A Long-Range Attractive Interaction of Rotons in Superfluid $^4$He

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With the use of the method of the collective description developed by one of the authors (N) for superfluid $^4$He, it is shown that a long-range interaction of rotons transmitted by phonons is attractive and yields a resonance state of a roton pair with the binding energy of the order of magnitude 0.12 K which is relevant to the recent experimental results of the Raman scattering. The effect of the short-range mutual interaction of rotons is also discussed. Some comments on the relationship to the other theories of the collective description are made in appendices.

§ 1. Introduction

Bohm and Salt (BS) and one of the authors (N) obtained interaction Hamiltonians of individual particles transmitted by phonons in their methods of collective description for liquid helium, respectively. The two results obtained independently are completely equivalent, if it is assumed that the phonon energies are nondispersive for wave numbers below a cutoff wave number $q_0$ and the energies of individual particles are free-particle like for wave numbers above $q_0$, which is given by $q_0 = (8N/V)^{1/2}$, where $\rho_0$ is the mean number density; $N/V$. This interaction can be considered to come from the backflow effect of individual particles, and the long-range part of this interaction potential has the same form as that of two electric dipoles.

The expression of this interaction potential can be modified by taking account of the dispersion effect of phonons and the effect of an effective mutual interaction between individual particles. Investigation of this interaction potential is of importance in view of a recent experimental result of Raman scattering from liquid helium II due to Greytak and Yan. According to their result, it appears possible that a roton pair with opposite momenta can have a bound state and the interaction between rotons is attractive. The binding energy of these rotons estimated by this experiment is 0.37 K.

In this paper, it will be shown that two individual particles with opposite momenta near the roton minimum yields a resonance state with a lower energy

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than twice the roton energy compatible with the experimental result, if the major part of the mutual interaction, which is responsible for the Raman scattering, is given by our interaction potential transmitted by phonons.

In previous papers referred to as I') and I', it was shown that excitation energies of individual particles are shifted owing to the interaction with phonons and that among individual particles themselves, which is assumed, in the lowest approximation, to yield the form factor and the Feynman energy having the same values as given by the x-ray or the neutron scattering experiment. The energy shift was calculated by using the perturbation theory in I. A more complete account of it was given by dealing with the self-energy operator of the one-particle Green's function of individual particles, as shown in another previous paper referred to as II). Our theory of investigating a system of these quasi-particles with energy shifts may be regarded as a microscopic version of Landau's quantum hydrodynamical-theory of rotons. Hereafter, we shall call these quasi-particles simply rotons.

As the first approximation, by neglecting the interactions with phonons and with particle pairs, the excitation energy of individual particles is given by the Bogoliubov energy obtained for an effective potential which is arranged so that the calculated form factor may become equal to the observed one numerically. We shall call the individual particles with the Bogoliubov energies bare rotons which are transformed into real rotons with the observed excitation energies after the above-mentioned interactions are switched on. These bare rotons may be called simply rotons as far as no confusion occurs.

According to a recent precise experiment of neutron scattering worked out by Graf et al., the line widths of rotons are surprisingly small even for wave numbers near 2.25 A⁻¹ at which the group velocity of the roton is equal to the sound velocity under pressure of 1.03 atm and at temperature of 1.08 K. This result implies that rotons near the roton minimum have sufficiently sharp spectra to yield a well-defined resonance state of a roton pair with opposite momenta.

As shown by Ruvalds et al. and Iwamoto, mutual interactions of rotons which exchange roton pairs with opposite momenta are important in analysing the experimental result of the Raman scattering from liquid helium due to Greytak and Yan. At the absolute zero temperature, as shown by Stephen and Nakajima, the light can be coupled only to the D-wave portion of the wave function for the roton pair.

In § 2 the unperturbed Hamiltonian of phonons and rotons with the renormalized energies are obtained by following the method of the phase operator approach for phonons and the Bogoliubov approximation for rotons. In § 3 the Hamiltonian of the long-range interaction of rotons transmitted by phonons is investigated and the resonance energy of the roton pair is estimated. As mentioned in I', the simple expression for the dipole type interaction does not account for the appearance of the resonance state, because the interaction given by this
expression becomes repulsive. If the form factors involved in the vertex functions for the interaction with phonons were put equal to unity for the wave numbers above \( q_0 \), the interaction transmitted by phonons would be reduced to the dipole type. The form factors used here have peaks near the wave number \( k = 2A^{-1} \) and make the interaction attractive. Furthermore, the \( D \)-wave portion of the coupling parameters of this interaction is of an order of magnitude \( 10^{-10} \text{erg/cm}^2 \) and capable of yielding a resonance state by neglecting the direct contribution from the short-range mutual interaction of rotons. The \( S \)-wave portion of these parameters is one-tenth as large in magnitude as that coming from the short-range potential which is obtained by taking account of the result of the pair theory.\(^1\) In \$4, we discuss the possible origins giving rise to the binding energy of the roton pair in the framework of the present theory. In Appendix A, brief survey is given over the method of the phase operator approach given by one of the authors (N)\(^1\) as this method seems to have largely been overlooked. In Appendix B, some comments are made on the quantum mechanical potential appearing in the phase operator approach and on the renormalization process for the phonon energy, in relation to the recent theories of Berdahl\(^1\) and Rajagopal and Grest.\(^1\) In Appendix C, a simplified derivation of the expression for the binding energy of the roton pair is shown, in order to clarify our notations used in this paper by keeping a close relation to Iwamoto’s theory.\(^1\)

\section*{§ 2. Phonons and rotons}

In the theory of the collective description, the total Hamiltonian is divided into three parts; the phonon part, the internal part and the interaction part. The phonon part is obtained from the Hamiltonian of the density-phase operator approach given by one of the authors (N) by expanding the number density \( \rho \) about the mean number density \( \rho_0 = N/V \) as \( \rho = \rho_0 + \rho' \). Chan and Valatin\(^2\) could show by using a nonunitary transformation that this Hamiltonian is equivalent to that of Bogoliubov and Zubarev\(^3\) which is also equivalent to that of Sunakawa’s curl free velocity field approach\(^4\) as pointed out by Kebukawa.\(^5\) It is obvious, without referring to the theory of Bogoliubov and Zubarev, that our Hamiltonian is equivalent to Sunakawa’s one. This Hamiltonian is exact in the high density limit, but it opens to question as yet whether this Hamiltonian is useful for real problems of liquid helium without restriction. From our point of view, liquid helium is not at so high a density and this Hamiltonian is relevant only to the problems associated with long-wave lengths, such as the propagation of phonons for low wave numbers (see Appendix B).

In order to evade the superfluous complex of the interactions among excitations with high wave numbers through a number of anharmonic terms, it will be reasonable to introduce a cutoff wave number \( q_0 \) for the Fourier transforms of the density and the phase operators and the excitations with higher wave numbers. Datasets with this cutoff wave number will be easier to deal with. The renormalization process for the phonon energy should be considered in connection with this cutoff wave number. This renormalization process is essential to the stability of the theory. In Appendix B, the renormalization process for the phonon energy is considered in relation to the recent theories of Berdahl\(^1\) and Rajagopal and Grest.\(^1\)}
numbers than \( q_0 \) are considered as furnished by the internal Hamiltonian of individual particles with a mutual effective potential. These individual particles can have zero momentum so that a well-defined condensate may be defined. We shall consider the Bogoliubov approximation and deal with bare rotons with the Bogoliubov energies at the first step of the approximation. These bare rotons interact among themselves through the condensate as well as with phonons through the interaction part.

When the interactions with phonons and with roton pairs through the condensate are switched on, we obtain an assembly of quasi-particles with the observed excitation energies which are identified with real rotons. For the roton region, by introducing separation parameters for the effective potential, as discussed in II, the calculated excitation energies can be fitted on to the observed energies. An observed excitation energy is given by a pole of one-particle Green's function determined by

\[
\varepsilon - \varepsilon^B - \Sigma(k, \varepsilon) = 0, \tag{2.1}
\]

where \( \Sigma(k, \varepsilon) \) is the self-energy operator including the effects of both the interactions with phonons and with roton pairs.

For the phonon region, the calculation of the excitation energy was made by Sunakawa et al. and more recently by Grest and Rajagopal for the Hamiltonian of the phase operator approach. Their results of the calculation agree fairly well with the experimental result below the cutoff wave number \( q_0 \), but become less exact above \( q_0 \). The results may be improved by employing an effective potential which yields the form factor with the observed values for low \( q \) values below \( q_0 \), as tried for the roton region. A more exact calculation of the phonon energy is left to another occasion. In the following, as the phonon energy, we may be allowed to use the observed excitation energies as the renormalized energies.

The renormalized energies \( \varepsilon_q \) and \( \varepsilon_k \) are introduced by following a renormalization process to replace the unperturbed energy given by the phase operator approach \( \varepsilon^p \) and that given by the Bogoliubov approximation for the effective potential \( \varepsilon^B \). The unperturbed Hamiltonian is arranged in the form

\[
H_0 = \sum_{\varepsilon < \varepsilon_0} \varepsilon_q B_q \dagger B_q + \sum_{\varepsilon_0 < \varepsilon} \varepsilon_k C_k \dagger C_k + d^p + d^R, \tag{2.2}
\]

where \( B_q \dagger \) and \( B_q \) are the field operators of phonons and \( C_k \dagger \) and \( C_k \) are those of rotons, and \( d^p \) and \( d^R \) are the renormalization terms for the phonon part and the roton part, respectively, defined by

\[
d^p = \sum_{\varepsilon < \varepsilon_0} \left( \varepsilon^p - \varepsilon_q \right) B_q \dagger B_q, \quad d^R = \sum_{\varepsilon_0 < \varepsilon} \left( \varepsilon^B - \varepsilon_k \right) C_k \dagger C_k. \tag{2.3}
\]

The renormalized energies \( \varepsilon_q \) and \( \varepsilon_k \) are determined so that the renormalization terms may vanish after the interactions are switched on, up to the desired order of accuracy. For the roton region, \( \varepsilon_k \) satisfies the dispersion equation (2.1), (see Appendix B).
§ 3. Interaction Hamiltonian of rotons

In order to introduce the model Hamiltonian for rotons, the expression for the interaction Hamiltonian transmitted by phonons are obtained from the vertex functions for the interactions with phonons and roton pairs listed in Table C I in I'. These vertex functions are given by Fourier coefficients of an effective potential which provides us with the observed form factor in the present theory. At the first step of the calculation, the form factor \( \lambda_k \) obtained in the lowest approximation is replaced by the observed one\(^{28} \) denoted by \( S_k \). In this way, the interaction Hamiltonian for rotons transmitted by phonons is obtained in the form

\[
H_{\text{r'}'} = -\frac{1}{2} \sum_{k, k'} V_q(k, k') C_k^l C_{k'}^{l'} C_{k + q}^l C_{k - q}^{l'},
\]

\( (3.1) \)

where \( M \) is the mass of the atom.

This expression is essentially the same as that given by \( (4.1) \) and \( (4.4) \) in I' except for the energy denominators. As we are interested in the mutual interaction of rotons which is responsible for the Raman scattering, we consider exclusively the Hamiltonian of the form

\[
H_{\text{r''}} = -\frac{1}{2} \sum_{k, k'} V(k, k') C_k^l C_{k'}^{l'} C_{k + q}^l C_{k - q}^{l'},
\]

\( (3.4) \)

In obtaining this expression, we have neglected the effect of the renormalization factor defined by

\[
z_k = [1 - \partial \Sigma(k, \epsilon)/\partial \epsilon]^{-1}, \quad 0 \leq z_k \leq 1,
\]

\( (3.5) \)

which has been considered as unity; \( z_k = 1 \). If this effect were not negligible, the parameter \( V(k, k') \) would have been multiplied by \( z_k z_{k'} \).

The resonance energy for the roton pair was obtained by Iwamoto for an interaction potential of type \( (3.1) \). To gain a great familiarity with his result, we would rederive the resonance energy in a simplified way in Appendix C.

The coupling parameter of the interaction \( V(k, k') \) is expanded in the Legendre polynomials. The values of the expansion coefficients are listed in Table I for some wave numbers near the roton minimum for \( l = 0, 2 \). The energy shift for the resonance energy of the roton pair at the roton minimum with the wave number \( k_0 = 1.91 \times 10^{-1} \) is obtained from \( (C.11) \)

\[
\epsilon_B = g^4(k_0) k_0^2 / (2h)^2,
\]

\( (3.6) \)
A Long-Range Attractive Interaction of Rotons in Superfluid \textsuperscript{4}He

Table I.

<table>
<thead>
<tr>
<th>$k \times 10^{-8}$ cm(^{-1})</th>
<th>1.90</th>
<th>1.91</th>
<th>1.95</th>
<th>2.00</th>
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Table II.

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<th>$k/q_0$</th>
<th>$N\nu_s^{(o)}$ (K)</th>
<th>$k/q_0$</th>
<th>$N\nu_s^{(o)}$ (K)</th>
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<th>$N\nu_s^{(o)}$ (K)</th>
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<td>1.6</td>
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<td>2.2</td>
<td>2.16</td>
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<td>2.3</td>
<td>3.60</td>
<td>2.9</td>
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<td>2.7</td>
<td>2.38</td>
<td>3.3</td>
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Table III.

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<tr>
<th>$k \times 10^{-8}$ cm(^{-1})</th>
<th>1.80</th>
<th>1.91</th>
<th>2.01</th>
<th>2.13</th>
</tr>
</thead>
<tbody>
<tr>
<td>$V_s^{(o)} (k, k) \times 10^{18}$ erg/cm(^8)</td>
<td>1.15</td>
<td>1.02</td>
<td>0.91</td>
<td>0.82</td>
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<tr>
<td>$V_s^{(o)} (k, k) \times 10^{18}$ erg/cm(^8)</td>
<td>0.68</td>
<td>-0.51</td>
<td>-0.92</td>
<td>-0.93</td>
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where the coupling parameter $g_s(k)$ is defined by (C·8) and the effective mass of the roton $\mu = 0.16M_{\text{He}}$ ($M_{\text{He}} = 6.64 \times 10^{-4}$ g) has been determined by the renormalized roton energy.

The so-called binding energy given by (3·6) is estimated as $\varepsilon_B = 0.12$ K by using the value of $g_s(k_0)$ listed in Table I. When we use the value of $g_s(k)$ for $k = 2.0$ A\(^{-1}\) in place of $g_s(k_0)$, the binding energy becomes 0.37 K.

Besides the above long-range interaction transmitted by phonons, we are left with the short-range mutual effective interaction which is supposed to give rise to the observed form factor. In order to obtain this effective interaction potential, the lowest Bogoliubov approximation is not sufficient, therefore we considered the pair theory approach in a previous paper,\(^{16}\) which keeps the framework of our theory unchanged but modifies the numerical values of the coupling
parameters for the effective potential. Here we employ a trial effective potential as shown by Fig. 1 and in Table II which yields the observed values, in the lowest approximation of the pair theory, for the form factor and for the roton energy at wave numbers near the roton minimum.\(^{16}\)

As the interaction Hamiltonian for the short-range interaction which is reasonable for the Raman scattering, we assume the following form:

\[
H_{r}(\kappa) = \frac{1}{2} \sum_{|\kappa + \kappa'| > \kappa} V_{\kappa + \kappa'} C_{\kappa} C_{\kappa'}^{\dagger} C_{\kappa'} C_{\kappa}^{\dagger},
\]

where the effects of the coherence factors have been neglected.\(^7\) The coefficients of the Legendre expansion given by (C-1) are listed in Table III for wave numbers near the roton minimum. The S-wave coefficients \((l = 0)\) listed in Table III are ten times as large as those listed in Table I for the long-range potential. These values of the order of magnitude \(10^{-38}\) erg/cm\(^3\) are relevant to those suggested by Landau and Khalatonikov\(^{24}\) in obtaining the viscosity coefficient for rotons (see § 4). The D-wave coefficients \((l = 2)\) listed in Table III are less than those given for the long-range potential, therefore we may consider that the major part of the binding energy detected by the Raman scattering comes from the long-range potential transmitted by phonons.

§ 4. Discussion

In this paper, we have obtained the coupling parameters for the scattering of rotons by rotons, which are relevant to the experimental results of the Raman scattering and of the viscosity coefficients. Landau and Khalatonikov\(^{24}\) estimated the magnitude of the coupling constant for the roton-roton scattering from the experimental data on the viscosity coefficients by assuming the interaction potential in the following simple form with a constant coupling parameter:

\[
V = V_{0} \delta(r - r').
\]

By subtracting the phonon component from the experimental values of the viscosity coefficient between 1.35 K and 1.9 K, they attributed the nearly constant residual part of the viscosity coefficient to the roton-roton scattering and estimated the mean collision time as \(\tau_{r} = 1.5 \times 10^{38} \text{s/cm}\(^3\)\) and the coupling constant as \(V_{0} = 0.5 \times 10^{-38} \text{erg/cm}\(^3\)\). When (4.1) is used in obtaining \(V_{0}(k_{0}, k_{0})\) we obtain \(V_{0} = 0.9 \times 10^{-38} \text{erg/cm}\(^3\)\) which is close to the value listed in Table III. Since the S-wave portion of the long-range potential is negligible compared with that of the short-range potential, we can conclude that the short-range effective potential is essential to obtain the transport coefficients.

It has been shown that the D-wave portion of the long-range potential is essential to obtain the resonance state of the roton pair. Ishikawa and Yamada\(^{25}\) obtained a similar result to ours about the interaction of rotons transmitted by phonons by following Landau's quantum hydrodynamical approach. They argue
that the main part of the attractive potential comes from the change in the roton energy $\Delta$ due to the density fluctuation; $\partial \Delta / \partial \rho$. Although any relationship of our result to theirs is not completely clear at present, we can point out that a part of this effect is included in the coupling parameter used here as the change of the quantum mechanical potential due to the density fluctuation. The more quantitative investigation on this effect is necessary in the framework of our theory of the collective description. The main part of the attractive potential given here comes from the modified dipole type interaction which is obtained by taking account of the short-range mutual interaction of rotons that affects the expression of the vertex function $\Gamma(k, q)$ for the interaction with phonons.

Recently, Ikushima and Ohbayashi succeeded in detecting the bound state of the roton pair by performing the Raman scattering experiment and they obtained a slightly larger binding energy at temperature of 1.51 K than that of Greytak obtained at 1.2 K.

As an origin of the discrepancy between the theoretical result and the experimental result, we can consider the effect of the change of the quantum mechanical potential due to the density fluctuation which modifies the expression of the vertex function for the interaction with phonons. As another origin, we may consider the effect of the short-range potential, which is, however, not unambiguous at present, especially about the $D$-wave coefficients. The further investigations of these problems are necessary.

Finally, we would make a remark on the mutual effective potential of rotons. The effective potential is so determined that it may yield the observed form factor. In practice, we have obtained it by taking account of the result of the pair theory which gives the expression for the form factor in the form

$$S_k = \left[ \frac{\xi_k - \eta_k}{\xi_k + \eta_k} \right]^{1/2},$$  \hspace{1cm} (4.2)$$

$$\xi_k = \frac{\hbar^2 k^2}{2M} + \sum_{k'} V_{k-k'}^{(0)} n_{k'} - \mu,$$  \hspace{1cm} (4.3)

where $\eta_k$, $n_k$ and $\mu$ are the pairing energy, the mean occupation number and the chemical potential, respectively. It is our next task to determine such an effective potential that can yield the available experimental results in a more complete manner by taking account of the interactions with phonons and roton pairs. The effective potential thus obtained will serve as a milestone guiding us to a completely microscopic theory.

The authors would like to express their thanks to Drs. K. Ishikawa and K. Yamada for sending one of the authors (N) a preprint of their work and to Drs. Ikushima and K. Ohbayashi for bringing their notice to the recent experimental results of the Raman scattering.
Appendix A

The Hamiltonian of the phase operator approach

We deal with the Hamiltonian of the phase operator approach to obtain the phonon excitation and the mutual interaction of rotons transmitted by phonons. The original expression of this Hamiltonian was given in a previous paper of one of the authors (N). This Hamiltonian reads

\[
H = \int \left\{ \frac{M}{2} \rho(r) \nabla \cdot \mathbf{v}(r) \rho(r) \nabla \cdot \mathbf{v}(r) \right\} + \frac{\hbar}{2M} \| \mathbf{v}(r) \|^2 \rho(r) + \frac{\hbar}{2i} \left[ \mathbf{v}(r) \cdot \nabla \rho(r) \right] - \mathbf{v}(r) \left[ \rho(r) - \delta(\mathbf{r} - \mathbf{r'}) \right] \mathbf{V}(\mathbf{r} - \mathbf{r'}) \, d\mathbf{r} d\mathbf{r'},
\]

where \( \rho(r) \) is the density operator and \( \mathbf{v}(r) \) is the velocity operator. This expression is exact except for a boundary effect of the region of zero density. As the use of this Hamiltonian has largely been overlooked, we would briefly summarize the results obtained in the previous papers and emphasize the necessary cautions in dealing with this Hamiltonian.

By noticing a commutation relation of the form

\[
[\rho(r), [\rho(r'), \mathbf{v}(r'')]] = 0,
\]

the original expression (A.1) turns out into the alternative form\(^7\)

\[
H = \int \left\{ \frac{M}{4} \left[ \mathbf{v}(r) \cdot \nabla \rho(r) + \nabla \rho(r) \cdot \mathbf{v}(r) \right] + \frac{\hbar}{8M} \| \mathbf{v}(r) \|^2 \rho(r) \\
+ \frac{\hbar}{4i} \left[ \mathbf{v}(r) \cdot \nabla \rho(r) - \nabla \rho(r) \cdot \mathbf{v}(r) \right] + \frac{1}{2} \mathbf{V}(\mathbf{r} - \mathbf{r'}) \rho(r) \left[ \rho(r') - \delta(\mathbf{r} - \mathbf{r'}) \right] \mathbf{V}(\mathbf{r} - \mathbf{r'}) \right\} d\mathbf{r} d\mathbf{r'},
\]

which is rederived by Kobe and Coomer\(^7\) by the current algebra approach.

The commutation relation between two velocity operators at different spatial points \( \mathbf{r} \) and \( \mathbf{r'} \) was obtained as a continuum limit of a commutation relation obtained in a lattice space. In general, the velocity field is not irrotational. In fact, the vortex motion can appear associated with the region of zero density. Furthermore, it can be shown that the vorticity is commutative with the density; \([\mathbf{V} \times \mathbf{v}(r), \rho(r')]] = 0\) and the commutation relation between two current operators is given by the irrotational part of the velocity operator.

It is very plausible that the vorticity can be neglected in considering the problems in the high density limit and those associated with long-wave lengths, therefore the velocity field for phonons is considered as irrotational. The Hamiltonian given in terms of the irrotational velocity field is called the Hamiltonian of the phase operator approach, because the irrotational part of the ve-
A Long-Range Attractive Interaction of Rotons in Superfluid $^4$He 1793

...operator is given by the phase operator of the field operator (quantized wave function). This Hamiltonian should not be applied, without restriction, to the problems of many-Boson systems not at so high a density, for which the excitations of short-wave lengths, inclusive of the vortex motion, become of importance. This is the reason why we have introduced the cutoff wave number $q_0$.

Appendix B

Quantum mechanical potential and renormalized energies

The unperturbed Hamiltonian of phonons is given by

$$H_p^{(0)} = \frac{N}{2M} \sum_{\xi \in \xi_0} q^2 P_q P_{-q} + \frac{1}{2} \sum_{\xi \in \xi_0} \left( V_q + 2T_q + \frac{\hbar^2 q^2}{4MN} \right) Q_q Q_{-q}$$

$$= \sum_{\xi \in \xi_0} \epsilon_q \left( B_q B_{-q} + \frac{1}{2} \right), \quad (B.1)$$

$$T_q = \frac{1}{V} \langle 0 | V_q \rho_0 - | 0 \rangle \rho - \frac{1}{\rho} | 0 \rangle \rho_0 | 0 \rangle, \quad (B.2)$$

$$\epsilon_q = \frac{\hbar^2 q^2}{2M \lambda_q} \left( \frac{\hbar^2 q^2}{2M} + 2N(V_q + 2T_q) \right)^{-1/2}, \quad (B.3)$$

where $P_q$ and $Q_q$ are the auxiliary variables for the Fourier transforms of the phase operator $\phi(r)$ and the density operator $\rho(r)$, respectively, $V_q$ the quantum mechanical potential; $\hbar^2 |\rho|^2/(8M\rho)$, $\langle 0 | A | 0 \rangle_\rho$ the average of an operator $A$ with respect to the ground state of rotons and $\lambda_q$ the lowest order approximation to the observed form factor $S_q$. The quantity $T_q$ remains finite as long as the system is stable. When $V_q/\rho^2$ and $1/\rho$ are expanded in $\rho'$ about $\rho = \rho_0$, we obtain the lowest approximation to $2T_q$ in the form

$$2T_q^{(0)} = S_q \left( \frac{\hbar^2}{4MN} \right) \sum_{\xi \in \xi_0} (q^2 + k^2) S_k. \quad (B.4)$$

The effects of this term to the excitation energy and the ground state energy have been investigated by Berdahl, Rajagopal, and Grest. By using the Rayleigh-Schrödinger perturbation expansion they have shown that the ground state energy becomes convergent and the excitation energy converges in the low $q$ limit.

In this paper, instead of following the usual perturbation theory, we consider a renormalization method which leads to a dispersion equation obtained by calculating the energy shift from the Feynman energy due to the three particle processes. The renormalized phonon energy is obtained by solving the following dispersion equation:

$$\epsilon_q - \epsilon_q^\prime - \frac{\hbar^2 q^2}{2M \left( S_q - \frac{1}{\lambda_q} \right)} + \epsilon_q^{(0)} = 0. \quad (B.5)$$
The form factor \( S_q \) in the third term of (B·5) and \( \varepsilon_q^{(\beta)} \) are calculated from the perturbation theory with the renormalized energy denominators up to second order. The expression for the renormalized phonon energy \( \varepsilon_q \) is essentially equivalent to the previous one given by (3·5) in \( I' \), except that the Feynman energies and the unperturbed energies involved in the energy denominators are replaced by the renormalized energies. At the present state of the problem, it is best to use the observed form factor instead of the lowest approximation \( \lambda_q \) or \( \lambda_k \) which are involved in the vertex functions for the three particle processes as listed in Table CI in \( I' \), because our knowledge about the Fourier transform of the interaction potential \( V_q \) and the averaged quantities for the ground state of rotons is rather poor. After this replacement the dispersion equation (B·5) assumes the form

\[
\begin{align*}
\varepsilon_q - \varepsilon_q^{(\beta)} &= 2 \sum_{\lambda=1}^{\infty} \left[ \Gamma_a(k, q)(\varepsilon_q - \varepsilon_k - \varepsilon_{k-q}) + \Gamma_b(k, q)(\varepsilon_q + \varepsilon_k + \varepsilon_{k-q}) \right] ^2 \\
&\times \left[ (\varepsilon_q + \varepsilon_k + \varepsilon_{k-q})(\varepsilon_q - \varepsilon_k - \varepsilon_{k-q}) \right], \\
\Gamma_a(k, q) &= \frac{1}{2} \Gamma_c(k, q) - \frac{\hbar^2}{4M} \left( S_k q S_q \right) ^{1/2} \left( \frac{k \cdot q}{S_q} + \frac{k^2 - k \cdot q}{S_k} \right), \\
\Gamma_b(k, q) &= \frac{1}{2} \Gamma_c(k, q) - \frac{\hbar^2}{4M} \left( S_k S_q \right) ^{1/2} \left( \frac{k^2 - q^2}{S_q} + \frac{k^2 - k \cdot q}{S_k} \right), \\
\Gamma_c(k, q) &= \frac{\hbar^2}{2M} S_q ^{1/2} \left( \frac{k \cdot q - q^2/2}{S_q} - \frac{q^2}{2} \right), \quad k \to \infty, \quad q \to 0.
\end{align*}
\]

In obtaining the renormalized roton energy from the dispersion equation (2·1), the higher order effect of the quantum mechanical potential should also be taken into account. In order to consider this effect, the parameter of the effective potential \( V_k \) should be replaced by \( V_k + 2T_{k'} \), where \( T_{k'} \) has the same expression as for (B·2) except that the averages are taken with respect to the ground state of phonons. The lowest approximation to \( 2T_{k'} \) reads

\[
2T_{k'} = (\hbar^2/4MN^2) S_k \sum_{\lambda=1}^{\infty} (k^2 + q^2) S_q,
\]

which is evaluated by the use of the observed form factor of the x-ray scattering obtained by Hallock to the effect

\[
2T_{k'} = N^{-1} (a + bk^2), \quad a = 0.53 \text{ K}, \quad b = 0.67 \times 10^{-18} \text{ K cm}^4
\]

which nearly completely cancels the contribution to the second order perturbation energy for the three particle processes coming from the vertex function \( \Gamma_a(k, q) \). A fuller presentation will be given elsewhere.

**Appendix C**

The resonance energy of the roton pair

As a wave function of roton pairs with the excitation energy \( E \) for the
A Long-Range Attractive Interaction of Rotons in Superfluid $^4$He

model Hamiltonian (3.4), we consider the following wave function:

$$u(E) = \sum_k \{ f_k C_k C_{-k} | 0 \} ,$$  

(C.1)

where $|0\rangle$ stands for the ground state of rotons. We confine ourselves to the roton pair states and obtain a linearized equation-of-motion for (3.4) expressed as

$$E u(E) = \sum_k \{ 2 \varepsilon_k f_k - \sum_{k'} V(k,k')f_{k'} \} C_k C_{-k} | 0 \} ,$$  

(C.2)

from which it follows that

$$E f_k = 2 \varepsilon_k f_k - \sum_{k'} V(k,k') f_{k'} .$$  

(C.3)

By expanding $f_k = f(k, \theta, \varphi)$ in the spherical harmonics $Y^m_l (\theta, \varphi)$ as

$$f_k = f(k, \theta, \varphi) = \sum_{l,m} u_{l,m} (k) Y^m_l (\theta, \varphi) ,$$  

(C.4)

and the coupling parameter $V(k,k')$ in the Legendre polynomials as

$$V(k,k') = \sum_l (l + \frac{1}{2}) V_l (k,k') P_l (\cos \Theta) ,$$  

(C.5)

we find the equation for $u_{l,m} (k)$ of the form

$$E u_{l,m} (k) = 2 \varepsilon_k u_{l,m} (k) - V/2\pi^2 \int_{0}^{\pi} V_l (k,k') u_{l,m} (k') k' dk' .$$  

(C.6)

where $\Theta$ is the angle between $k$ and $k'$ and we have used the addition theorem:

$$P_l (\cos \Theta) = \frac{4 \pi}{2l + 1} \sum_m Y_l^m (\theta, \varphi) Y_l^m (\theta', \varphi') .$$  

(C.7)

When we assume that the expansion coefficient $V_l (k,k')$ is separable as

$$V_l (k,k') = g_l (k) g_l (k') / V ,$$  

(C.8)

the dispersion equation is derived from (C.6) in the form

$$1 = \frac{1}{(2\pi)^2} \int \frac{g_l^2 (k)}{2 \varepsilon_k - E} k^2 dk .$$  

(C.9)

In order to consider the resonance state of the roton pair with the wave number $k_0 = 1.91 \text{ A}^{-1}$, we assume the renormalized energy in the form

$$\varepsilon_k = A + \frac{k^2}{2\mu} (k - k_0)^2 ,$$  

(C.10)

and obtain the energy shift of the resonance state of the form
which is called the binding energy of the roton pair by Greytak. This result is completely equivalent to Iwamoto's one which is obtained from his dispersion equation

\[ -\frac{1}{g} = R(E) = \pi V_i^2(k_0) \sqrt{\frac{\mu}{2\Delta - E}}, \]  

by noticing that he wrote \(-\frac{1}{g}W_i(k, k')/V\) in place of \(2\pi kk'V_i(k, k')\) given in (C.5), \(\Delta\) as \(\Delta/2\), \(\mu\) as \(2\mu\) and put \(W_i(k, k') = gV_i(k)V_i(k')\), \(\hbar = 1\), therefore we should read

\[ -gV_i(k)V_i(k') = kk'g_1(k)g_1(k')/(2\pi)^2.\] 

The observed excitation energies used in obtaining the coupling parameters of the interaction are those given by Cowley and Woods. [9]

**References**


8) L. D. Landau, J. Phys. 5 (1941), 71.


18) P. Berdahl, Ph. D. Thesis, Stanford University (1972), Unpublished. We thank Dr. Berdahl for sending us a copy of this thesis.


T. Kebukawa, private communication.
A Long-Range Attractive Interaction of Rotons in Superfluid $^4$He

26) A. Ikushima and K. Ohbayashi, private communication.

Note added in proof: In the above list of references, Ref. 19 should be supplemented by the following two references published after this paper was submitted.

Recently, A. K. Rajagopal, A. Bachi and J. Ruvalds [Phys. Rev. A9 (1974), 2707] obtained the binding energy of the roton pair by using the Sunakawa Hamiltonian to find an energy value ten times as large as the observed one. From our point of view, they have overestimated the contributions to this energy value coming from the high-momentum states.