional waves, phonons of energy $\hbar KC$ for wave number K, where C is the sound velocity. The specific heat variation as T^3 (below $0.7°k$) shows there are no other states of low energy. Why this is so is seen as follows.

The wave function must not be altered by any change which simply interchanges the atoms. Yet the excited state must be orthogonal to the ground state. Starting at any configuration A, and supposing the amplitude to be positive, one must find a new configuration B to which we can assign a negative amplitude, and which differs from the old configuration A by just a stirring of the atoms without change of mean density (to omit phonon states). It is clear that every such configuration is close to the original one, albeit with some atoms interchanged. So it is hard to find a configuration to give a negative amplitude which is sufficiently far (in configuration space) from the original one of positive amplitude to result in a low gradient of amplitude and thus a low energy. The lowest state will have B differ as much as possible from A.

Configuration B is furthest from A if all of the atoms in B are between the sites occupied in A. The transition from positive amplitude for A to equal negative amplitude for B is as smooth as possible if the amplitude for other intermediate configurations is simply proportional to the number of atoms on A sites minus the number on B sites. Density fluctuations and overlapping atoms must be avoided just as in the ground state. It is therefore deduced that the wave function of the excited states will, to a good approximation, be of the form

$$\Psi = \sum_i f(\vec{R_i}) \, \Psi \qquad (1)$$

where Ψ is the ground state function and $f(\vec{R})$ is $+1$ if R is at an A site and -1 if at a B site, and the sum is taken over all the atoms, coor-

dinates $\vec{R_i}$.

Other chains of reasoning starting from other viewpoints concur in the conclusion that (1) is a good approximation to the wave function with $f(\vec{R})$ some function with variations predominately of wave length equal to the atomic spacing.

Knowing that (1) is the form of the function, we turn to a mathematical argument to obtain a detailed evaluation of the best choices for $f(\vec{R})$ and the energies to which they belong. We shall compute the fraction

$$E = \langle \Psi^*, H\Psi \rangle / \langle \Psi^*, \Psi \rangle \tag{2}$$

in terms of f and find the f's which make it stationary. Measuring energies above E_0, the ground state energy, the hamiltonian is

$$H = -(\hbar^2/2m)\sum_i \nabla^2_i + V - E_0 \tag{3}$$

From (1) and (3), using $H\Psi = 0$, we find

$$H\Psi = -(\hbar^2/2m)\sum_i (\Psi\nabla^2_i f(\vec{R_i}) + 2\nabla_i\Psi \cdot \nabla \cdot f(\vec{R_i}))$$

Substituting into (2), noting that Ψ is real and that $2\Psi\nabla\Psi = \nabla\Psi^2$ and integrating by parts, one gets

$$E = \frac{(\hbar^2/2m)(\sum_i \int \Psi^2 \nabla_i f^*(\vec{R_i}) \cdot \nabla_i f(\vec{R_i}) d^N V}{\sum_i \sum_j \Psi^2 f^*(\vec{R_i}) f(\vec{R_i}) d^N V} \tag{4}$$

The integral $d^N V$ is over all configuration of all the atoms. In the denominator we can first integrate Ψ^2 over all variables except i, j. This gives a result proportional to the correlation function $p(\vec{R_i} - \vec{R_j})$ for the ground state (that is, $p(\vec{R} - \vec{R'})$ is the probability per unit volume of finding an atom at $\vec{R'}$ if one is known to be at $(\vec{R})$. Similarly the numerator is integrated first over all variables but $\vec{R_i}$, giving the chance to find an atom at $\vec{R_i}$, which is constant. Thus (4) reduces to

$$E = \frac{(\hbar^2/2m) \int \nabla f^*(\vec{R}) \cdot \nabla f(\vec{R}) d^3\vec{R}}{\iint p(\vec{R} \to \vec{R'}) f^*(\vec{R}) f(\vec{R'}) d^3\vec{R} d^3\vec{R'}}$$

This is stationary if f satisfies

$$-(\hbar^2/2m)\nabla^2 f(\vec{R}) = E\int p(\vec{R} + \vec{R'}) f(\vec{R'}) d^3\vec{R'}$$

where S(K) is the liquid form factor for He at absolute zero, the fourier transform of the correlation function;

$$S(\overline{K}) = \quad p(R) \exp(iK \cdot R) \, d^3 R$$

The function S(K) can be obtained directly from X-ray or neutron scattering experiments. The behaviour for small $\underline{K}$ can be obtained theoretically from its relation to the zero point density fluctuations of the sound field. One gets $S(K) = hK/2mc$, so that $E_K = h\,KC$, the energy of a phonon. This must check because the form (1) for low $\underline{K}$ is also exactly the form of the wave function for the first excited state of the sound field.

For very high $\underline{K}$, S(K) approaches 1 because $p(R)$ contains a delta function at the origin. For intermediate $\underline{K}$, S(K) rises to a maximum and falls away, with perhaps other subsidiary oscillations, as a result of the local order occasioned by the tendency of the atoms to stay apart. This maximum makes a ring in the X-ray scattering corresponding to a value of $\underline{K}$ of order $2/a$.

Therefore, E_K rises first linearly with $\underline{K}$, but then falls to a minimum and rises again. The states available at low temperatures are therefore either phonons, or else excitations near the minimum of the curve (where it has the parabolic form

$$:+ (H^2/2)(K - K_0)^2.$$

Landau has shown that this is just the kind of an energy curve which will qualitatively and quantitatively describe the properties of helium II. The kinetic aspects of the two fluid model are also readily understood starting from this point.

1 - R.P. Feynman, Phys. Rev. (to be published).