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On the Energy Spectrum in Quantum Hydrodynamics and the Theory of Helium II

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Summary: The eigenvalue spectrum of the quantum-mechanical Hamiltonian of non-viscous fluids is calculated in the approximation of large sound velocity and for low densities of phonons and rotons. The anharmonic potential energy in the Hamiltonian has no influence on the roton energies in the approximation considered; all contributions due to the term $\sim (\varrho - \varrho_0)^3$ cancel and the term $\sim (\varrho - \varrho_0)^4$ only gives rise to a renormalization of the sound velocity. Several procedures to cut off large wave numbers are discussed. They lead to different results, but they all yield positive rest energies of the rotons and, when applied to He II, energy spectra of the right form and order of magnitude to fit the experimental data on specific heat up to temperatures near the λ-point.

§ 1. Introduction.

After the energy spectrum of liquid helium postulated by LANDAU¹)²) had proven to be so successful in explaining and predicting many properties of He II, several attempts have been made to give this energy spectrum a more secure foundation. One of these attempts consists in quantizing the hydrodynamical equations of a non-viscous fluid and looking for the eigenvalues of the corresponding Hamiltonian. For the case of irrotational motion this has been done by KRONIG and THELLUNG³), and the concept of phonons has thereby become clarified. The theory has been extended by THELLUNG⁴) and by ZIMAN⁵) so as to include vortex motions. The total Hamiltonian is then found to consist of three parts: The phonon part of irrotational hydrodynamics, which can approximately be diagonalized, a roton part, and an interaction between phonons and rotons. ZIMAN⁵) succeeded in finding certain eigenvalues of the roton part, i. e. the eigenvalues for one roton present. It is also possible to calculate the eigenvalues of the roton part when two rotons are present, but this problem is rather academic as long as the interaction part of the Hamiltonian is neglected, which is easily seen to modify the energy spectrum by amounts of the same order of magnitude as the eigenvalues of the roton part. In order to avoid a perturbation treatment of the interaction we have first tried a method analogous to the BLOCH-NORDSIECK transformation in quantum electrodynamics[6]). However, it turns out that the remaining nondiagonal term in the transformed Hamiltonian, which is a small perturbation in electrodynamics, is here as big as the original interaction. Therefore nothing is gained and it is, in fact, simpler to use conventional perturbation theory for the original interaction energy. In the case of liquid helium we shall see that this is not a bad approximation. One might also try to calculate the quantum-hydrodynamical partition function directly without knowing the explicit energy eigenvalues. However, it is easier first to determine the eigenvalues approximately.

Meanwhile a paper by ALLCOCK and KUPER[7])*) (to be referred to as AK) appeared which gives the energy spectrum for an incompressible liquid (sound velocity $c_0 = \infty$). For c_0 large but not infinite they treat the case of one roton present, passing from second quantization to the representation of the roton in configuration space. They follow a method of LEE, LOW and PINES[8]) and ZIENAU[9]) (which is similar to the BLOCH-NORDSIECK transformation[6])) to obtain a development in negative powers of c_0. Setting the anharmonic potential energy in the Hamiltonian equal to zero, they give an explicit expression for the rest energy of a roton $\sim c_0^{-1}$ (the rest energy of order c_0^0 disappears), without however evaluating the integrals involved. Even its sign is uncertain.

In this paper we calculate the kinetic and rest energies of the rotons to the first non vanishing order in negative powers of c_0 (i.e. $\sim c_0^0$ for the kinetic and $\sim c_0^{-1}$ for the rest energy). We do not abandon second quantization and we use conventional perturbation theory from the very beginning. The contributions of the anharmonic terms in the potential energy are fully taken into account to order c_0^{-1}.

In § 2 of this paper we present the basic Hamiltonian. Two special questions are discussed in § 3 and § 4, namely a renormalization problem arising from the anharmonic potential energy and the order of factors in the Hamiltonian. § 5 and § 6 contain the calculation of the roton energies according to a cut-off method proposed by ZIMAN. In § 7 other cut-off procedures are examined, and in § 8 the results are discussed and compared with experimental data.

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*) The author is indebted to Dr. G. R. ALLCOCK and Dr. C. G. KUPER for sending him a preliminary form of their manuscript.

§ 2. The Hamiltonian.

In the quantum hydrodynamics of a non-viscous fluid the Hamiltonian is known to be simply the sum of the kinetic and potential energies[4])[5]).

$$H = \int_V d^3x \left(\tfrac{1}{2}\, \boldsymbol{v}\, \varrho\, \boldsymbol{v} + E_p(\varrho) \right). \tag{1}$$

It is most convenient to express the velocity $\boldsymbol{v}$ in terms of a scalar potential φ, the density ϱ and ZIMAN's[5]) variables Ψ, Ψ^*,

$$\boldsymbol{v} = -\nabla\varphi - \frac{i\hbar}{2\varrho}\{\Psi^* \nabla\Psi - \nabla\Psi^* \Psi\}. \tag{2}$$

The four fields introduced fulfil the following commutation relations[5])

$$[\varrho(\boldsymbol{x}), \varphi(\boldsymbol{x}')] = \frac{\hbar}{i}\,\delta(\boldsymbol{x}-\boldsymbol{x}'),\ [\Psi(\boldsymbol{x}), \Psi^*(\boldsymbol{x}')] = \delta(\boldsymbol{x}-\boldsymbol{x}'), \tag{3}$$

all other commutators vanishing. We substitute (2) into (1) and expand all functions of ϱ in rising powers of the deviation of ϱ from its equilibrium value ϱ_0, in particular

$$\frac{1}{\varrho} = \frac{1}{\varrho_0} - \frac{\varrho-\varrho_0}{\varrho_0^2} + \frac{(\varrho-\varrho_0)^2}{\varrho_0^3} - \cdots \tag{4}$$

and (see for instance KRONIG and THELLUNG[3]) equ. (31))

$$E_p(\varrho) = \frac{1}{2!}\frac{c_0^2}{\varrho_0}(\varrho-\varrho_0)^2 + \frac{1}{3!}\left(\frac{d}{d\varrho}\frac{c^2}{\varrho}\right)_0 (\varrho-\varrho_0)^3 + \frac{1}{4!}\left(\frac{d^2}{d\varrho^2}\frac{c^2}{\varrho}\right)_0 (\varrho-\varrho_0)^4 + \cdots \tag{5}$$

The Hamiltonian is then split up into a sum of terms similar to expressions (1·7a)—(1·7g) of AK, viz.

$$\left.\begin{aligned}
H_{\mathrm{ph}} &= \int_V d^3x \left\{ \frac{1}{2}\varrho_0 (\nabla\varphi)^2 + \frac{1}{2}\frac{c_0^2}{\varrho_0}(\varrho-\varrho_0)^2 \right\} && \text{(a)}\\
H_{\mathrm{rot}} &= \int_V d^3x \left(-\frac{\hbar^2}{8\varrho_0}\right) \{\Psi^* \nabla\Psi - \nabla\Psi^* \Psi\}^2 && \text{(b)}\\
H_{\mathrm{int}} &= \int_V d^3x \frac{i\hbar}{2} \nabla\varphi \{\Psi^* \nabla\Psi - \nabla\Psi^* \Psi\} && \text{(c)}\\
H'_{\mathrm{ph}} &= \int_V d^3x \left\{ \frac{1}{2}\nabla\varphi\,(\varrho-\varrho_0)\,\nabla\varphi + \frac{1}{3!}\left(\frac{d}{d\varrho}\frac{c^2}{\varrho}\right)_0 (\varrho-\varrho_0)^3 \right\} && \text{(d)}\\
H''_{\mathrm{ph}} &= \int_V d^3x \frac{1}{4!}\left(\frac{d^2}{d\varrho^2}\frac{c^2}{\varrho}\right)_0 :(\varrho-\varrho_0)^4: && \text{(e)}\\
&\cdots\cdots\\
H'_{\mathrm{int}} &= \int_V d^3x \frac{\hbar^2}{8\varrho_0^2}(\varrho-\varrho_0)\{\Psi^* \nabla\Psi - \nabla\Psi^* \Psi\}^2 && \text{(f)}\\
H''_{\mathrm{int}} &= \int_V d^3x \left(-\frac{\hbar^2}{8\varrho_0^3}\right)(\varrho-\varrho_0)^2 \{\Psi^* \nabla\Psi - \nabla\Psi^* \Psi\}^2 && \text{(g)}\\
&\cdots\cdots
\end{aligned}\right\} \quad (6)$$

The symbol $:(\varrho-\varrho_0)^4:$ in (6e) means that later, when $(\varrho-\varrho_0)^4$ will be expressed in terms of creation and annihilation operators, we shall have to write this expression in the form of an S-product as defined by WICK[10]), i.e. with all creation operators to the left and all annihilation operators to the right. This results from a renormalization that has to be carried out on the sound velocity, and will be explained in § 3.

In (6a)—(6g) the terms with a suffix ph contain only the phonon fields ϱ and φ. H_{rot} depends exclusively on the roton fields Ψ, Ψ^*, whereas the terms denoted by a suffix int contain both fields. The primed and double primed expressions are subsequent terms of the expansion in powers of $\varrho-\varrho_0$. In classical hydrodynamics $\varrho-\varrho_0$ is very small compared with ϱ_0 for vortex motions and sound waves of moderate amplitude, so we would expect that also in quantum hydrodynamics the first three terms (6a)—(6c) should give the main contributions to the low energy eigenvalues.

Assuming all field quantities to be periodic in a cube of volume V we decompose them into Fourier series

$$\left.\begin{aligned}\varphi &= \frac{1}{V^{1/2}}\sum_{\boldsymbol{k}}\sqrt{\frac{c_0\hbar}{2\varrho_0 k}}\,(a_{\boldsymbol{k}}+a^*_{-\boldsymbol{k}})\,e^{i\boldsymbol{k}\boldsymbol{x}}\\ \varrho-\varrho_0 &= \frac{1}{V^{1/2}}\sum_{\boldsymbol{k}}\sqrt{\frac{\varrho_0\hbar k}{2c_0}}\,i\,(a^*_{\boldsymbol{k}}-a_{-\boldsymbol{k}})\,e^{-i\boldsymbol{k}\boldsymbol{x}}\end{aligned}\right\} \tag{7}$$

$$\Psi=\frac{1}{V^{1/2}}\sum_{\boldsymbol{k}} b_{\boldsymbol{k}}\,e^{i\boldsymbol{k}\boldsymbol{x}},\quad \Psi^*=\frac{1}{V^{1/2}}\sum_{\boldsymbol{k}} b^*_{\boldsymbol{k}}\,e^{-i\boldsymbol{k}\boldsymbol{x}}\,. \tag{8}$$

Here we have introduced at once the operators a^*, a, b^*, b, which are seen from (3) to obey the commutation relations characterizing creation and absorption operators, i.e.

$$\left.\begin{gathered}[a_{\boldsymbol{k}},a^*_{\boldsymbol{k}'}]=[b_{\boldsymbol{k}},b^*_{\boldsymbol{k}'}]=\delta_{\boldsymbol{k}\boldsymbol{k}'},\\ \text{all other commutators being zero.}\end{gathered}\right\} \tag{9}$$

Then H_{ph} becomes diagonal[3]),

$$H_{\text{ph}}=\sum_{\boldsymbol{k}}\hbar c_0 k\left(n_{\boldsymbol{k}}+\frac{1}{2}\right), \tag{10}$$

where $n_{\boldsymbol{k}}\equiv a^*_{\boldsymbol{k}}a_{\boldsymbol{k}}$ are the numbers of phonons of wave vector $\boldsymbol{k}$. ZIMAN[5]) has shown that H_{rot} takes the form

$$\begin{aligned}H_{\text{rot}}=\frac{\hbar^2}{8\varrho_0 V}\Bigg\{&\sum_{\boldsymbol{k},\boldsymbol{m}}(k^2+m^2)\,b^*_{\boldsymbol{m}}b_{\boldsymbol{m}}+\\ &+\sum_{\boldsymbol{k},\boldsymbol{l},\boldsymbol{m},\boldsymbol{n}}(\boldsymbol{k}+\boldsymbol{n})\,(\boldsymbol{l}+\boldsymbol{m})\,b^*_{\boldsymbol{m}}b^*_{\boldsymbol{n}}b_{\boldsymbol{k}}b_{\boldsymbol{l}}\,\delta_{\boldsymbol{k}+\boldsymbol{l},\boldsymbol{m}+\boldsymbol{n}}\Bigg\}\,.\end{aligned} \tag{11}$$

Here one has to use a cut-off method which allows for the atomistic structure of the liquid and the finite number of degrees of freedom. ZIMAN has made it plausible that the Fourier series for φ, ϱ and Ψ should all be cut off at the same maximum wave number K_0 so that all sums in (7) and (8) are to be taken only over $\boldsymbol{k}$'s with $k \equiv |\boldsymbol{k}| < K_0$. K_0 is determined by the condition that the number of possible $\boldsymbol{k}$'s should equal the number of degrees of freedom, i.e.

$$\sum_{\substack{\boldsymbol{k} \\ k < K_0}} 1 = 3\, N_{\mathrm{at}}\,. \tag{12}$$

N_{at} is the number of atoms in the volume V. We are going to use this cut-off method troughout in our calculations, except in § 7. Replacing the sum in (12) by an integral, we obtain for liquid helium

$$K_0 = \sqrt[3]{18\,\pi^2 \frac{\varrho_0}{m_{\mathrm{He}}}} = 1.57 \times 10^8 \ \mathrm{cm}^{-1} \tag{13}$$

(m_{He} = mass of the helium atom; ϱ_0 = density in the absence of excitations, i.e. at the absolute zero, $\approx 0{\cdot}145 \ \mathrm{g\ cm}^{-3}$ [11])). H_{rot} can be written as

$$H_{\mathrm{rot}} = \sum_{\substack{\boldsymbol{m} \\ m < K_0}} (\Delta_0 + B_0 m^2)\, N_{\boldsymbol{m}} + \\ + \frac{\hbar^2}{8\,\varrho_0 V} \sum_{\substack{\boldsymbol{k},\boldsymbol{l},\boldsymbol{m},\boldsymbol{n} \\ k,l,m,n < K_0}} (\boldsymbol{k}+\boldsymbol{n})\,(\boldsymbol{l}+\boldsymbol{m})\, b^*_{\boldsymbol{m}}\, b^*_{\boldsymbol{n}}\, b_{\boldsymbol{k}}\, b_{\boldsymbol{l}}\, \delta_{\boldsymbol{k}+\boldsymbol{l},\,\boldsymbol{m}+\boldsymbol{n}}\,, \tag{14}$$

where

$$\Delta_0 = \frac{\hbar^2}{8\,\varrho_0 V} \sum_{\substack{\boldsymbol{k} \\ k < K_0}} k^2, \quad B_0 = \frac{\hbar^2}{8\,\varrho_0 V} \sum_{\substack{\boldsymbol{k} \\ k < K_0}} 1. \tag{15}$$

$N_{\boldsymbol{m}} \equiv b^*_{\boldsymbol{m}} b_{\boldsymbol{m}}$ is the number of rotons of wave vector $\boldsymbol{m}$. For liquid helium, the numerical values of the roton rest energy Δ_0 and the maximum kinetic energy $B_0 K_0{}^2$, divided by Boltzmann's constant $\varkappa$, become (using (13))

$$\frac{\Delta_0}{\varkappa} = 6.7^0, \quad \frac{B_0 K_0^2}{\varkappa} = 11.2^0. \tag{16}$$

In comparison, the maximum phonon energy is

$$\frac{\hbar c_0 K_0}{\varkappa} = 28.6^0 \tag{17}$$

($c_0 = 239 \ \mathrm{m\ sec}^{-1}$ [12])).

H_{rot} is diagonal for the states where the total number of rotons

$$N_{\mathrm{rot}} \equiv \sum_{\boldsymbol{m}} N_{\boldsymbol{m}} \tag{18}$$

(which is a constant of the motion) is 0 or 1. The eigenvalues of H_{rot} can also be exactly determined for $N_{\text{rot}} = 2$*). The result is that the eigenvalues show very minor deviations from the spectrum

$$2\,\Delta_0 + B_0\,(m^2 + m'^2) \tag{19}$$

(where $\boldsymbol{m}$ and $\boldsymbol{m}'$ are any wave vectors) which one would have if only the first term on the right hand side of (14) were present. This is not surprising, as, roughly speaking, for $N_{\text{rot}} \ll 3\,N_{\text{at}}$ the second term on the right hand side of (14) gives contributions only of the relative order of magnitude $N_{\text{rot}}/3\,N_{\text{at}}$. For the application to sufficiently low temperatures, when the density of rotons is small, this term is negligible. In what follows we shall ignore it. It can be shown that this is completely legitimate for the calculation of the thermodynamic functions of helium below the λ-temperature.

Thus we have reached the result that the transformations (7) and (8) diagonalize H_{ph} and, to a very good approximation (if $N_{\text{rot}} \ll 3\,N_{\text{at}}$), also H_{rot}. Simultaneously the total momentum

$$\boldsymbol{G} = \int_V d^3x\,\frac{1}{2}\{\varrho\boldsymbol{v} + \boldsymbol{v}\varrho\} \tag{20}$$

becomes diagonal and takes the form

$$\boldsymbol{G} = \sum_{\boldsymbol{k}} \hbar\boldsymbol{k}\,n_{\boldsymbol{k}} + \sum_{\boldsymbol{k}} \hbar\boldsymbol{k}\,N_{\boldsymbol{k}}\,, \tag{21}$$

which shows that the phonons and rotons of wave vector $\boldsymbol{k}$ carry a (linear) momentum $\boldsymbol{p} = \hbar\boldsymbol{k}$.

However, H_{int} (6c) changes the energy spectrum considerably (see also AK). These corrections will be calculated in §§ 5 and 6. Allcock and Kuper have stated that for the calculation of the roton rest energy even the terms (6d)—(6g) cannot be neglected; they will be taken into account in § 6. We finish this section by expressing (6c)—(6g) in terms of the creation and annihilation operators by means of (7) and (8):

$$H_{\text{int}} = -i\sqrt{\frac{\hbar^3 c_0}{8\varrho_0 V}} \sum_{\substack{\boldsymbol{k},\boldsymbol{m}\\ k,m,|\boldsymbol{k}+\boldsymbol{m}|<k_0}} \frac{1}{\sqrt{k}}\,(2\boldsymbol{k}\boldsymbol{m} + k^2)\,(a_{\boldsymbol{k}} + a^*_{-\boldsymbol{k}})\,b^*_{\boldsymbol{k}+\boldsymbol{m}}\,b_{\boldsymbol{m}}\,, \tag{22}$$

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*) The autor is indebted to Professor W. Pauli for very helpful advice in that question.

$$\left.\begin{aligned} H'_{\mathrm{ph}} = &-i\sqrt{\frac{\hbar^3 c_0}{8\varrho_0 V}}\Bigg\{\sum_{\substack{\boldsymbol{k}+\boldsymbol{l}+\boldsymbol{m}=0\\ k,l,m<K_0}}\sqrt{k\,l\,m}\,\frac{1}{6}\,f(\boldsymbol{k},\boldsymbol{l},\boldsymbol{m})\,(a^*_{\boldsymbol{k}}\,a^*_{\boldsymbol{l}}\,a^*_{\boldsymbol{m}} - a_{\boldsymbol{k}}\,a_{\boldsymbol{l}}\,a_{\boldsymbol{m}}) + \\ &+\sum_{\substack{\boldsymbol{m}=\boldsymbol{k}+\boldsymbol{l}\\ k,l,m<K_0}}\sqrt{k\,l\,m}\,\frac{1}{2}\,f(\boldsymbol{k},\boldsymbol{l},\boldsymbol{m})\,(a^*_{\boldsymbol{m}}\,a_{\boldsymbol{k}}\,a_{\boldsymbol{l}} - a^*_{\boldsymbol{k}}a^*_{\boldsymbol{l}}\,a_{\boldsymbol{m}})\Bigg\}, \\ f(\boldsymbol{k},\boldsymbol{l},\boldsymbol{m}) \equiv &\,\frac{\boldsymbol{k}\boldsymbol{l}}{k\,l} + \frac{\boldsymbol{l}\boldsymbol{m}}{l\,m} + \frac{\boldsymbol{m}\boldsymbol{k}}{m\,k} + \frac{\varrho_0^2}{c_0^2}\left(\frac{d}{d\varrho}\,\frac{c^2}{\varrho}\right)_0. \end{aligned}\right\} \quad (23)$$

The term

$$\frac{\varrho_0^2}{c_0^2}\left(\frac{d}{d\varrho}\,\frac{c^2}{\varrho}\right)_0$$

is due to the first anharmonic term in the potential energy. From experiments by ATKINS and STASIOR¹³) its value is found to be about 5; therefore it cannot be neglected a priori.

$$\begin{aligned} H''_{\mathrm{ph}} = \frac{1}{4!}\,\frac{\varrho_0^3}{c_0^2}\left(\frac{d^2}{d\varrho^2}\,\frac{c^2}{\varrho}\right)_0\frac{\hbar^2}{4\varrho_0 V}&\sum_{\substack{\boldsymbol{k}+\boldsymbol{l}+\boldsymbol{m}+\boldsymbol{n}=0\\ k,l,m,n<K_0}}\sqrt{k\,l\,m\,n}\,(a^*_{\boldsymbol{k}}\,a^*_{\boldsymbol{l}}\,a^*_{\boldsymbol{m}}\,a^*_{\boldsymbol{n}} - \\ &-4\,a^*_{\boldsymbol{k}}\,a^*_{\boldsymbol{l}}a^*_{\boldsymbol{m}}a_{-\boldsymbol{n}} + 6\,a^*_{\boldsymbol{k}}\,a^*_{\boldsymbol{l}}\,a_{-\boldsymbol{m}}\,a_{-\boldsymbol{n}} - \\ &-4\,a^*_{\boldsymbol{k}}\,a_{-\boldsymbol{l}}\,a_{-\boldsymbol{m}}\,a_{-\boldsymbol{n}} + a_{-\boldsymbol{k}}\,a_{-\boldsymbol{l}}\,a_{-\boldsymbol{m}}\,a_{-\boldsymbol{n}}). \end{aligned} \quad (24)$$

Here we have arranged the operators in the form of an S-product¹⁰) as mentioned before. Further we have

$$\begin{aligned} H'_{\mathrm{int}} = &-i\sqrt{\frac{\hbar}{2\varrho_0 V c_0}}\sum_{\substack{\boldsymbol{k},\,\boldsymbol{m}\\ k,m,\,|\boldsymbol{k}+\boldsymbol{m}|<K_0}}\sqrt{k}\,(a^*_{-\boldsymbol{k}} - a_{\boldsymbol{k}})\,b^*_{\boldsymbol{k}+\boldsymbol{m}}\,b_{\boldsymbol{m}}\,(\varDelta_0 + B_0\,(\boldsymbol{k}+\boldsymbol{m})\,\boldsymbol{m}) - \\ &-i\,\frac{\hbar^2}{8\varrho_0 V}\sqrt{\frac{\hbar}{2\varrho_0 V c_0}}\sum_{\substack{\boldsymbol{j},\,\boldsymbol{k},\,\boldsymbol{l},\,\boldsymbol{m},\,\boldsymbol{n}\\ j,k,l,m,n<K_0}}\sqrt{j}\,(a^*{}_{\boldsymbol{j}} - a_{-\boldsymbol{j}})\,\times \\ &\times b^*_{\boldsymbol{m}}\,b^*_{\boldsymbol{n}}\,b_{\boldsymbol{k}}\,b_{\boldsymbol{l}}\,(\boldsymbol{k}+\boldsymbol{n})\,(\boldsymbol{l}+\boldsymbol{m})\,\delta_{\boldsymbol{k}+\boldsymbol{l},\,\boldsymbol{j}+\boldsymbol{m}+\boldsymbol{n}}\,. \end{aligned} \quad (25)$$

Of H''_{int} we shall only need the expectation value for no phonons present, so we can immediately take the vacuum expectation value of $(\varrho - \varrho_0)^2$. This yields

$$\begin{aligned} \langle H''_{\mathrm{int}}\rangle_{\text{ph vac.}} = \Bigg(\frac{\hbar^2}{8\varrho_0 V}\sum_{\substack{\boldsymbol{j}\\ j<K_0}} j\Bigg)\Bigg\{&\frac{4}{\hbar c_0}\sum_{\substack{\boldsymbol{m}\\ m<K_0}}(\varDelta_0 + B_0 m^2)\,b^*_{\boldsymbol{m}}\,b_{\boldsymbol{m}} + \\ &+\frac{\hbar}{2\varrho_0 V c_0}\sum_{\substack{\boldsymbol{k},\,\boldsymbol{l},\,\boldsymbol{m},\,\boldsymbol{n}\\ k,l,m,n<K_0}}(\boldsymbol{k}+\boldsymbol{n})\,(\boldsymbol{l}+\boldsymbol{m})\,b^*_{\boldsymbol{m}}\,b^*_{\boldsymbol{n}}\,b_{\boldsymbol{k}}\,b_{\boldsymbol{l}}\,\delta_{\boldsymbol{k}+\boldsymbol{l},\,\boldsymbol{m}+\boldsymbol{n}}\Bigg\}. \end{aligned} \quad (26)$$

Again, as in (14), the terms $\sim b^*\,b^*\,b\,b$ in (25) and (26) can be ignored for small roton densities.

§ 3. Renormalization of the sound velocity.

The term $\sim (\varrho - \varrho_0)^4$ in the development (5) of the potential energy leads to a renormalization problem. This question is independent of the roton fields and, to the approximation considered here, it is also independent of the third order term for the phonons, H'_{ph}. We therefore omit them in this section and investigate only the Hamiltonian

$$\tilde{H} = \int_V d^3x \left\{ \frac{1}{2} \varrho_0 (\nabla \varphi)^2 + \frac{c_0'^2}{2\varrho_0} (\varrho - \varrho_0)^2 + \lambda (\varrho - \varrho_0)^4 \right\}, \tag{27}$$

$$\lambda = \frac{1}{4!} \left(\frac{d^2}{d\varrho^2} \frac{c^2}{\varrho} \right)_0, \tag{28}$$

where $(\varrho - \varrho_0)^4$ is now to be written as it comes from the development of E_p (5) (*not* as an S-product). A new symbol c_0' has been introduced in (27), because the quantity denoted by this will turn out to be different from c_0 of § 2. We develop φ and $\varrho - \varrho_0$ in Fourier series analogous to (7)

$$\left.\begin{aligned} \varphi &= \frac{1}{V^{1/2}} \sum_{\boldsymbol{k}} \beta_k (a_{\boldsymbol{k}} + a^*_{-\boldsymbol{k}})\, e^{i\boldsymbol{k}\boldsymbol{x}} \\ \varrho - \varrho_0 &= \frac{1}{V^{1/2}} \sum_{\boldsymbol{k}} \gamma_k\, i\, (a^*_{\boldsymbol{k}} - a_{-\boldsymbol{k}})\, e^{-i\boldsymbol{k}\boldsymbol{x}}, \end{aligned}\right\} \tag{29}$$

where $a_{\boldsymbol{k}}$ and $a^*_{\boldsymbol{k}}$ are supposed to be annihilation and creation operators respectively, thus obeying the commutation relations for the a's and a^*'s in (9). The functions β_k and γ_k are left undetermined for the moment; we merely assume them to be real c-numbers which depend only on the length of the vector $\boldsymbol{k}$. The commutation rule (3) for ϱ and φ requires that

$$2\, \beta_k \gamma_k = \hbar\,. \tag{30}$$

Now we substitute (29) into (27). By rearranging the a's and a^*'s so as to get all terms into the form of S-products (all a^*'s to the left, all a's to the right) we obtain supplementary terms due to the commutators, and the final result is

$$\begin{aligned} \tilde{H} = {} & \frac{1}{2} \varrho_0 \sum_{\boldsymbol{k}} \beta_k^2 k^2 (a_{\boldsymbol{k}} a_{-\boldsymbol{k}} + a^*_{-\boldsymbol{k}} a^*_{\boldsymbol{k}} + 2\, a^*_{\boldsymbol{k}} a_{\boldsymbol{k}} + 1) + \\ & + \frac{1}{2} \frac{c_0'^2}{\varrho_0} \sum_{\boldsymbol{k}} \gamma_k^2 (- a_{\boldsymbol{k}} a_{-\boldsymbol{k}} - a^*_{-\boldsymbol{k}} a^*_{\boldsymbol{k}} + 2\, a^*_{\boldsymbol{k}} a_{\boldsymbol{k}} + 1) + \\ & + \frac{\lambda}{V} \Big(\sum_{\boldsymbol{m}} \gamma_m^2 \Big) \sum_{\boldsymbol{k}} \gamma_k^2 (- 6\, a_{\boldsymbol{k}} a_{-\boldsymbol{k}} - 6\, a^*_{-\boldsymbol{k}} a^*_{\boldsymbol{k}} + 12\, a^*_{\boldsymbol{k}} a_{\boldsymbol{k}} + 3) + \\ & + \frac{\lambda}{V} \sum_{\boldsymbol{k}+\boldsymbol{l}+\boldsymbol{m}+\boldsymbol{n}=0} \gamma_k \gamma_l \gamma_m \gamma_n (a^*_{\boldsymbol{k}} a^*_{\boldsymbol{l}} a^*_{\boldsymbol{m}} a^*_{\boldsymbol{n}} - 4\, a^*_{\boldsymbol{k}} a^*_{\boldsymbol{l}} a^*_{\boldsymbol{m}} a_{-\boldsymbol{n}} + \\ & + 6\, a^*_{\boldsymbol{k}} a^*_{\boldsymbol{l}} a_{-\boldsymbol{m}} a_{-\boldsymbol{n}} - 4\, a^*_{\boldsymbol{k}} a_{-\boldsymbol{l}} a_{-\boldsymbol{m}} a_{-\boldsymbol{n}} + a_{-\boldsymbol{k}} a_{-\boldsymbol{l}} a_{-\boldsymbol{m}} a_{-\boldsymbol{n}}). \end{aligned} \tag{31}$$

Now we can bring all terms quadratic in a and a^* into diagonal form by choosing β_k and γ_k so that

$$\frac{1}{2}\varrho_0\,\beta_k^2\,k^2 = \left(\frac{1}{2}\,\frac{c_0'^2}{\varrho_0} + 6\,\frac{\lambda}{V}\sum_{\boldsymbol{m}}\gamma_m^2\right)\gamma_k^2. \tag{32}$$

Of the quadratic terms in (31) then only those $\sim a_{\boldsymbol{k}}^*\,a_{\boldsymbol{k}} = n_{\boldsymbol{k}}$ are left. From (30) and (32) β_k and γ_k can be determined. Elimination of β_k yields γ_k as a function of $\hbar$ and the constants occuring in (27) and of $\sum_{\boldsymbol{k}}\gamma_k^2 \equiv \Gamma$. By taking the square and summing over $\boldsymbol{k}$ one obtains an equation of the third degree for Γ. It is, however, much simpler to define a new quantity c_0 by

$$c_0 = \sqrt{c_0'^2 + 12\,\frac{\lambda\varrho_0}{V}\sum_{\boldsymbol{m}}\gamma_m^2} \tag{33}$$

and to express β_k and γ_k in terms of c_0. This is also much more reasonable, for we shall see that c_0 is the physical sound velocity (i.e. the quantity that has to be identified with the speed of sound measured experimentally), whereas c_0' is only an auxiliary quantity which can be expressed in terms of the physical quantities by means of (33). With the definition (33), equ. (30) and (32) yield

$$\beta_k = \sqrt{\frac{\hbar c_0}{2\varrho_0 k}}\,, \quad \gamma_k = \sqrt{\frac{\hbar\varrho_0 k}{2c_0}}\,, \tag{34}$$

and the Hamiltonian takes the following form (where :...: denotes the S-product)

$$\tilde{H} = \sum_{\boldsymbol{k}}\hbar c_0 k\left(a_{\boldsymbol{k}}^*\,a_{\boldsymbol{k}} + \frac{1}{2}\right) - 3\,\frac{\lambda}{V}\left(\sum_{\boldsymbol{k}}\frac{\hbar\varrho_0}{2c_0}\,k\right)^2 + $$

$$+ \frac{\lambda}{V}\left(\frac{\hbar\varrho_0}{2c_0}\right)^2\sum_{\boldsymbol{k}+\boldsymbol{l}+\boldsymbol{m}+\boldsymbol{n}=0}\sqrt{klmn}\,:(a_{\boldsymbol{k}}^* - a_{-\boldsymbol{k}})\,(a_{\boldsymbol{l}}^* - a_{-\boldsymbol{l}})\,(a_{\boldsymbol{m}}^* - a_{-\boldsymbol{m}})\,(a_{\boldsymbol{n}}^* - a_{-\boldsymbol{n}}): \tag{35}$$

or in $\boldsymbol{x}$-space:

$$\tilde{H} = \int_V d^3x\left\{\frac{1}{2}\varrho_0(\nabla\varphi)^2 + \frac{c_0^2}{2\varrho_0}(\varrho - \varrho_0)^2 + \lambda:(\varrho - \varrho_0)^4:\right\} - 3\,\frac{\lambda}{V}\left(\sum_{\boldsymbol{k}}\frac{\hbar\varrho_0}{2c_0}k\right)^2. \tag{36}$$

The equations of motion are

$$\left.\begin{aligned} \dot{\varrho} &\equiv \frac{i}{\hbar}\left[\tilde{H}, \varrho\right] = \varrho_0\,\Delta\varphi \\ \dot{\varphi} &\equiv \frac{i}{\hbar}\left[\tilde{H}, \varphi\right] = \frac{c_0^2}{\varrho_0}\,(\varrho - \varrho_0) + 4\,\lambda:(\varrho - \varrho_0)^3:, \end{aligned}\right\} \tag{37}$$

the commutator of an S-product with an operator linear in a and a^* being again an S-product.

From (37), we gather that sound waves of phase velocity c_0 are possible if the influence of the anharmonic term $4\,\lambda : (\varrho - \varrho_0)^3 :$ is sufficiently small. We shall see that there are cases where this term may be neglected, although c_0 is not even approximately equal to c_0'.

To show this, let us consider a Schrödinger function of the system, which, at a given time, say $t = 0$, is

$$\Phi_{t=0} = D \sum_{n=0}^{\infty} e^{-d(n-n_0)^2 + in\delta} \frac{(a_{\boldsymbol{k}}^*)^n}{\sqrt{n!}} \,| 0 > . \tag{38}$$

$| 0 >$ and $(n!)^{-\frac{1}{2}} (a_{\boldsymbol{k}}^*)^n | 0 >$ are normalized eigenvectors of the operators $a_{\boldsymbol{m}}^* \, a_{\boldsymbol{m}} = n_{\boldsymbol{m}}$, the first for all $n_{\boldsymbol{m}} = 0$, and the second for $n_{\boldsymbol{k}} = n$ and all other $n_{\boldsymbol{m}} = 0$ ($\boldsymbol{m} \neq \boldsymbol{k}$). D is determined by the condition

$$D^2 \sum_{n=0}^{\infty} e^{-2d(n-n_0)^2} = 1 \tag{39}$$

in order that Φ be normalized, too. Further we assume

$$\sqrt{d} \cdot n_0 \gg 1, \qquad \sqrt{d} \ll 1; \tag{40}$$

this means that $D^2 e^{-2d(n-n_0)^2}$ is practically a δ-function*). From (29), (34) and (38) the expectation values of $\varrho - \varrho_0$ and φ at $t = 0$ are seen to be

$$\langle \varrho - \varrho_0 \rangle_{t=0} = A \sin(\boldsymbol{k}\boldsymbol{x} + \delta), \quad \langle \varphi \rangle_{t=0} = \frac{c_0}{\varrho_0 k} A \cos(\boldsymbol{k}\boldsymbol{x} + \delta), \tag{41}$$

where

$$A = \sqrt{\frac{2\,\hbar\,\varrho_0\,k\,n_0}{V c_0}}, \tag{42}$$

terms of relative order $1/n_0$ being neglected. The equations of motion (37), which are knwon to hold for the expectation values as well[14]), give for $t = 0$

$$\left.\begin{aligned} \left[\frac{\partial}{\partial t} \langle \varrho - \varrho_0 \rangle\right]_{t=0} &= \langle \dot{\varrho} \rangle_{t=0} = -c_0\, k\, A \cos(\boldsymbol{k}\boldsymbol{x} + \delta) \\ \left[\frac{\partial}{\partial t} \langle \varphi \rangle\right]_{t=0} &= \langle \dot{\varphi} \rangle_{t=0} = \frac{c_0^2}{\varrho_0} A \sin(\boldsymbol{k}\boldsymbol{x} + \delta) + 4\lambda\, A^3 \sin^3(\boldsymbol{k}\boldsymbol{x} + \delta)\,. \end{aligned}\right\} \tag{43}$$

Evidently, if there were no anharmonic term in (37), the expectation values for any time t would be

$$\langle \varrho - \varrho_0 \rangle_t = A \sin(\boldsymbol{k}\boldsymbol{x} - c_0 k t + \delta), \quad \langle \varphi \rangle_t = \frac{c_0}{\varrho_0 k} A \cos(\boldsymbol{k}\boldsymbol{x} - c_0 k t + \delta). \tag{44}$$

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*) For our purpose, however, we cannot take a state where the number $n_{\boldsymbol{k}}$ is exactly given at $t = 0$, because the expectation values of $\varrho - \varrho_0$ and φ would then be zero.

But even with the anharmonic term present, (44) is an approximate solution during a time t not too long but still containing many periods $2\,\pi/c_0 k$, provided that

$$|\lambda|\,A^2 \ll \frac{c_0^2}{\varrho_0}\,. \tag{45}$$

If we suppose $|\lambda|$ (28) to be of the order of c_0^2/ϱ_0^3 (its experimental value is uncertain, but probably negative[13])), condition (45) requires (see (42))

$$n_0 \ll \frac{\varrho_0 V c_0}{\hbar k} \approx 10^{30}\,\mathrm{cm}^{-4}\,.\,\frac{V}{k} \text{ for liquid He.} \tag{46}$$

Hence for a macroscopic volume ($V \approx 1$ cm^3), one can easily find an n_0 that satisfies (45) and (40) simultaneously, even if $|\lambda|$ is several orders of magnitude larger than c_0^2/ϱ_0^3 and k an ultrasonic wave number ($k \gg 1$ cm^{-1}). Thus we have demonstrated that states exist which correspond to macroscopic sound waves of phase velocity c_0.

The proof that in certain cases the terms arising from the expression $4\,\lambda\!:\!(\varrho-\varrho_0)^3\!:$ in (37) are negligible has only been possible because this term is an S-product. If we had simply $4\,\lambda\,(\varrho-\varrho_0)^3$ instead, the terms with an a^* to the right of an a would give rise to the creation and annihilation of virtual quanta. They would produce supplementary terms linear in A in the lower equation (43), which, in general, would not at all be negligible. This statement is equivalent to the statement that c_0 may be quite different from c_0'.

To see this let us look at equation (33). We have to compare c_0^2 and $12\,(\lambda\,\varrho_0/V)\,\sum\limits_m \gamma_m^2$. According to (34), $\sum\limits_m \gamma_m^2$ diverges without a cut-off, hence the mathematical quantity c_0' would have to be infinite (λ being negative). But also with the cut-off of § 2 and λ of the order of c_0^2/ϱ_0^3 the quantity $12\,(|\lambda|\,\varrho_0/V)\,\sum\limits_m \gamma_m^2$ is seen to be larger than c_0^2 for the helium data.

By comparing (41) and (43) with the classical equations of motion derived from the Hamiltonian (27), we see that λ, in contrast to c_0', means the same physical quantity in quantum hydrodynamics as in the classical theory. Further terms with higher powers of $\varrho-\varrho_0$ in the Hamiltonian (27), e.g. a term $\sim(\varrho-\varrho_0)^6$, would of course renormalize λ as well as c_0'.

As the Hamiltonian (36) is identical with $H_{\mathrm{ph}} + H''_{\mathrm{ph}}$ (6), apart from the irrelevant constant $-\,3\,(\lambda/V)\,(\sum\limits_k \hbar\,\varrho_0\,k/2\,c_0)^2$, we see that c_0 in § 2 already means the physical (renormalized) sound velocity.

§ 4. Remarks on the order of factors in H.

An alternative treatment of the problem of § 3 consists in immediately writing the fourth order term in the Hamiltonian (27) as an S-product and omitting the commutators by the argument that classically the order of factors is irrelevant. Then the results of § 3 are obtained without any renormalization. It is perhaps not very natural to write an S-product a priori because in $\boldsymbol{x}$-space this is a complicated non-local expression. But in $\boldsymbol{k}$-space it is very simple.

This opens the question of what happens if we alter the order of factors in other terms of the basic Hamiltonian (6), e.g. by writing them as S-products (which is probably the only reasonable ordering different from the one used in (6)).

In H_{ph} (6a) the reordering of factors can only produce irrelevant additive constants. In H_{int} (6c) and H'_{ph} (6d) the a's and a^*'s can be permuted arbitrarily, since all commutators vanish (see (22) and (23)). The order of factors in H_{rot} (6b) has been studied by ALLCOCK and KUPER. They conclude that any non-trivial alteration in (6b) violates all of the three requirements that H_{rot} shall be positive-definite*), gauge-invariant (i.e. invariant under simultaneous transformations of φ, Ψ and Ψ^* which do not alter the velocity (2)), and shall lead to the correct equations of motion for $\boldsymbol{v}$ and ϱ**). As to (6f) and (6g), they arise from multiplication of $\{\Psi^* \nabla \Psi - \nabla \Psi^* \Psi\}^2$ in (6b) by the successive terms of the expansion (4) of $1/\varrho$. Consequently the arrangement of the Ψ's and Ψ^*'s in (6f) and (6g) must be the same as in (6b). The last possibility is to arrange the a's and a^*'s in $(\varrho - \varrho_0)^2$, equation (6g), differently. But if we multiply the expansion on the right hand side of (4) by $\varrho = \varrho_0 + (\varrho - \varrho_0)$, the result must, by definition, be equal to unity. This is only true if no term in (4) is altered.

Thus the investigations of §§ 3 and 4 have given a full justification of the Hamiltonian (6), and we are now ready to calculate its lowest eigenvalues.

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*) It is easy to see that H_{rot} (6b), when written as an S-product, has negative eigenvalues for $N = 2$. Also, if $H_{\mathrm{ph}} + H_{\mathrm{rot}} + H_{\mathrm{int}}$ (which classically is positive definite) is taken as an S-product, it has negative eigenvalues in the perturbation approximation for large c_0.

**) This can only be understood if one has a definite opinion about the order of factors in the equations of motion.

§ 5. The roton energy to order $\mathbf{c_0^0}$.

We take

$$H_0 = H_{\mathrm{ph}} + H_{\mathrm{rot}} \tag{47}$$

as unperturbed energy with the eigenvalues

$$E_\alpha = \sum_{\substack{\boldsymbol{k} \\ k < K_0}} \hbar\, c_0\, k \left(n_{\boldsymbol{k}} + \frac{1}{2}\right) + \sum_{\substack{\boldsymbol{m} \\ m < K_0}} (\Delta_0 + B_0\, m^2)\, N_{\boldsymbol{m}}\,. \tag{48}$$

α is characterized by the quantum numbers $n_{\boldsymbol{k}}$ and $N_{\boldsymbol{m}}$. All other terms of (6),

$$H' = H_{\mathrm{int}} + H'_{\mathrm{ph}} + H''_{\mathrm{ph}} + \cdots + H'_{\mathrm{int}} + H''_{\mathrm{int}} + \cdots, \tag{49}$$

are considered as a perturbation. As $\varrho - \varrho_0$ is proportional to $c_0^{-\frac{1}{2}}$ (see (7)), (6) can be considered as a development in negative powers of c_0. The different constituents of H are proportional to the powers of c_0 written below as follows

$$\left.\begin{array}{ccccccccc} H_0 & H_{\mathrm{int}} & H'_{\mathrm{ph}} & H''_{\mathrm{ph}} & \cdots & H'_{\mathrm{int}} & H''_{\mathrm{int}} & & \cdots \\ c_0 & c_0^{\frac{1}{2}} & c_0^{\frac{1}{2}*)} & c_0^{0*)} & \cdots & c_0^{-\frac{1}{2}} & c_0^{-1} & & \cdots \end{array}\right\} \tag{50}$$

A perturbative treatment of H' will therefore yield an expansion of the energy eigenvalues in negative powers of c_0, as Allcock and Kuper's method does. The *dimensionless* perturbation parameter in question turns out to be the ratio of the maximum kinetic energy of the unperturbed rotons to the maximum phonon energy

$$\varepsilon = \frac{B_0 K_0^2}{\hbar\, c_0 K_0}\,. \tag{51}$$

For $c_0 \gg B K_0/\hbar$ we may expect good results. In the case of liquid helium the data (16) and (17) give

$$\varepsilon = 0{\cdot}4\,, \tag{52}$$

so we might obtain at least something of the right order of magnitude.

For all perturbed energies (phonon energy, rest and kinetic energies of the roton) we only calculate the highest term in c_0 that is different from zero. Nothing of the order c_0 is added to the unperturbed energies, so we do not compute any correction to the phonon energy.

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*) We have assumed that $(d/d\varrho\; c^2/\varrho)_0$ and $(d^2/d\varrho^2\; c^2/\varrho)_0$ are of the order of magnitude of c_0^2/ϱ_0^2 and c_0^2/ϱ_0^3 respectively. For liquid helium this is justified for the first term[13]); for the second term it is a reasonable supposition.

The only correction to the roton energy $\sim c_0^0$ comes from the second order perturbation expression

$$W_{\alpha\alpha}^{(2)} = \sum_{\beta}{}' \frac{H'_{\alpha\beta} H'_{\beta\alpha}}{E_\alpha - E_\beta} \qquad (53)$$

through the term

$$E'_\alpha = \sum_{\beta} \frac{|(H_{\mathrm{int}})_{\beta\alpha}|^2}{E_\alpha - E_\beta} . \qquad (54)$$

The terms of the form $\sum\limits_{\beta} (H'_{\mathrm{ph}})_{\alpha\beta} \, (H_{\mathrm{int}})_{\beta\alpha} / (E_\alpha - E_\beta)$ would seem to give a contribution $\sim c_0^0$ too, but in view of (22) and (23) they vanish. (54) and (22) give

$$\begin{aligned} E'_\alpha = \frac{\hbar^3 c_0}{8 \varrho_0 V} \sum_{\substack{\boldsymbol{k},\boldsymbol{m} \\ k,m,|\boldsymbol{k}+\boldsymbol{m}|<K}} \frac{(2\boldsymbol{k}\boldsymbol{m}+k^2)^2}{k} (N_{\boldsymbol{k}+\boldsymbol{m}}+1) N_{\boldsymbol{m}} \times \\ \times \left[\frac{n_{\boldsymbol{k}}}{\hbar c_0 k - B_0 (k^2 + 2\boldsymbol{k}\boldsymbol{m})} + \frac{n_{-\boldsymbol{k}}+1}{-\hbar c_0 k - B_0 (k^2 + 2\boldsymbol{k}\boldsymbol{m})} \right] . \end{aligned} \qquad (55)$$

In the case of liquid helium the denominators can never vanish because of (51), (52) and the condition k, m, $|\boldsymbol{k}+\boldsymbol{m}| < K_0$. For the same reason as earlier we neglect in (55) the terms of higher than the first degree in the N's and n's, i.e. we take only*)

$$E'_\alpha \cong - \frac{\hbar^2}{8 \varrho_0 V} \sum_{\substack{\boldsymbol{k},\boldsymbol{m} \\ k,m,|\boldsymbol{k}+\boldsymbol{m}|<K_0}} \frac{(2\boldsymbol{k}\boldsymbol{m}+k^2)^2}{k^2} N_{\boldsymbol{m}} \frac{1}{1 + \dfrac{B_0 (k^2 + 2\boldsymbol{k}\boldsymbol{m})}{\hbar c_0 k}} . \qquad (56)$$

For a fixed $\boldsymbol{m}$ we replace the sum over $\boldsymbol{k}$ by an integral and introduce polar coordinates with $\boldsymbol{m}$ as axis ($z = \cos\vartheta = \boldsymbol{k}\boldsymbol{m}/km$). This leads to an integral of the form

$$\int_0^{K_0} k^2 \, dk \int_{-1}^{+1} dz \ldots$$

$$(k^2 + 2 k m z + m^2 < K_0^2)$$

As long as $k + m < K_0$, z may vary between -1 and $+1$. If

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*) For small k, $n_{\boldsymbol{k}}$ may be large even at low temperatures, but in the calculation of the thermodynamic functions the influence of small k's is strongly reduced by the factor k^2 in $\int_0^{K_0} k^2 \, dk \cdots$. An exact analysis shows that it is completely negligible for helium below the λ-temperature.

$k + m > K_0$, z is restricted to values between -1 and $(K_0^2 - k^2 - m^2)/2\,km$. Therefore we get finally

$$E'_\alpha \cong -\sum_{\substack{m \\ m<K_0}} N_m \frac{\hbar^2}{8\varrho_0 V} \frac{V}{(2\pi)^3} \cdot 2\pi \times$$

$$\times \left(\int_0^{K_0-m} dk \int_{-1}^{+1} dz + \int_{K_0-m}^{K_0} dk \int_{-1}^{\frac{K_0^2-k^2-m^2}{2km}} dz \right) \frac{(2\,kmz+k^2)^2}{1+\dfrac{B_0(k^2+2\,kmz)}{\hbar c_0 k}} \,. \tag{57}$$

This integral can of course be evaluated analytically, but gives a rather involved expression. However, we can develop the denominator in powers of $B_0(k^2 + 2\,kmz)/\hbar c_0 k$ (which is always smaller than 1); this gives just the expansion in powers of ε. Besides we are interested only in small wave numbers m, so we expand (57) also in powers of m. This yields

$$\begin{aligned} E'_\alpha \cong \sum_{\substack{m \\ m<K_0}} N_m \Big[& -\Delta_0 \left(1 - \frac{5}{6}\varepsilon + \frac{5}{7}\varepsilon^2 - \cdots\right) + \\ & + B_0 K_0 m \left(\frac{3}{4} - \frac{3}{4}\varepsilon + \frac{3}{4}\varepsilon^2 - \cdots\right) + \\ & + B_0 m^2 \left(\frac{1}{6} + \frac{3}{4}\varepsilon - \frac{9}{5}\varepsilon^2 \cdots\right) + \cdots \Big] . \end{aligned} \tag{58}$$

We have thus reached the result of AK that to order c_0^0 the rest energy ($m = 0$) of the roton in (48) is exactly compensated by (58). Therefore we have to carry the calculation of the rest energy further to order c_0^{-1}, and all terms written down in (49) and (50) have to be taken into account. Fortunately this is not necessary for the kinetic energy (terms $\sim m, m^2$).

If one evaluates (57) exactly in ε, but develops in powers of m, one obtains for $\varepsilon = 0{\cdot}4$

$$E'_\alpha \cong \sum_{\substack{m \\ m<K_0}} N_m [-0{\cdot}76\,\Delta_0 + 0{\cdot}54\,B_0 K_0 m + 0{\cdot}29\,B_0 m^2 + \cdots], \tag{59}$$

which shows that already the first terms of the expansions in (58) give good results.

The restriction of the calculations to small m is sufficient for low temperature investigations. The factors $\exp[-(\Delta + B_0 m^2)/kT]$ in the partition function give only minor contributions for large m, because $B_0 K_0^2/\varkappa T = 11{\cdot}2^0/T$; therefore the exact shape of the energy for large m is not important, unless the unperturbed energy for large m is strongly modified by H_{int}. But an exact evaluation of (56) for $m = K_0$ shows that the correction to $\varDelta_0 + B_0 K_0^2$ is only $- 0{\cdot}51\ \varDelta_0$ for $\varepsilon = 0{\cdot}4$.

We have only calculated the energy corrections due to the *diagonal* elements of the second order perturbation matrix (53). There exist non-diagonal elements of $W^{(2)}$

$$W^{(2)}_{\gamma\alpha} = \sum_{\beta}{}' \frac{H'_{\gamma\beta} H'_{\beta\alpha}}{E_\alpha - E_\beta} \tag{60}$$

"on the energy shell" (i.e. for $E_\gamma = E_\alpha$), corresponding to scattering between rotons and phonons. These non-diagonal elements influence the energy eigenvalues, but again, for the case of small phonon and roton densities, they can be neglected.

§ 6. The rest energy of the rotons to order c_0^{-1}.

In order to avoid unnecessary complications, we consider now a state α where N_0 rotons of wave number $\boldsymbol{0}$ are present, all other $N_{\boldsymbol{m}}$'s being zero. This is sufficient because we do not calculate the kinetic roton energy to order c_0^{-1}. We also suppose all $n_{\boldsymbol{k}}$'s to be zero. The argument is the same as in § 5: For small phonon densities the terms $\sim n_{\boldsymbol{k}} N_{\boldsymbol{m}}$ can be neglected.

We expect contributions from the perturbation matrices of first, second, third and fourth order, viz.

$$W^{(1)}_{\alpha\alpha} = H'_{\alpha\alpha}, \tag{61a}$$

$$W^{(2)}_{\alpha\alpha} = \sum_{\beta}{}' \frac{H'_{\alpha\beta} H'_{\beta\alpha}}{E_\alpha - E_\beta}, \tag{61b}$$

$$W^{(3)}_{\alpha\alpha} = \sum_{\beta,\gamma}{}' \frac{H'_{\alpha\gamma} H'_{\gamma\beta} H'_{\beta\alpha}}{(E_\alpha - E_\beta)(E_\alpha - E_\gamma)}, \tag{61c}$$

$$W^{(4)}_{\alpha\alpha} = \sum_{\beta,\gamma,\delta}{}' H'_{\alpha\delta} H'_{\delta\gamma} H'_{\gamma\beta} H'_{\beta\alpha} \left\{ \frac{1}{(E_\alpha - E_\beta)(E_\alpha - E_\gamma)(E_\alpha - E_\delta)} \bigg|_{E_\gamma \neq E_\alpha} - \right.$$
$$\left. - \frac{1}{2} \frac{1}{(E_\alpha - E_\beta)^2 (E_\alpha - E_\delta)} \bigg|_{E_\gamma = E_\alpha} - \frac{1}{2} \frac{1}{(E_\alpha - E_\beta)(E_\alpha - E_\delta)^2} \bigg|_{E_\gamma = E_\alpha} \right\}. \tag{61d}$$

For the particular state α, characterized above, there are no non-diagonal matrix elements $W^{(s)}_{\varepsilon\alpha}$, similar to (60), on the energy shell. The reason is that all constituents of H' conserve the total number of rotons. The energy E_α of the state α is $N_0\ \varDelta_0$ (apart from the zero point energy of the phonons). Hence the energy E_ε of the state ε is $N_0\ \varDelta_0$ + kinetic roton energies + energies of phonons produced, which are all positive contributions. E_ε is equal to E_α only if there are no rotons with a momentum $\hbar \boldsymbol{m} \neq 0$ and no phonons in the state ε, i.e. if $\varepsilon = \alpha$.

Now let us look at the different parts of H' (49). Their orders of magnitude are given by (50) and their structures in the creation and annihilation operators by (22)—(26). It is easy to see that there are no energy corrections of order $c_0^{-\frac{1}{2}}$. The contributions of order c_0^{-1} to the $W^{(s)}$, (61a)–(61d), arise from the following terms (apart from the contribution calculated in § 5):

$$W^{(1)}_{\alpha\alpha}: \qquad (H''_{\text{int}})_{\alpha\alpha} \tag{62a}$$

$$W^{(2)}_{\alpha\alpha}: \qquad \sim H_{\text{int}}\, H'_{\text{int}} \tag{62b}$$

$$W^{(3)}_{\alpha\alpha}: \qquad \text{no contributions} \tag{62c}$$

$$W^{(4)}_{\alpha\alpha}: \qquad \sim H^4_{\text{int}}, \ \sim H^3_{\text{int}}\, H'_{\text{ph}}, \ \sim H^2_{\text{int}}\, H'^2_{\text{ph}}. \tag{62d}$$

It is obvious what is meant by the symbols used here: For instance $\sim H^3_{\text{int}}\, H'_{\text{ph}}$ means that three of the factors $H'_{\sigma\tau}$ in (61d) are replaced by $(H_{\text{int}})_{\sigma\tau}$ and one by $(H'_{\text{ph}})_{\sigma\tau}$, of course in all possible permutations. Other contributions $\sim c_0^{-1}$ than (62a)—(62d) do not occur. In particular, there is no term $\sim H^2_{\text{int}}\, H''_{\text{ph}}$ in (62c), just *because* H''_{ph} (24) *is an S-product.* So we have the result that H''_{ph} does not give any contribution to the roton energy in order c_0^{-1}.

The calculation of (62a) and (62b) is simple. By using (26) and taking into account that

$$\frac{\hbar^2}{8\,\varrho_0 V} \sum_{\substack{\boldsymbol{k} \\ k < K_0}} k = \frac{3}{4}\, B_0 K_0 \tag{63}$$

(look at (15) and replace the sums by integrals) we get

$$(H''_{\text{int}})_{\alpha\alpha} = 3\, \Delta_0\, \varepsilon\, N_0 . \tag{64}$$

In view of (22) and (25) the contribution to $W^{(2)}_{\alpha\alpha}$ (62b) becomes

$$\sum_\beta \frac{(H_{\text{int}})_{\alpha\beta} (H'_{\text{int}})_{\beta\alpha}}{E_\alpha - E_\beta} + \sum_\beta \frac{(H'_{\text{int}})_{\alpha\beta} (H_{\text{int}})_{\beta\alpha}}{E_\alpha - E_\beta} =$$

$$= -3\, \Delta_0\, \varepsilon \left[1 - \frac{4}{5}\, \varepsilon + \frac{4}{6}\, \varepsilon^2 - \cdots \right] N_0 . \tag{65}$$

In order to evaluate (62d), we first take the term $\sim H^4_{\text{int}}$ i. e. equation (61d) with each H' replaced by H_{int}. Now if we look at (22) and remember our special state α, we see that the state β (see

(61 d)) can only be of the following type: There are N_0-1 rotons of momentum $\boldsymbol{0}$, one roton of momentum $\hbar\boldsymbol{k}$ and one phonon of momentum $-\hbar\boldsymbol{k}$. $\boldsymbol{k}$ may be any wave vector for which $k < K_0$. For the state γ, however, there are several possibilities. For instance, there may still be N_0-1 rotons of momentum $\boldsymbol{0}$, one roton of momentum $\hbar(\boldsymbol{k}+\boldsymbol{m})$ and two phonons of momenta $-\hbar\boldsymbol{k}$ and $-\hbar\boldsymbol{m}$ respectively. $\boldsymbol{m}$ is subject to the restrictions $m < K_0$ and $|\boldsymbol{k}+\boldsymbol{m}| < K_0$. As δ must be an intermediate state between γ and α there are two possibilities in the case of the γ chosen above, namely (A) δ is identical with β or (B) δ contains one roton of momentum $\hbar\boldsymbol{m}$ and one phonon of momentum $-\hbar\boldsymbol{m}$, apart from the N_0-1 rotons of momenta $\boldsymbol{0}$. In the first case the contribution to (61 d) is

$$(A) \qquad C \sum_{\substack{\boldsymbol{k},\boldsymbol{m} \\ k,m,|\boldsymbol{k}+\boldsymbol{m}|<K_0}} \left[-\frac{k\,(2\,\boldsymbol{k}\boldsymbol{m}+m^2)^2}{m\,(k+m)}\right] N_0$$

with the abbreviation

$$C = \left(-i\sqrt{\frac{\hbar^3 c_0}{8\,\varrho_0 V}}\right)^4 \frac{1}{(\hbar c_0)^3} = \left(\frac{\hbar^2}{8\,\varrho_0 V}\right)^2 \frac{1}{\hbar c_0}\,, \tag{66}$$

and in the second case

$$(B) \qquad C \sum_{\substack{\boldsymbol{k},\boldsymbol{m} \\ k,m,|\boldsymbol{k}+\boldsymbol{m}|<K_0}} \left[-\frac{(2\,\boldsymbol{k}\boldsymbol{m}+k^2)\,(2\,\boldsymbol{k}\boldsymbol{m}+m^2)}{k+m}\right] N_0\,.$$

In the energy denominators the roton energies are neglected; they only yield corrections $\sim c_0^{-2}$ to $W_{\alpha\alpha}^{(4)}$.

Another possible state γ is the following one. There are N_0-2 rotons of momenta $\boldsymbol{0}$, one roton of momentum $\hbar\boldsymbol{k}$ and one of momentum $\hbar\boldsymbol{m}$, and two phonons of momenta $-\hbar\boldsymbol{k}$ and $-\hbar\boldsymbol{m}$ respectively. Here we have only the conditions $k < K_0$ and $m < K_0$, but *not* $|\boldsymbol{k}+\boldsymbol{m}| < K_0$. For δ there are the same two possibilities as before. So we obtain two further contributions to (61 d), namely

$$(C) \qquad C \sum_{\substack{\boldsymbol{k},\boldsymbol{m} \\ k,m<K_0}} \left[-\frac{k\,m^3}{k+m}\right] N_0\,(N_0-1)$$

and

$$(D) \qquad C \sum_{\substack{\boldsymbol{k},\boldsymbol{m} \\ k,m<K_0}} \left[-\frac{k^2 m^2}{k+m}\right] N_0\,(N_0-1).$$

The last possibility is that γ is identical with α, and δ contains

N_0-1 rotons of momenta $\boldsymbol{0}$, one roton of momentum $\hbar\boldsymbol{m}$ and one phonon of momentum $-\hbar\boldsymbol{m}$. This gives

$$(E) \qquad C\sum_{\substack{\boldsymbol{k},\boldsymbol{m}\\ k,m<K_0}}\left[\frac{1}{2}\,k\,m^2+\frac{1}{2}\,k^2\,m\right]N_0^2 .$$

Again, there is no correlation between $\boldsymbol{k}$ and $\boldsymbol{m}$.

(A), (B), (C), (D) and (E) are all contributions to (61 d) due to H_{int} alone. We have not considered the terms where $\boldsymbol{k}=\boldsymbol{m}$ or where γ contains no phonons but two rotons of opposite momenta $\hbar\boldsymbol{k}$ and $-\hbar\boldsymbol{k}$. These terms are of the type $1/V^2\sum_{\boldsymbol{k}}\ldots$, not $1/V^2\sum_{\boldsymbol{k}}\sum_{\boldsymbol{m}}\ldots$, and therefore they give an energy contribution of relative order $1/3\ N_{\text{at}}$ (N_{at} = number of atoms in V) which tends to zero for a macroscopic sample of the liquid.

Adding up (C) and (D), we see that the denominator is cancelled by a factor $k+m$ in the numerator. Taking into account that $\boldsymbol{k}$ and $\boldsymbol{m}$ in each term may be interchanged, we see that the terms $\sim N_0^2$ in (C), (D) and (E) cancel. The final result of (A) + (B) + (C) + (D) + (E) is:

$$C\left\{\sum_{\substack{\boldsymbol{k},\boldsymbol{m}\\ k,m,\,|\boldsymbol{k}+\boldsymbol{m}|<K_0}}\left[-\frac{4\,(\boldsymbol{k}\,\boldsymbol{m})^2}{k}-4\,m\,(\boldsymbol{k}\boldsymbol{m})-k\,m^2\right]+\sum_{\substack{\boldsymbol{k},\boldsymbol{m}\\ k,m<K_0}}k\,m^2\right\}N_{\boldsymbol{0}} \qquad (67)$$

The contributions $\sim H_{\text{int}}^3\,H'_{\text{ph}}$ and $\sim H_{\text{int}}^2\,H'^2_{\text{ph}}$ in (62 d) are evaluated in a similar way. First we take those with one factor H'_{ph} in (61 d). The terms $\sim (H'_{\text{ph}})_{\alpha\delta}(H_{\text{int}})_{\delta\gamma}(H_{\text{int}})_{\gamma\beta}(H_{\text{int}})_{\beta\alpha}$ and $\sim (H_{\text{int}})_{\alpha\delta}\times\times(H_{\text{int}})_{\delta\gamma}(H_{\text{int}})_{\gamma\beta}(H'_{\text{ph}})_{\beta\alpha}$ together yield (see (22) and (23))

$$(A') \qquad 2\,C\sum_{\substack{\boldsymbol{k}+\boldsymbol{l}+\boldsymbol{m}=0\\ k,l,m<K_0}}k\,(2\,\boldsymbol{k}\,\boldsymbol{l}+l^2)\,(-\,m^2)\,\frac{f(\boldsymbol{k},\boldsymbol{l},\boldsymbol{m})}{(k+l)\,(k+l+m)}\,N_{\boldsymbol{0}},$$

and the terms $\sim(H_{\text{int}})_{\alpha\delta}(H'_{\text{ph}})_{\delta\gamma}(H_{\text{int}})_{\gamma\beta}(H_{\text{int}})_{\beta\alpha}$ and $\sim(H_{\text{int}})_{\alpha\delta}(H_{\text{int}})_{\delta\gamma}\times\times(H'_{\text{ph}})_{\gamma\beta}(H_{\text{int}})_{\beta\alpha}$ give

$$(B') \qquad 2\,C\sum_{\substack{\boldsymbol{k}+\boldsymbol{l}+\boldsymbol{m}=0\\ k,l,m<K_0}}k\,(2\,\boldsymbol{k}\,\boldsymbol{l}+l^2)\,m^2\,\frac{f(\boldsymbol{k},\boldsymbol{l},-\boldsymbol{m})}{(k+l)\,m}\,N_{\boldsymbol{0}}.$$

Then we take the contributions due to two factors H'_{ph} in (61 d). The terms $\sim(H'_{\text{ph}})_{\alpha\delta}(H'_{\text{ph}})_{\delta\gamma}(H_{\text{int}})_{\gamma\beta}(H_{\text{int}})_{\beta\alpha}$ and $\sim(H_{\text{int}})_{\alpha\delta}(H_{\text{int}})_{\delta\gamma}(H'_{\text{ph}})_{\gamma\beta}$ $(H'_{\text{ph}})_{\beta\alpha}$ yield

$$(C') \qquad 2\,C\left\{\sum_{\substack{\boldsymbol{k}\\ k<K_0}}\ \sum_{\substack{\boldsymbol{l}+\boldsymbol{m}+\boldsymbol{n}=0\\ l,m,n<K_0}}k^3\,l\,m\,n\cdot\frac{1}{6}\,f^2(\boldsymbol{l},\boldsymbol{m},\boldsymbol{n})\times\right.$$
$$\times\left[\frac{1}{2}\,\frac{1}{k^2(l+m+n)}+\frac{1}{2}\,\frac{1}{k\,(l+m+n)^2}\right]+$$
$$\left.+\sum_{\substack{\boldsymbol{k}+\boldsymbol{l}+\boldsymbol{m}=0\\ k,l,m<K_0}}k^4\,l\,m\,\frac{f(-\boldsymbol{k},\boldsymbol{l},\boldsymbol{m})\,f(\boldsymbol{k},\boldsymbol{l},\boldsymbol{m})}{2\,k^2(k+l+m)}\right\}N_{\boldsymbol{0}},$$

and the terms $\sim (H'_{\mathrm{ph}})_{\alpha\delta}(H_{\mathrm{int}})_{\delta\gamma}(H'_{\mathrm{ph}})_{\gamma\beta}(H_{\mathrm{int}})_{\beta\alpha}$ and $\sim (H_{\mathrm{int}})_{\alpha\delta}(H_{\mathrm{ph}})_{\delta\gamma} \times$ $\times (H_{\mathrm{int}})_{\gamma\beta}(H'_{\mathrm{ph}})_{\beta\alpha}$ give

$$(D')\qquad 2\,C\Bigg\{\sum_{\substack{\boldsymbol{k}\\ k<K_0}}\;\sum_{\substack{\boldsymbol{l}+\boldsymbol{m}+\boldsymbol{n}=0\\ l,\,m,\,n<K_0}} k^3\,l\,m\,n\left[-\frac{(1/6)\,f^2(\boldsymbol{l},\boldsymbol{m},\boldsymbol{n})}{k(l+m+n)\,(k+l+m+n)}\right]+$$

$$+\sum_{\substack{\boldsymbol{k}+\boldsymbol{l}+\boldsymbol{m}=0\\ k,\,l,\,m<K_0}} k^4\,l\,m\left[-\frac{(1/2)\,f^2(\boldsymbol{k},\boldsymbol{l},\boldsymbol{m})}{k\,(k+l+m)\,(2\,k+l+m)}+\frac{(1/2)\,f(\boldsymbol{k},\boldsymbol{l},\boldsymbol{m})\,f(-\boldsymbol{k},\boldsymbol{l},\boldsymbol{m})}{k\,(l+m)\,(k+l+m)}\right]\Bigg\}\,N_0\,.$$

From the term $\sim (H_{\mathrm{int}})_{\alpha\delta}(H'_{\mathrm{ph}})_{\delta\gamma}(H'_{\mathrm{ph}})_{\gamma\beta}(H_{\mathrm{int}})_{\beta\alpha}$ we obtain the contribution

$$(E')\qquad C\Bigg\{\sum_{\substack{\boldsymbol{k}\\ k<K_0}}\;\sum_{\substack{\boldsymbol{l}+\boldsymbol{m}+\boldsymbol{n}=0\\ l,\,m,\,n<K_0}} k^3\,l\,m\,n\left[-\frac{(1/6)\,f^2(\boldsymbol{l},\boldsymbol{m},\boldsymbol{n})}{k^2(k+l+m+n)}\right]+$$

$$+\sum_{\substack{\boldsymbol{k}+\boldsymbol{l}+\boldsymbol{m}=0\\ k,\,l,\,m<K_0}} k^4\,l\,m\left[-\frac{(1/2)\,f^2(\boldsymbol{k},\boldsymbol{l},\boldsymbol{m})}{k^2(2\,k+l+m)}-\frac{(1/2)\,f^2(-\boldsymbol{k},\boldsymbol{l},\boldsymbol{m})}{k^2(l+m)}\right]\Bigg\}\,N_0$$

and from the term $\sim (H'_{\mathrm{ph}})_{\alpha\delta}(H_{\mathrm{int}})_{\delta\gamma}(H_{\mathrm{int}})_{\gamma\beta}(H'_{\mathrm{ph}})_{\beta\alpha}$

$$(F')\qquad C\Bigg\{\sum_{\substack{\boldsymbol{k}\\ k<K_0}}\;\sum_{\substack{\boldsymbol{l}+\boldsymbol{m}+\boldsymbol{n}=0\\ l,\,m,\,n<K_0}} k^3\,l\,m\left[-\frac{(1/6)\,f^2(\boldsymbol{l},\boldsymbol{m},\boldsymbol{n})}{(l+m+n)^2\,(k+l+m+n)}\right]+$$

$$+\sum_{\substack{\boldsymbol{k}+\boldsymbol{l}+\boldsymbol{m}=0\\ k,\,l,\,m<K_0}} k^4\,l\,m\left[-\frac{(1/2)\,f^2(\boldsymbol{k},\boldsymbol{l},\boldsymbol{m})}{(k+l+m)^2\,(2\,k+l+m)}-\frac{(1/2)\,f^2(\boldsymbol{k},\boldsymbol{l},\boldsymbol{m})}{(k+l+m)^2\,(l+m)}\right]\Bigg\}\,N_0\,.$$

(A')—(F') are all contributions to (62d) $\sim H^3_{\mathrm{int}}\,H'_{\mathrm{ph}}$ and $\sim H^2_{\mathrm{int}}\,H'^2_{\mathrm{ph}}$. Again terms of the relative order $1/3\,N_{\mathrm{at}}$ have been omitted. On the other hand, there are even terms of the relative order $3\,N_{\mathrm{at}}$ with respect to the ordinary ones (which are independent of N_{at}), viz. the first terms in (C'), (D'), (E'), and (F'), but they are easily seen to cancel. When (A')—(F') are added up many terms compensate and we obtain the very simple result for $(A') + (B') + (C') + (D') + (E') + (F')$:

$$C\sum_{\substack{\boldsymbol{k},\,\boldsymbol{m}\\ k,\,m,\,|\boldsymbol{k}+\boldsymbol{m}|<K_0}}\left[4\,\frac{(\boldsymbol{k}\,\boldsymbol{m})^2}{k}+4\,m(\boldsymbol{k}\boldsymbol{m})\right]N_0\,. \tag{68}$$

According to the expression (23) for $f\,(\boldsymbol{k},\boldsymbol{l},\boldsymbol{m})$, (A') — (F') contain linear and quadratic terms in $(\varrho_0^2/c_0^2)\,(d/d\varrho\;c^2/\varrho)_0$. It is remarkable that all these terms have cancelled in (68). This means that also the anharmonic potential energy of the third degree in $\varrho - \varrho_0$ is without influence on the roton energies in the approximation considered here.

The contributions (62a)—(62d) to the roton rest energy $\sim c_0^{-1}$ are now given by (64), (65), (67), and (68). (64) and (65) compensate each other to order c_0^{-1} *), (67) and (68) give in view of (66)

$$E''_\alpha = \left(\frac{\hbar^2}{8\varrho_0 V}\right)^2 \frac{1}{\hbar c_0} \Bigg\{ \sum_{\substack{\boldsymbol{k},\boldsymbol{m} \\ k,m<K_0}} k\,m^2 - \sum_{\substack{\boldsymbol{k},\boldsymbol{m} \\ k,m,|\boldsymbol{k}+\boldsymbol{m}|<K_0}} k\,m^2 \Bigg\} N_{\boldsymbol{0}}\,. \tag{69}$$

This can be calculated similarly to (56) in § 5 and yields

$$E''_\alpha = \frac{29}{63}\,\Delta_0\,\varepsilon\,N_{\boldsymbol{0}}\,. \tag{70}$$

(58) and (70) now show that the unperturbed energy spectrum (48) is transformed by H' (49) into

$$E_\alpha + E'_\alpha + E''_\alpha = \sum_{\substack{\boldsymbol{k} \\ k<K_0}} \hbar\,c_0\,k\left(n_{\boldsymbol{k}} + \frac{1}{2}\right) + $$

$$+ \sum_{\substack{\boldsymbol{m} \\ m<K_0}} (\Delta + A\,m + B\,m^2 + \cdots)\,N_{\boldsymbol{m}} + \cdots, \tag{71}$$

where to order c_0^{-1}

$$\Delta = \Delta_0\left(\frac{5}{6} + \frac{29}{63}\right)\varepsilon \tag{72}$$

and to order c_0^0

$$A = \frac{3}{4}\,B_0\,K_0\,, \qquad B = \frac{7}{6}\,B_0\,. \tag{73}$$

The rest energy of the rotons is now proved to be positive for small ε. In contrast to the second energy spectrum proposed by LANDAU[2]) Δ is positive here. For He II ($\varepsilon = 0{\cdot}4$) the numerical value of (72) is according to (16)

$$\frac{\Delta}{\varkappa} = 3{\cdot}5^0\,. \tag{74}$$

If the contributions of (58) and (65) to Δ are calculated exactly (instead of taking only the first terms of the expansion in ε) one obtains

$$\frac{\Delta}{\varkappa} = 4{\cdot}8^0\,. \tag{75}$$

But this is not very consistent since for the rest of our calculation Δ is only computed to order ε.

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*) This is probably not accidental, for in classical hydrodynamics (6a)—(6c) give an absolutely sufficient description of an only slightly excited liquid, so that one might be tempted to omit (6d)—(6g) in quantum theory too. It is therefore surprising that (6d)—(6g) give a noticeable contribution at all. Maybe a cut-off method that corresponds better to physical reality makes this difference vanish.

§ 7. Different cut-off procedures.

Artmann*) has suggested an alternative cut-off method. He observed that the roton fields Ψ and Ψ^* occur exclusively in the combination $\Psi^* \nabla \Psi - \nabla \Psi^* \Psi$, and it is only this expression (not Ψ and Ψ^* themselves) which has a direct physical meaning (being a momentum density apart from a constant factor). Therefore it seems more natural to cut off this whole expression, not Ψ and Ψ^* separately, by putting

$$\left.\begin{aligned} \Psi^* \nabla \Psi - \nabla \Psi^* \Psi &= \frac{1}{V} \sum_{\substack{\boldsymbol{k},\boldsymbol{m} \\ |\boldsymbol{m}-\boldsymbol{k}| < K_0}} b_{\boldsymbol{k}}^* b_{\boldsymbol{m}}\, i\,(\boldsymbol{k}+\boldsymbol{m})\, e^{i(\boldsymbol{m}-\boldsymbol{k})\boldsymbol{x}} = \\ &= \frac{1}{V} \sum_{\substack{\boldsymbol{k}',\boldsymbol{m}' \\ k' < K_0}} b_{\boldsymbol{k}'+\boldsymbol{m}'}^* b_{\boldsymbol{m}'}\, i(\boldsymbol{k}' + 2\,\boldsymbol{m}')\, e^{-i\boldsymbol{k}'\boldsymbol{x}}. \end{aligned}\right\} \quad (76)$$

For φ and $\varrho - \varrho_0$ the same cut-off as previously is used. As $\boldsymbol{m}'$ in (76) is not restricted, an infinite number of degrees of freedom is left in the theory, but all the same this does not lead to any divergencies.

This cut-off method and the previous one do not give equal results. If we use the same K_0 in (76) as for φ and $\varrho - \varrho_0$ (this means that the "resolving power" of the liquid due to its "graininess" (Ziman[5]), p. 264) is supposed to be the same for the Fourier components of φ, $\varrho - \varrho_0$ and the expression (76)) we obtain for the roton Hamiltonian (6b)

$$H_{\text{rot}} = \sum_{\boldsymbol{m}} (\varDelta_0 + 4\, B_0\, m^2)\, N_{\boldsymbol{m}} + \sim b^* b^* b\, b \quad (77)$$

instead of (14). Thus the rest energy of the unperturbed rotons is the same, but their mass is already different. Moreover, with the cut-off (76) the sums (55) and (56) are only subject to the condition $k < K_0$ (not $m < K_0$ nor $|\boldsymbol{k}+\boldsymbol{m}| < K_0$) and B_0 is to be replaced by $4\, B_0$. Consequently one obtains instead of (58)

$$E'_\alpha \cong \sum_{\boldsymbol{m}} N_{\boldsymbol{m}} \left[-\varDelta_0 \left(1 - \frac{5}{6}\, 4\, \varepsilon + \cdots\right) + B_0\, m^2 \left(-\frac{4}{3} + \cdots\right) + \cdots \right]. \quad (78)$$

Furthermore, the condition $|\boldsymbol{k}+\boldsymbol{m}| < K_0$ in (A) and (B) of § 6 is dropped. The other expressions (C)—(E) and (A')—(F') remain unaltered. So, instead of (70), the contribution to (62d) becomes

$$E''_\alpha = \varDelta_0 \left(-1 - \frac{39}{224}\right) \varepsilon\, N_0\,. \quad (79)$$

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*) Private communication from Mr. F. Artmann, T. H. Delft.

Also H'_{int} now takes a form different from (25), and the contributions $\sim \varepsilon$ to (62a) and (62b) do not cancel. In this way Artmann's method yields an energy spectrum of the type (71), too, where now to the same order in ε as (72) and (73)

$$\Delta = \frac{6725}{2016} \Delta_0 \varepsilon, \quad A = 0, \quad B = \frac{8}{3} B_0. \tag{80}$$

In the case of an incompressible medium ($\varepsilon = 0$) this result is identical with the result of AK (3·6) obtained by using their "incompressible" Hamiltonian (3·4) from the very beginning. This is *not* the case when Ziman's cut-off method is employed (see (73)). Thus Artmann's cut-off seems to be preferable for an incompressible liquid. However, if one deals with a compressible fluid (ϱ not constant) it is doubtful which method is the better, because Artmann's method is also unable to cut off *all* physical quantities in the same way. If for example a momentum density is cut off according to (76), the corresponding velocity, which differs by a factor $1/\varrho$, is cut off in a different way. From the point of view of pure hydrodynamics it is probably impossible to see which cut-off procedure corresponds better to physical reality. An investigation of that problem would go far beyond the framework of the present article.

If one carries out the transition from second quantization to the representation of the roton in configuration space (AK equation (4·2)), Artmann's cut-off is simpler to take into account than Ziman's. In the case of He II, however, there are practical reasons for using Ziman's cut-off procedure. It is of course possible to calculate (56) as modified by Artmann's method without a development in powers of $4\,\varepsilon$ (which would be wrong because $4\,\varepsilon = 1{\cdot}6$). But in none of the energy denominators in (A)—(E) and (A')—(F') of § 6 may the roton energies be neglected. The calculations would therefore become very cumbersome. Besides, the whole expansion (6) of the Hamiltonian in rising powers of $\varrho - \varrho_0$ looks rather questionable in quantum mechanics, if the maximum kinetic energy of the rotons is larger than the maximum energy of the phonons. The only thing one could do is simply to omit (6d)—(6g) by the argument used before that classically (6a)—(6c) give a sufficient description of a but slightly excited liquid.

A third cut-off procedure consists in combining Ziman's and Artmann's methods by putting

$$\Psi^* \nabla \Psi - \nabla \Psi^* \Psi = \frac{1}{V} \sum_{\substack{\boldsymbol{k},\boldsymbol{m} \\ k, m, |\boldsymbol{m}-\boldsymbol{k}| < K_0}} b_{\boldsymbol{k}}^* b_{\boldsymbol{m}}\, i\,(\boldsymbol{k} + \boldsymbol{m})\, e^{i(\boldsymbol{m}-\boldsymbol{k})\boldsymbol{x}}. \tag{81}$$

This yields still another H_{rot}, namely

$$H_{\mathrm{rot}} = \sum_{\substack{\boldsymbol{m} \\ m < K_0}} \left(\varDelta_0 - \frac{3}{4} B_0 K_0 m + \frac{5}{2} B_0 m^2 \right) N_{\boldsymbol{m}} + \sim b^* b^* b\, b \tag{82}$$

and leads again to a spectrum of the type (71), where now ($\varDelta$ to order ε, A and B to order ε^0)

$$\varDelta = \frac{499}{168} \varDelta_0\, \varepsilon, \quad A = 0, \quad B = \frac{8}{3} B_0. \tag{83}$$

Like (80), it gives the correct limit for an incompressible liquid.

For practical reasons, we have always cut off sharply. Instead, one might introduce smooth cut-off factors, but this cannot change the energy spectrum drastically.

§ 8. Discussion of the results.

With the energy spectrum (71), (72), (73) we can calculate the partition function and the thermodynamic properties of the fluid. For He II, (72) and (73) can only be expected to give the right order of magnitude because $\varepsilon = 0{\cdot}4$ (instead of $\varepsilon \ll 1$), and because of the arbitrariness introduced by the cut-off procedure. If $\varDelta/\varkappa$ is chosen $\approx 7^0$ and A and B considerably smaller than in (73) (but still of the same order of magnitude) the theory gives the correct specific heat[15]) from absolute zero up to temperatures even near the λ-point. Also the spectra of § 7, which are of the same form as LANDAU's first spectrum ($A = 0$)[1]), have the right order of magnitude to fit the specific heat data.

The theory of the two-fluid model[1])[16]) can also be applied to the spectrum (71), and one can calculate e.g. the velocity of second sound. The result agrees qualitatively with experiment when values for $\varDelta$, A and B fitting the specific heat are used*).

Unlike in DEBYE's theory of solids, the numerical results here depend considerably on how one cuts off the momenta of the excitations. The reason is that the constants $\varDelta$, A and B in (71) are determined by sums over virtual quanta which also have high energies.

We have simply tried to find the energy spectrum of hydrodynamics. We have not discussed the question whether the hydrodynamical variables are suitable coordinates to describe an ensemble of atoms in a liquid. This problem is much more difficult here than

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*) The author wishes to thank Dr. W. R. THEIS for some numerical calculations.

in the theory of solids. The investigations by FEYNMAN[17]) seem to indicate that hydrodynamics provides a fair description of a Bose liquid at low temperatures. On the other hand, the hydrodynamical description of an ensemble of Fermi particles seems at least to be very incomplete. It is probably at this place that the difference between ^{3}He and ^{4}He comes into play. (In hydrodynamics one does not speak about the statistics of the particles composing the liquid. The phonons and rotons as defined here must obey Bose statistics, since a quantization with anticommutators would never yield the limit of classical hydrodynamics.)

One should therefore try to give the hydrodynamical approach to He II a secure foundation. If this is found, it will perhaps also yield a better cut-off method.

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