

## Three-roton bound states

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The existence and binding energy of three-roton bound states with a vanishing total momentum are investigated. In the presence of attractive roton-roton interaction, however weak it may be, three-roton bound states of  $s$ - and  $d$ -wave symmetry are necessarily formed. Those binding energies can be expected to be about 1 K. The observability in experiments such as Raman scattering is also discussed. Further, the effects of four- and five-excitation states on the Raman spectrum are briefly discussed.

### I. INTRODUCTION

Landau<sup>1</sup> proposed that superfluid <sup>4</sup>He, He II could be understood as an interacting phonon-roton gas. From this viewpoint, understanding the interaction between phonons and rotons is essential to explain the thermodynamical and transport properties of He II.

Raman scattering<sup>2,3</sup> has been a useful tool to investigate the interaction between excitations in He II. Theoretically, Iwamoto<sup>4</sup> and Ruvalds and Zawadowski<sup>5,6</sup> showed that the Raman spectrum  $I_R$  should have cusps or inflections with infinite derivatives at  $E = 2\Delta_0$  and  $2\Delta_1$ ;  $E$  is the energy transferred from the incident light to He II, and  $\Delta_0$  and  $\Delta_1$  denote the minimum and the maximum energies of the phonon-roton dispersion curve, i.e., the roton and the maxon energies, respectively. Furthermore, they argued that a resonance should appear below  $E = 2\Delta_0$  if the interaction between two rotons was attractive. This resonance was clearly observed by Murray, Woerner, and Greytak.<sup>7</sup>

Recently, Ohbayashi and his co-workers<sup>8</sup> have performed Raman scattering experiments with a fairly high resolution around  $E = 2\Delta_0$  and also at higher-energy regions and observed several abrupt changes in  $dI_R/dE$  at energies higher than  $2\Delta_0$  and  $2\Delta_1$ . By taking account of three-excitation states, Hirashima and Iwamoto<sup>9</sup> showed that the Raman spectrum should also have cusps or inflections with infinite derivatives at  $E = 3\Delta_0$ ,  $2\Delta_0 + \Delta_1$ ,  $\Delta_0 + 2\Delta_1$ , and  $3\Delta_1$ . In a refined experiment by Ohbayashi *et al.*<sup>10</sup> values of  $E$  at which structures appear agree fairly with those values mentioned above. In this paper we investigate the possibility of the formation of three-roton bound states.

In Raman scattering the produced excitations have a vanishing total momentum,  $K=0$ , and are dominantly of  $d$ -wave symmetry. Thus the above-mentioned result, i.e., confirmation of the existence of a two-roton resonance, means that the interaction between two rotons with  $K=0$  and of  $d$ -wave symmetry is attractive. Even between two rotons with  $K=0$ , however, there can be many interact-

ing channels other than the  $d$ -wave one; the total angular momentum  $l$  can be any even integer. (The fact that it should be even comes from the Bose statistics.) Neither Raman scattering nor neutron scattering provides us with any information of the interaction at  $K=0$  in the channels other than the  $d$ -wave one.

For a finite  $K$ , there can also be several interacting channels between two rotons. Since the rotational invariance in momentum space is broken in this case,  $l$  is no longer a good quantum number. In particular, for a large  $K$ ,  $K \gtrsim p_0$ ,  $p_0$  being the roton momentum, channels are characterized by the magnetic quantum number  $m$  around  $K$ ; again only channels with even  $m$  are relevant due to the Bose statistics. Indeed several authors<sup>11,12</sup> argued that, to explain the experimentally observed roton lifetime and energy shift consistently, it was essential to work with a roton-roton interaction which is of a finite range (not a  $\delta$ -function type introduced first by Landau and Khalatnikov<sup>13,14</sup>) and is of several channels.

One can also deduce the quantitative information on the roton-roton interaction at large  $K$  by studying the roton linewidth (or viscosity) and the roton energy shift. It was shown<sup>11,12</sup> that to explain the linewidth the interaction at a large  $K$  should be large compared with that at  $K=0$  in the  $d$ -wave channel deduced from Raman scattering. Furthermore, the sign of the energy shift (decreasing with the temperature increasing) implies that the dominant interaction is attractive. Note that, however, those results are obtained after the thermal average in contrast to the results obtained from Raman and neutron scatterings, where one can see the elementary processes at least at the absolute zero,  $T=0$ .

Owing to the peculiar dispersion, in the presence of attractive interaction, however weak it may be, two rotons with a finite  $K$  also form bound states.<sup>15</sup> If it is clearly observed in neutron scattering, it will give us definite information on the roton-roton interaction with a finite  $K$ . In addition to the experimental resolution, however, single roton linewidth present at finite temperatures has prevented us from drawing any definite conclusion on the

existence of two-roton bound states (resonances) at a finite  $K$ . Actually Smith *et al.*<sup>16</sup> analyzed the neutron data using the theory of Zawadowski *et al.*<sup>6</sup> and reported that the roton-roton interaction at large  $K$ 's ( $2.7 \text{ \AA}^{-1} < K/\hbar < 3.3 \text{ \AA}^{-1}$ ) was repulsive. (See also Refs. 17 and 18).

So far we have given a brief summary of the present understanding of the roton-roton interaction. Details on the subject were reviewed by Zawadowski.<sup>19</sup> A brief but recent review was given by Bedell, Pines, and Zawadowski<sup>20</sup> (hereafter referred to as BPZ) (see also Refs. 21 and 22).

Now we return to Raman scattering. Confining ourselves to two-excitation states we get information only on the interaction between two rotons with  $K=0$  and  $l=2$  as mentioned before. However, three-excitation states with a vanishing total momentum,  $P=0$ , can also be involved in Raman scattering. (Note that we denote the total momentum of *three*-roton states by  $\mathbf{P}$  while that of *two*-roton ones by  $\mathbf{K}$  in this paper.) In the presence of attractive roton-roton interaction, then, we can expect that three-roton bound states (boson analog of a triton) are formed and will be observed in the experiment. We should note that, as far as three-roton states with  $P=0$  are concerned, as in this paper, relevant interaction is not one between two rotons with  $K=0$ , but one with  $K \simeq p_0$ . Observation of three-roton bound states [strictly speaking, resonant states (see Sec. III D)] would thus enable us to directly estimate the strength of roton-roton interaction with  $K \simeq p_0$ . This would, needless to say, give us valuable information to deepen our understanding of the roton-roton interaction and thereby of the various properties of He II.

As we will see, in the presence of attractive interaction between two rotons, three-roton bound states are necessarily formed just like two-roton ones. Those binding energies are much larger than those of the two-roton bound states with  $K \simeq p_0$  for the same coupling constants. On the other hand, it is not clear whether they are larger or smaller than those of two-roton bound states with  $K=0$ , because the relevant interactions are different for each case.

In this connection we should mention the recent work by BPZ.<sup>20</sup> They calculated the strength of the interaction between two rotons with large  $K$ 's as well as that with  $K=0$  using the polarization potential approach.<sup>23</sup> Their results showed that the former was attractive and larger (by almost an order of magnitude) than the latter. Note that their results are not inconsistent with those obtained from the analysis of the roton linewidth and the energy shift already mentioned. Using their values for the coupling constants we will see that the three-roton binding energy is about 1 K, which is large compared with the observed *d*-wave two-roton binding energy of 0.27 K.<sup>7,24</sup>

Investigation of the three-roton bound state is in itself of great interest, because the roton is a unique excitation due to its peculiar dispersion. Indeed two-roton bound states (resonances) also originate from this peculiarity.

In this paper we are mainly concerned with three-excitation (roton) states. We, however, have no firm

reason to truncate more than three excitation states; those states can also be involved in Raman scattering. Indeed, in a recent experiment,<sup>10</sup> Ohbayashi *et al.* suggested that there might also appear structures at  $E = n\Delta_0 + m\Delta_1$  with  $n + m \geq 4$  in the Raman spectrum. In this paper we touch on effects of four- and five-excitation states on the Raman spectrum by simply extending the discussion made by Hirashima and Iwamoto.<sup>9</sup>

The paper is organized as follows: In Sec. II we give an appropriate form of two-roton interaction for a large  $K$  and wave functions describing three-roton states with  $P=0$  and angular momentum  $l$ . In Sec. III we solve the Schrödinger equation to investigate the existence and the binding energy of three-roton bound states with  $l=0, 1$ , and 2, and then discuss several points including the observability of those states. Section IV is devoted to a brief discussion on four- and five-excitation states. In Sec. V we give a summary of the paper. Throughout the paper we restrict ourselves to the case with  $T=0$ .

## II. ROTON-ROTON INTERACTION FOR $K \simeq p_0$ AND THREE-ROTON WAVE FUNCTIONS

Before studying three-roton bound states, in this section we first give the interaction between two rotons with a large  $K$  and then construct wave functions describing three rotons with  $P=0$  as preliminaries.

### A. Roton-roton interaction for a large $K$ ( $K \gtrsim p_0$ )

Since we are mainly interested in Raman scattering, we concern ourselves exclusively with three-roton states with  $P=0$ . It is then sufficient to consider the interaction between two rotons with  $K \simeq p_0$ . For  $K \gtrsim p_0$ , the interaction  $v(\mathbf{p}_1, \mathbf{p}_2, \mathbf{p}_3, \mathbf{p}_4; \mathbf{K})$ , which is depicted in Fig. 1, should take the following form:<sup>25</sup>

$$v(\mathbf{p}_{12}, \mathbf{p}_{34}; \mathbf{K}) = \Omega^{-1} \sum_{m=-\infty}^{\infty} v_{|m|}(K) \exp[-im(\varphi_{12} - \varphi_{34})], \quad (1)$$

where  $\mathbf{p}_{ij} = (\mathbf{p}_i - \mathbf{p}_j)/2$ ,  $\Omega$  is the system volume, and  $\varphi_{ij}$  the azimuthal angle of  $\mathbf{p}_{ij}$  around  $\mathbf{K}$ . (See Fig. 2.) All  $p_i$ 's ( $i=1-4$ ) take the value

$$p_0 - \Delta p_c \leq p_i \leq p_0 + \Delta p_c,$$

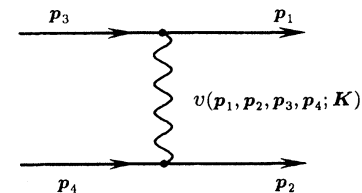


FIG. 1. Interaction between two rotons;  $\mathbf{p}_1 + \mathbf{p}_2 = \mathbf{p}_3 + \mathbf{p}_4 = \mathbf{K}$ .

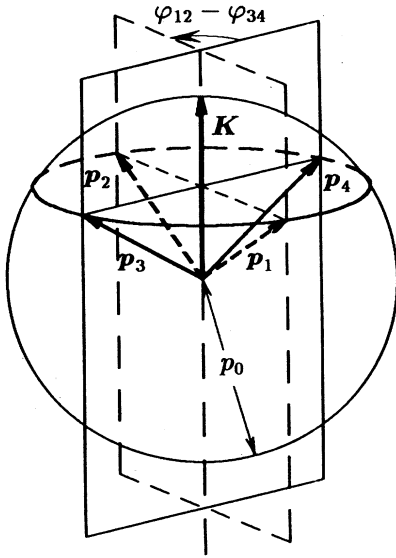


FIG. 2. Scattering of a roton pair ( $\mathbf{p}_3, \mathbf{p}_4$ ) into another pair ( $\mathbf{p}_1, \mathbf{p}_2$ );  $\mathbf{K} = \mathbf{p}_1 + \mathbf{p}_2 = \mathbf{p}_3 + \mathbf{p}_4$  and  $K \gtrsim p_0$ . All  $\mathbf{p}_i$ 's lie approximately on the sphere with a radius  $p_0$ .

$\Delta p_c$  being the cutoff momentum,  $\Delta p_c \approx 0.2p_0$ . If all  $p_i$ 's lie exactly on the sphere with a radius  $p_0$ , the Bose statistics require that  $m$  in (1) should be even, which we assume in the following; this amounts to neglecting terms of order  $(\Delta p_c/p_0)$  (see Sec. III D). Note that in general there also exists three-roton interaction, which cannot be expressed as a sum of two-roton interactions. In this paper we disregard that interaction.

$$D_{mm'}^l(\alpha, \beta, \gamma) = \langle lm | \exp(-i\alpha l_z) \exp(-i\beta l_y) \exp(-i\gamma l_z) | lm' \rangle^* \\ = \exp(i\alpha m) d_{mm'}^l(\beta) \exp(i\gamma m'), \quad (3)$$

with

$$d_{mm'}^l(\beta) = \langle lm' | \exp(i\beta l_y) | lm \rangle. \quad (4)$$

In Eq. (2) (and from now on) we do not explicitly write the condition  $\mathbf{P} = \sum_{i=1}^3 \mathbf{p}_i = 0$ .

To obtain the symmetrized wave function we add up the unsymmetrized ones with the arguments permuted,

$$\Psi_m^l(\mathbf{p}_1, \mathbf{p}_2, \mathbf{p}_3) = \psi_m^l(\mathbf{p}_1, \mathbf{p}_2, \mathbf{p}_3) + \psi_m^l(\mathbf{p}_1, \mathbf{p}_3, \mathbf{p}_2) \\ + \psi_m^l(\mathbf{p}_2, \mathbf{p}_3, \mathbf{p}_1) + \dots,$$

where  $\psi_m^l$  is the unsymmetrized wave function.

Now we have to determine how to take the body-fixed coordinates for the given arguments ( $\mathbf{p}_i, \mathbf{p}_j, \mathbf{p}_k$ ) ( $i, j, k = 1, 2, 3$ ).<sup>28</sup> Note that the order of the arguments is important. First we take the  $z$  axis to be parallel with the first argument  $\mathbf{p}_i$ , and then the  $y$  axis with  $\mathbf{p}_i \times \mathbf{p}_j$ ; conse-

### B. Three-roton wave functions

In three-roton states with  $P=0$ , the total angular momentum  $l$  is a good quantum number. In this subsection we give the wave function describing the three-roton states with  $P=0$  and with any  $l$ . Here we should note that in the three-roton case, the Bose statistics do not preclude odd  $l$  states, in contrast with the two-roton case. In the following we give the derivation of the three-roton wave functions in some detail, because it is not a trivial task.

Since, besides  $l$ , its projection  $m$  is also a good quantum number, the wave function of three rotors with  $P=0$  is specified by  $l$  and  $m$ ,  $\Psi_m^l(\mathbf{p}_1, \mathbf{p}_2, \mathbf{p}_3; \mathbf{P} = \sum_{i=1}^3 \mathbf{p}_i = 0)$ . Owing to the condition  $\mathbf{P}=0$ ,  $\Psi_m^l$  is expressed by six variables. It is convenient to take as the variables the magnitude of  $\mathbf{p}_i$  ( $i=1, 2, 3$ ),  $p_1, p_2$ , and  $p_3$ , and the Euler angles ( $\alpha, \beta$ , and  $\gamma$ ) to specify the orientation of the triangle formed by  $\mathbf{p}_1, \mathbf{p}_2$ , and  $\mathbf{p}_3$ . For the definition of the Euler angles, we follow the convention taken by Bohr and Mottelson<sup>26</sup> or Rose.<sup>27</sup> We denote the space-fixed coordinates by  $(XYZ)$  and the body-fixed ones by  $(xyz)$ .

The wave function  $\Psi_m^l$  is a superposition of states specified with  $l$  and its projection  $m'$  onto the body-fixed  $z$  axis. We denote the corresponding wave function by  $u_{m'}^l(p_1, p_2, p_3)$ , which is a function of  $p_1, p_2$ , and  $p_3$ ; we assume that it is symmetric under any permutations of  $p_i$ 's. The wave function  $\Psi_m^l$  is then expressed in terms of  $u_{m'}^l$  as follows:<sup>26</sup>

$$\Psi_m^l(\mathbf{p}_1, \mathbf{p}_2, \mathbf{p}_3) = \mathcal{S} \sum_{m'=-l}^l D_{mm'}^l(\alpha, \beta, \gamma) u_{m'}^l(p_1, p_2, p_3), \quad (2)$$

where  $\mathcal{S}$  stands for the symmetrization with respect to the permutations of the  $\mathbf{p}_i$ 's. The  $D$  function is, following Bohr and Mottelson,<sup>26</sup> defined by

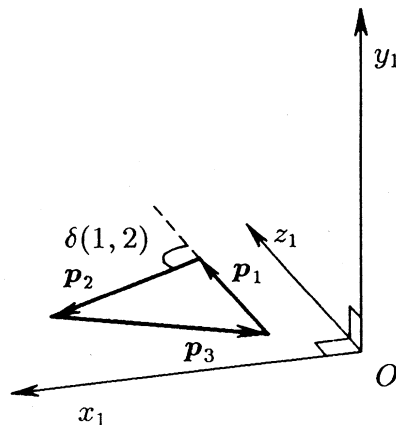


FIG. 3. Body-fixed coordinates  $(x_1, y_1, z_1)$ . The triangle formed by  $\mathbf{p}_1, \mathbf{p}_2$ , and  $\mathbf{p}_3$  lies on the  $x_1$ - $z_1$  plane.  $\delta(1,2)$  is the angle made by  $\mathbf{p}_1$  and  $\mathbf{p}_2$ .

quently the  $y$  axis is perpendicular to the plane on which the  $\mathbf{p}_1$ - $\mathbf{p}_2$ - $\mathbf{p}_3$  triangle lies. The  $x$  axis is uniquely determined by the requirement that the  $(xyz)$  coordinates are right-handed ones. We denote the body-fixed coordinates defined in this way for  $(\mathbf{p}_1, \mathbf{p}_2, \mathbf{p}_3)$  by  $(x_1, y_1, z_1)$  (see Fig. 3) and the corresponding Euler angles by  $(\alpha_1, \beta_1, \gamma_1)$ , and for

$(\mathbf{p}_1, \mathbf{p}_3, \mathbf{p}_2)$  by  $(x'_1, y'_1, z'_1)$  and  $(\alpha'_1, \beta'_1, \gamma'_1)$ . Similarly, we can define  $(x_2, y_2, z_2)$  and  $(\alpha_2, \beta_2, \gamma_2)$ , and  $(x_3, y_3, z_3)$  and  $(\alpha_3, \beta_3, \gamma_3)$ , etc.; the  $x_2$  axis is parallel with  $\mathbf{p}_2$  and the  $y_2$  axis with  $\mathbf{p}_2 \times \mathbf{p}_3$ , for example.

Since we have assumed that  $u_m^l$  is symmetric, we see that  $\Psi_m^l$  reduces to the following:

$$\Psi_m^l(\mathbf{p}_1, \mathbf{p}_2, \mathbf{p}_3) = \sum_{m'=-l}^l [D_{mm'}^l(\alpha_1, \beta_1, \gamma_1) + D_{mm'}^l(\alpha'_1, \beta'_1, \gamma'_1) + D_{mm'}^l(\alpha_2, \beta_2, \gamma_2) + \cdots] u_{m'}^l(p_1, p_2, p_3),$$

where we assume  $u_m^l$  is properly normalized.

It is convenient to express the five  $D_{mm'}^l$ 's in terms of the remaining  $D_{mm'}^l$ , e.g.,  $D_{mm'}^l(\alpha_1, \beta_1, \gamma_1)$ . Firstly, since  $x'_1 = -x_1$  and  $y'_1 = -y_1$ , in other words,  $\gamma'_1 = \gamma_1 + \pi$  (see Fig. 3), we have

$$D_{mm'}^l(\alpha'_1, \beta'_1, \gamma'_1) = D_{mm'}^l(\alpha_1, \beta_1, \gamma_1 + \pi) = D_{mm'}^l(\alpha_1, \beta_1, \gamma_1) e^{im'\pi} = (-1)^{m'} D_{mm'}^l(\alpha_1, \beta_1, \gamma_1). \quad (5)$$

Next, since  $(x_2, y_2, z_2)$  is given by the rotation of  $(x_1, y_1, z_1)$  with  $\delta(12)$  around the  $Y$  axis [ $\delta(12)$  is the angle made by  $\mathbf{p}_1$  and  $\mathbf{p}_2$ ,  $\cos\delta(12) = \mathbf{p}_1 \cdot \mathbf{p}_2 / (p_1 p_2)$ ],  $D_{mm'}^l(\alpha_2, \beta_2, \gamma_2)$  is given by

$$\begin{aligned} D_{mm'}^l(\alpha_2, \beta_2, \gamma_2) &= \langle lm | \exp(-i\alpha_1 l_Z) \exp(-i\beta_1 l_Y) \exp(-i\gamma_1 l_Z) \exp[-i\delta(12) l_Y] | lm' \rangle^* \\ &= \sum_{m''=-l}^l D_{mm''}^l(\alpha_1, \beta_1, \gamma_1) d_{m''m'}^l(\delta(12)). \end{aligned} \quad (6)$$

By similarly considering the remaining permutations and noting that the same result is also obtained in terms of  $(\alpha_1, \beta_2, \gamma_2)$  and  $(\alpha_3, \beta_3, \gamma_3)$ , we finally have the symmetrized three-boson (roton) wave function with the angular momentum  $l$  and its projection  $m$  onto the  $Z$  axis as

$$\begin{aligned} \Psi_m^l(\mathbf{p}_1, \mathbf{p}_2, \mathbf{p}_3) &= \sum_{m', m''=-l}^l D_{mm''}^l(\alpha_1, \beta_1, \gamma_1) \Delta_{m''m'}^l(p_1, p_2, p_3) u_{m'}^l(p_1, p_2, p_3) \\ &= \sum_{m', m''=-l}^l D_{mm''}^l(\alpha_2, \beta_2, \gamma_2) \Delta_{m''m'}^l(p_2, p_3, p_1) u_{m'}^l(p_1, p_2, p_3) \\ &= \sum_{m', m''=-l}^l D_{mm''}^l(\alpha_3, \beta_3, \gamma_3) \Delta_{m''m'}^l(p_3, p_1, p_2) u_{m'}^l(p_1, p_2, p_3), \end{aligned} \quad (7)$$

where  $\Delta_{mm'}^l(p_1, p_2, p_3)$  is defined by

$$\Delta_{mm'}^l(p_1, p_2, p_3) = [\delta_{mm'} + d_{mm'}^l(\delta(12)) + d_{mm'}^l(-\delta(31))][1 + (-1)^{m'}]. \quad (8)$$

Note that the dependence of  $\Delta_{mm'}^l$  on  $p_1$ ,  $p_2$ , and  $p_3$  comes through that of  $\delta(ij)$  on them; e.g.,  $\delta(12) = \arccos[(p_3^2 - p_1^2 - p_2^2)/2p_1 p_2]$ . Since states with a definite  $l$  but with different  $m$  are degenerate, we drop the suffix  $m$  attached to  $\Psi_m^l$  from now on.

### III. THREE-ROTON BOUND STATES AND THEIR BINDING ENERGIES

We denote the ground state and the one-excitation state of He II by  $|0\rangle$  and  $b_p^\dagger|0\rangle$ , respectively. We require that  $b_p$  and  $b_p^\dagger$  should satisfy the Bose commutation relations. The effective Hamiltonian describing two interacting rotors is given by

$$\mathcal{H} = \sum_p \omega(p) b_p^\dagger b_p + \frac{1}{2} \sum_{p, p', \mathbf{K}} v(\mathbf{p}, \mathbf{p}'; \mathbf{K}) b_{\mathbf{K}/2+p}^\dagger b_{\mathbf{K}/2-p}^\dagger b_{\mathbf{K}/2-p} b_{\mathbf{K}/2+p}, \quad (9)$$

where  $\omega(p)$  is the experimentally observed roton dispersion; for the roton dispersion we use the parabola expression,  $\omega(p) = \Delta_0 + (p - p_0)^2 / (2\mu)$ , for  $p_0 - \Delta p_c \leq p \leq p_0 + \Delta p_c$  in this paper. For large  $K$  expression (1) can be used for  $v(\mathbf{p}, \mathbf{p}'; \mathbf{K})$  in (9) as noted in the preceding section. We approximately express the three-roton states with  $P=0$  and the angular momentum  $l$  as<sup>29</sup>

$$\Psi^l = \frac{1}{3!} \sum_{p_1, p_2} \Psi^l(\mathbf{p}_1, \mathbf{p}_2, \mathbf{p}_3) b_{p_1}^\dagger b_{p_2}^\dagger b_{p_3}^\dagger |0\rangle,$$

where  $\Psi^l(\mathbf{p}_1, \mathbf{p}_2, \mathbf{p}_3)$  is given in the preceding section [Eq. (7)] and the factor  $1/3!$  is introduced to avoid overcounting the identical states. Minimizing  $\langle \Psi^l | \mathcal{H} | \Psi^l \rangle - E \langle \Psi^l | \Psi^l \rangle$ , i.e.,  $\delta(\langle \Psi^l | \mathcal{H} | \Psi^l \rangle - E \langle \Psi^l | \Psi^l \rangle) = 0$ , readily leads to the

Schrödinger equation for  $\Psi^l(\mathbf{p}_1, \mathbf{p}_2, \mathbf{p}_3)$ ,

$$[E - \omega_3(p_1, p_2, p_3)]\Psi^l(\mathbf{p}_1, \mathbf{p}_2, \mathbf{p}_3) = \Omega^{-1} \sum_{m=\text{even}} v_{|m|} \left[ e^{-im\varphi_{23}} \sum_{\mathbf{p}'_{23}} e^{im\varphi'_{23}} \Psi^l(\mathbf{p}_1, \mathbf{p}'_2, \mathbf{p}'_3) + e^{-im\varphi_{31}} \sum_{\mathbf{p}'_{31}} e^{im\varphi'_{31}} \Psi^l(\mathbf{p}'_1, \mathbf{p}_2, \mathbf{p}_3) + e^{-im\varphi_{12}} \sum_{\mathbf{p}'_{12}} e^{im\varphi'_{12}} \Psi^l(\mathbf{p}'_1, \mathbf{p}'_2, \mathbf{p}_3) \right], \quad (10)$$

where (1) has been used because the total momentum of any pair is about  $p_0$ , e.g.,  $|\mathbf{p}_1 + \mathbf{p}_2| = p_3 \approx p_0$ ,  $E$  is the energy of the state  $\Psi^l$ , and  $\omega_3(p_1, p_2, p_3) = \sum_{i=1}^3 \omega(p_i)$ . Furthermore, we have assumed  $v_{|m|}(K)$  to be constant,  $v_{|m|}(K) \approx v_{|m|}(p_0) = v_{|m|}$ .

Owing to the condition  $P=0$ , the summations on the right-hand side of (10) are restricted by the triangular inequalities, e.g.,  $|p'_2 - p'_3| \leq p_1 \leq p'_2 + p'_3$ . Since all  $p_i$ 's are close in magnitude to  $p_0$ ,  $p_0 - \Delta p_c \leq p_i \leq p_0 + \Delta p_c$ , however, the inequalities are automatically satisfied. Hence, it is sufficient to perform the summations with the condition  $p_0 - \Delta p_c \leq p_i \leq p_0 + \Delta p_c$  but without any further restrictions.

The three-body Schrödinger equation is exactly solvable, i.e., without the variational method for example, for a separable interaction.<sup>30</sup> Similarly, we can solve Eq. (10) exactly. It should be noted, however, that the form of the interaction (1) is *not assumed* to solve the problem, but it naturally results from the symmetry considerations. (Moreover, it is required to explain the experimental results as mentioned in Sec. I.)

As usual we transform the summation in Eq. (10) into integration; in doing so it is convenient to take the variables as follows:

$$\sum_{\mathbf{p}'_{23}} \rightarrow \frac{\Omega}{(2\pi\hbar)^3} \int d\mathbf{p}'_{23} = \frac{\Omega}{(2\pi\hbar)^3} \frac{1}{p_1} \int_c p'_2 dp'_2 \int_c p'_3 dp'_3 \int_0^{2\pi} d\gamma_1,$$

where  $c$  means  $p_0 - \Delta p_c \leq p'_i \leq p_0 + \Delta p_c$  ( $i=2,3$ ). Note that  $\varphi'_{23} = -\gamma_1$ . Substituting (7) on the right-hand side of Eq. (10) we find that it is reduced to

$$\Psi^l(\mathbf{p}_1, \mathbf{p}_2, \mathbf{p}_3) = [E - \omega_3(p_1, p_2, p_3)]^{-1} \sum_{m'=-l, \text{even}}^l \frac{v_{|m'|}}{(2\pi\hbar)^3} \sum_{j=1}^3 D_{mm'}^l(\alpha_j, \beta_j, \gamma_j) \frac{2\pi}{p_j} F_{m'}^l(p_j), \quad (11)$$

with

$$F_{m'}^l(p) = \sum_{m''=-l}^l \int_c p' dp' \int_c p'' dp'' \Delta_{m'm''}^l(p, p', p'') u_{m''}^l(p, p', p''). \quad (12)$$

Since we are interested only in bound states, i.e., those states with  $E < \omega_3(p_1, p_2, p_3)$  (but see the following), no homogeneous term appears on the right-hand side of Eq. (11). Noting the orthogonality of  $D_{mm'}^l$  and the relations of  $D_{mm'}^l(\alpha_1, \beta_1, \gamma_1)$ ,  $D_{mm'}^l(\alpha_2, \beta_2, \gamma_2)$ , and  $D_{mm'}^l(\alpha_3, \beta_3, \gamma_3)$  [see (6)], we have, after a straightforward manipulation, a set of integral equations for  $F_{m'}^l(p)$ ,

$$F_{m'}^l(p_1) = - \sum_{m''=-l, \text{even}}^l \frac{2\pi v_{|m''|}}{(2\pi\hbar)^3} \left[ \delta_{m'm''} \int_c \frac{p_2 dp_2 p_3 dp_3}{\omega_3(p_1, p_2, p_3) - E} \frac{F_{m''}^l(p_1)}{p_1} + \int_c \frac{[1 + (-1)^{m'-m''}] d_{m'm''}^l(\delta(12)) dp_2 p_3 dp_3}{\omega_3(p_1, p_2, p_3) - E} F_{m''}^l(p_2) \right], \quad (13)$$

where the relation  $d_{mm'}^l(\beta) = (-1)^{m-m'} d_{mm'}^l(-\beta)$  has been used. If Eq. (13) has an eigenvalue  $E$  such that  $E < 3\Delta_0$  (but see the following), we have a bound state and the binding energy is given by  $E_B = 3\Delta_0 - E (> 0)$ .

Before proceeding we make a simplification. In deriving (1) we neglected terms of order  $(\Delta p_c/p_0)$ . In according with it we also neglect such terms in Eq. (13) to have  $\delta(12) = \frac{2}{3}\pi$ . We then see that  $\Delta_{m'm''}^l(p_1, p_2, p_3)$  defined by Eq. (8) becomes constant,

$$\Delta_{m'm''}^l = [\delta_{m'm''} + d_{m'm''}^l(\frac{2}{3}\pi) + d_{m'm''}^l(-\frac{2}{3}\pi)][1 + (-1)^{m'}] = \{\delta_{m'm''} + [1 + (-1)^{m-m'}] d_{m'm''}^l(\frac{2}{3}\pi)\}[1 + (-1)^{m'}], \quad (14)$$

i.e.,  $\Delta_{m'm''}^l$  is finite for even  $m$  and  $m'$ , and otherwise vanishes. Consequently  $F_{m'}^l$  also survives only for even  $m'$  and Eq. (13) is rewritten as

$$F_{m'}^l(p) = - \sum_{m''=-l, \text{even}}^l \frac{2\pi v_{|m''|}}{(2\pi\hbar)^3} \left[ \delta_{m'm''} \int_c \frac{p' dp' p'' dp''}{\omega_3(p, p', p'') - E} \frac{F_{m''}^l(p)}{p} + 2d_{m'm''}^l(\frac{2}{3}\pi) \int_c \frac{dp' p'' dp''}{\omega_3(p, p', p'') - E} F_{m''}^l(p') \right]. \quad (15)$$

Although Eq. (15) is valid for any  $l$ , we study only the cases with  $l=0, 1$ , and  $2$  in the following; only  $s$ - and  $d$ -wave states are observable in Raman scattering at  $T=0$  as will be discussed in Sec. III D.

From now on we set  $v_{|m|}$ 's to be negative; they are assumed to be attractive.

A. *s*-wave case

For the *s*-wave ( $l=0$ ),  $d_{00}^0(\beta)=1$ . Equation (15) is then reduced to

$$\alpha(E;p)F_0^0(p) + \int_c dp' \beta(E;p,p')F_0^0(p') = \left[ \frac{|v_0|}{(2\pi\hbar)^3} \right]^{-1} F_0^0(p), \quad (16)$$

where

$$\alpha(E;p) = \frac{2\pi}{p} \int_c dp' \int_c dp'' \frac{p'p''}{\omega_3(p,p',p'')-E} \quad (17)$$

and

$$\beta(E;p,p') = 4\pi \int_c dp'' \frac{p''}{\omega_3(p,p',p'')-E}. \quad (18)$$

Equation (16) is of a similar form with the ordinary Schrödinger equation for a two-body problem, but in contrast to it, where the eigenvalue  $E$  is determined for a given coupling constant, in Eq. (16) the coupling constant  $|v_0|$ , actually its inverse, is the eigenvalue for a given  $E$ .

We can then make an interpretation of Eq. (16) resorting to the analogy with the Schrödinger equation. We see that  $F(p)$  (suffixes dropped) stands for the wave function for a free roton with  $p$  with the remaining two interacting rotors. The second term on the left-hand side represents the effect of the "interaction"; the free roton represented by  $F(p)$  also interacts with both of the remaining two rotors. Indeed in the absence of the second term Eq. (16) gives the following expression for  $E$ :

$$2\Delta_0 - E = C^2 \frac{\Delta p_c^2}{2\mu} \exp \left[ - \left( \frac{\mu p_0^2}{2\pi\hbar^3 p} \right)^{-1} |v_0|^{-1} \right] - \left[ \Delta_0 + \frac{(p-p_0)^2}{2\mu} \right], \quad (19)$$

where  $C$  is a number weakly depending on  $E$  and  $p$  ( $C \approx 1.12$ ). The first term is the binding energy of *two* rotors with  $K=p$  and the second term the free roton energy.

Now it becomes clear that indeed the continuum threshold is not  $E=3\Delta_0$ , but  $E=2\Delta_0-E_c$ , where  $E_c$  is the maximum of the right-hand side of Eq. (19). In other words, if a state has the energy  $E$  less than  $3\Delta_0$  but larger than  $2\Delta_0-E_c$ ,  $2\Delta_0-E_c < E < 3\Delta_0$ , it is not a *three-roton* bound state, but a state where *two* rotors form a bound state with a scattering roton; it is a state in the continuum. Since the right-hand side of Eq. (19) takes the maximum value for  $p \approx p_0$ , the continuum threshold is approximately given by

$$3\Delta_0 - E_c = C^2 \frac{\Delta p_c^2}{2\mu} \exp \left[ - \left( \frac{\mu p_0}{2\pi\hbar^3} \right)^{-1} |v_0|^{-1} \right]. \quad (20)$$

The relation of  $E_B$ ,  $E_B=3\Delta_0-E$ , and  $|v_0|$ , obtained numerically from Eq. (16), is shown in Fig. 4, where dimensionless quantities

$$\varepsilon_B = E_B / (p_0^2 / 2\mu)$$

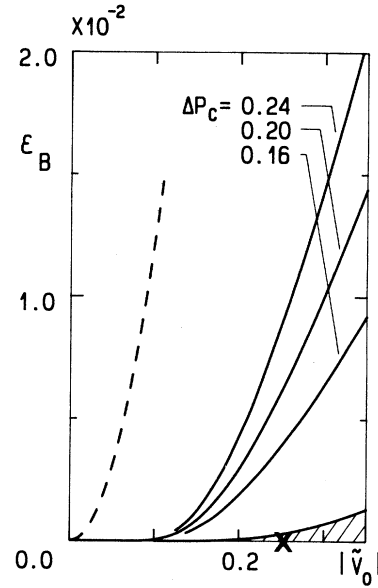


FIG. 4. Three-roton binding energy of the *s*-wave state as a function of  $|\bar{v}_0|$  for three different values of  $\Delta p_c$ :  $\Delta p_c=0.16$ ,  $0.20$ , and  $0.24$ . The binding energy and the strength of the interaction are respectively normalized as  $\varepsilon_B = E_B / (p_0^2 / 2\mu)$  and  $|\bar{v}_0| = |v_0| / (2\mu p_0 / \pi^2 \hbar^3)$ . The  $\times$  on the abscissa stands for the value of  $|\bar{v}_0|$  obtained by BPZ at zero pressure. The hatched region represents the continuum states. The dashed curve is the two-roton binding energy for  $K=0$  (see the text).

and

$$|\bar{v}_0| = |v_0| / (2\mu p_0 / \pi^2 \hbar^3)$$

are introduced. Using the values for  $p_0$  and  $\mu$ ,  $p_0/\hbar = 1.92$  ( $\text{\AA}^{-1}$ ) and  $\mu = 0.16m_4$  ( $m_4$  being the mass of a  ${}^4\text{He}$  atom), we have  $E_B = 140\varepsilon_B(K)$  and

$$|v_0| = 2.69 \times 10^{-38} |\bar{v}_0| (\text{erg cm}^3).$$

In Fig. 4 we have shown the  $\varepsilon_B - |\bar{v}_0|$  curve for three different values of  $\Delta p_c$ ;  $\Delta p_c=0.16$ ,  $0.20$ , and  $0.24$ . The continuum states for  $\Delta p_c=0.20$  noted above are also shown. Furthermore, for comparison, we show the two-roton binding energy  $\varepsilon_B^{2,l}$  with  $K=0$  and angular momentum  $l$ ; it should be noted that for this case the abscissa should be considered to represent  $|\bar{v}^l|$ , which is the strength of the interaction between two rotors with  $K=0$  and the angular momentum  $l$ ;  $\varepsilon_B^{2,l} = (\pi^2/8) |\bar{v}^l|^2$ .

From Fig. 4 we first note that  $\varepsilon_B$  varies exponentially for small  $|\bar{v}_0|$  as expected from Eq. (19), and that for the same values of  $|\bar{v}_0|$  and  $|\bar{v}^l|$   $\varepsilon_B$  is much smaller than  $\varepsilon_B^{2,l}$ . The latter fact is easily understood by considering the available momentum space; for the three-roton case, or for the case with two rotors with a finite  $K$ , the momentum space in which two interacting rotors can move is restricted, as shown in Fig. 5, in contrast with the case with two rotors with  $K=0$ , where two rotors can move on the whole sphere.

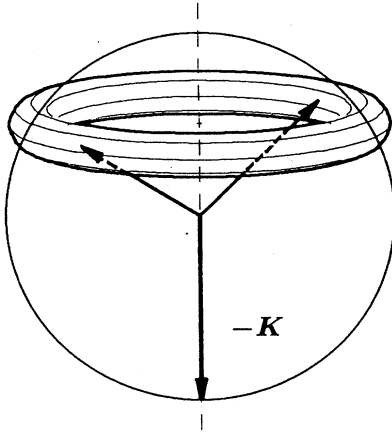


FIG. 5. Available momentum space for interacting two rotons with  $K \simeq p_0$ .

On the other hand,  $\varepsilon_B$  is much larger than the two-roton binding energy with  $K \simeq p_0$ , which is approximately given by the continuum threshold (20). Furthermore, we note that for large  $|\bar{v}_0|$ ,  $|\bar{v}_0| > 0.1$ ,  $\varepsilon_B$  sensitively depends on the cutoff  $\Delta p_c$ . Since  $|\bar{v}_0|$  may take such a large value (as will be discussed in Sec. III D), a calculation without using the parabola approximation for the roton dispersion (and thereby without the introduction of the cutoff) may be desired.

$$\alpha(E; p)F_{2-}^2(p) + [d_{22}^2(\frac{2}{3}\pi) - d_{2-2}^2(\frac{2}{3}\pi)] \int_c dp' \beta(E; p, p') F_{2-}^2(p') = \left[ \frac{|v_2|}{(2\pi\hbar)^3} \right]^{-1} F_{2-}^2(p) \quad (22)$$

and

$$\begin{aligned} \alpha(E; p)F_0^2(p) + d_{00}^2(\frac{2}{3}\pi) \int_c dp' \beta(E; p, p') F_0^2(p) + |v_2||v_0|^{-1} d_{20}^2(\frac{2}{3}\pi) \int_c dp' \beta(E; p, p') F_{2+}^2(p') &= \left[ \frac{|v_0|}{(2\pi\hbar)^3} \right]^{-1} F_0^2(p), \\ \alpha(E; p)F_{2+}^2(p) + [d_{22}^2(\frac{2}{3}\pi) + d_{2-2}^2(\frac{2}{3}\pi)] \int_c dp' \beta(E; p, p') F_{2+}^2(p') + 2|v_0||v_2|^{-1} d_{20}^2(\frac{2}{3}\pi) \int_c dp' \beta(E; p, p') F_0^2(p') & \\ &= \left[ \frac{|v_2|}{(2\pi\hbar)^3} \right]^{-1} F_{2+}^2(p), \end{aligned} \quad (23)$$

where

$$F_{2\pm}^2(p) = F_2^2(p) \pm F_{2-2}^2(p)$$

and the relations

$$d_{mm'}^l(\beta) = (-1)^{m-m'} d_{m'm}^l(\beta) = (-1)^{m-m'} d_{-m-m'}^l(\beta)$$

have been used. Substituting the values,  $d_{00}^2(2\pi/3) = -\frac{1}{8}$ ,  $d_{2-2}^2(2\pi/3) = \frac{9}{16}$ ,  $d_{20}^2(2\pi/3) = 3\sqrt{6}/16$ , and  $d_{22}^2(2\pi/3) = \frac{1}{16}$ , we first note that Eq. (22) yields no bound states because  $d_{22}^2(2\pi/3) - d_{2-2}^2(2\pi/3)$  is negative.

### B. *p*-wave case

Since only terms with even  $m'$  and  $m''$  appear in Eq. (15), we can consider only the  $m' = m'' = 0$  component for  $l = 1$ . The resultant equation reads as

$$\alpha(E; p)F_0^1(p) + d_{00}^1(\frac{2}{3}\pi) \int_c dp' \beta(E; p, p') F_0^1(p') = \left[ \frac{|v_0|}{(2\pi\hbar)^3} \right]^{-1} F_0^1(p). \quad (21)$$

Since

$$d_{00}^1(\beta) = [4\pi/(2l+1)]^{1/2} Y_{10}(\beta, 0),$$

we have

$$d_{00}^1(2\pi/3) = -\frac{1}{2}.$$

In analogy with the Schrödinger equation done in the preceding subsection, we see that the "interaction" represented by the second term on the left-hand side of Eq. (21) is *repulsive* and consequently that three-roton bound state is not formed in the *p*-wave states; the two-roton bound states are also formed though. Since the wave function changes its sign in the momentum space, it effectively feels repulsive interaction though  $v_0$  itself is attractive.

### C. *d*-wave case

In this case we must consider  $m' = -2, 0$ , and 2 components. After a little manipulation we can decouple the  $3 \times 3$  coupled equations to the following one decoupled and  $2 \times 2$  coupled equations:

We proceed to investigate the coupled Eqs. (23). The numerical result for  $\Delta p_c = 0.20$  is given in Fig. 6. We have found a bound state for a given set of  $(|\bar{v}_2|, |\bar{v}_0|)$ . Note that, however, if  $|\bar{v}_2|$  vanishes, there appears no bound state only with attractive interaction  $v_0$  in the  $m = 0$  channel, because  $d_{00}^2(2\pi/3)$  is negative. In Fig. 6 a finite value of  $\varepsilon_B$  is given even for  $|\bar{v}_2| = 0$ ; this should be regarded as the continuum threshold mentioned before.

### D. Discussions

We have found that three-roton bound states do exist in the presence of the attractive roton-roton interaction

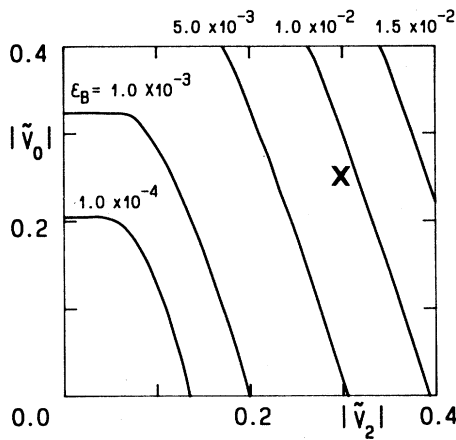


FIG. 6. Equibinding-energy curve for the  $d$ -wave three-roton bound states. The  $\times$  stands for the values of  $(|v_2|, |v_0|)$  obtained by BPZ at zero pressure.

and obtained the relation between the binding energy and the strength of the interaction. In this subsection we give some discussion on the results obtained so far.

We have just assumed that the roton-roton interaction for  $K \simeq p_0$  is attractive. Recently BPZ (Ref. 20) calculated the roton-roton interaction by means of the polarization potential approach.<sup>23</sup> They found that the roton-roton interaction for large  $K$ ,  $v_{|m|}(K \simeq p_0)$ , was attractive (at least at small pressures), and that its strength was larger by almost an order of magnitude than that of the interaction for  $K=0$ ,  $v^l$ . If we use their values of  $v_0$  and  $v_2$ , which are identified with their  $g_4^0$  and  $g_4^2$ , respectively, we find that the three-roton binding energy has a value around 1 K for both  $s$ - and  $d$ -wave cases. We noted in Sec. III A that if  $v_{|m|}$  were of the same magnitude as  $v^l$ , three-roton binding energy would be much smaller than the two-roton one with  $K=0$ . However, the three-roton binding energy can be much larger than the two-roton binding energy under the assumption of the large values of  $v_{|m|}$ 's. In Figs. 4 and 6 the values of  $v_0$  and  $v_2$  at zero pressure obtained by BPZ (Ref. 20) are depicted by crosses.

Next we discuss the observability of the three-roton bound states in Raman scattering. Actually, to discuss the Raman spectrum taking account of three-roton bound states (and two-roton bound states with a scattering roton) we should study the full three-body problem, in other words, the inhomogeneous Faddeev equation;<sup>31</sup> what we have done is simply equivalent to solving the homogeneous Faddeev equation. Unfortunately we have not been able to formulate it in a transparent way as in the two-excitation case.<sup>4-6</sup> We should thus content ourselves with qualitative discussions, but they are sufficient for the present purpose.

First, as mentioned in the Introduction, three-excitation states are also involved in Raman scattering; there should be a direct coupling between a photon and three-excitation states and that between two- and three-

excitation states, even if they might be small. In principle the three-roton bound states are also observable in Raman scattering.

What symmetry do the observable three-roton states have then,  $l=0, 1, 2$ , or  $\dots$ ? Since a photon has a spin 1, the conservation of the angular momentum leads to  $1=l+1$ ; we have treated the electromagnetic field with the dipole approximation because the wavelength of the incident light is much longer than the atomic scale. We see that  $l$  is either 0, 1, or 2. Since the parity conservation excludes  $l=1$  states, however, we have  $l=0$  ( $s$ -wave) and  $l=2$  ( $d$  wave) states as the final states of Raman scattering.

At the same time we should note that the three-roton bound states cannot be observed as sharp peaks, but instead as broad resonances. In addition to the coupling between three-roton states and two-excitation (phonon) states already mentioned, that between three-roton and three-phonon states, etc. give a width to the three-roton bound states; we have discarded those couplings so far. Furthermore, it is probable that the two broad peaks corresponding to the  $s$ - and  $d$ -wave resonances are merged into one depending on the experimental resolution and the temperature.

Taking account of the above circumstances we expect that the three-roton bound states (resonances) will be observed at most as a broad and not so large peak below the cusp (or inflection with infinite derivative) at  $E=3\Delta_0$ .<sup>9</sup> Note that, however, once their existence is unambiguously confirmed, it will be manifest evidence that the roton-roton interaction for  $K \simeq p_0$  is attractive and further allow us to estimate the strength of the attractive interaction.

Looking at the experimental data by Ohbayashi *et al.*,<sup>10</sup> we note that there seems to appear a broad hump below  $E=3\Delta_0$ . Needless to say, however, it is still premature to draw any conclusion on the existence of the three-roton resonances at the present stage, and it is hoped that further experiments will provide us with more information.

It is worth mentioning that the three-roton resonances can also be observed in a neutron scattering experiment. Since the situation is rather different from Raman scattering, e.g., the total momentum of the produced excitations is nonzero in neutron scattering, we give no further discussion on the subject, but it may deserve further investigation.

Lastly we mention the effects of the terms of order  $(\Delta p_c/p_0)$  neglected so far. Allowing for those terms we see that in (1) odd- $m$  terms also contribute. At the same time  $\Delta_{mm'}^l$  with odd  $m$  and/or  $m'$  does not vanish, so that in Eq. (13) there also appears  $F_m^l(p)$ 's with odd  $m'$ ; they couple only among themselves, but not with  $F_m^l(p)$ 's with even  $m'$ . We can then expect that three rotors are also bound in odd- $m'$  states, that is, for a given  $l$  another bound state(s) characterized by odd projection  $m'$  of  $l$  onto the body-fixed  $z$  axis may appear. However, those binding energies would be much smaller than those of even- $m'$  states discussed here, because  $v_{|m|}$  with odd  $m$  is smaller by an order of  $(\Delta p_c/p_0)$  than those with even  $m$  after all.



Three-roton states with even  $m'$  will also be affected. By relaxing the restriction  $\delta(ij)=2\pi/3$  we can take account of the vibrational motion in momentum space in addition to the rotational one discussed so far. It may be interesting to study the vibrational effects, but they will not be so relevant.

#### IV. EFFECTS OF FOUR- AND FIVE-EXCITATION STATES

In this section we give a brief discussion on effects of four- and five-excitation states on the Raman spectrum; this subject is quite disconnected from the discussions so far. The appearance of cusps or inflections with infinite derivatives at  $E=E_3^c$ ,  $E_3^c=3\Delta_0$ ,  $2\Delta_0+\Delta_1$ ,  $\Delta_0+2\Delta_1$ , or  $3\Delta_1$ , directly results from the analytic behavior of the *free*-three-excitation propagator around  $E=E_3^c$ ; it has a term proportional to  $|E-E_3^c|^{1/2}$  both above and below  $E=E_3^c$ .<sup>9,32</sup>

In regard to four-excitation states, we see that at  $E=E_4^c$ ,  $E_4^c=4\Delta_0$ ,  $3\Delta_0+\Delta_1$ ,  $2\Delta_0+2\Delta_1$ ,  $\Delta_0+3\Delta_1$ , and  $4\Delta_1$ , the *free*-four-excitation propagator has a term proportional to  $(E-E_4^c)\ln|E-E_4^c|$ . This term results in the appearance only of inflections with infinite derivatives, but never cusps, in the Raman spectrum. Similar argument leads to the conclusion that at  $E=5\Delta_0$  there appears no structure; only the second derivative diverges.

These results contradict the suggestion by Ohbayashi *et al.*<sup>10</sup> In the previously mentioned argument we have assumed the four- and five-excitation vertices to be slowly

varying around  $E=E_3^c$  and  $E_4^c$ . This assumption is not so justifiable because we have taken no account of the two- and three-excitation (roton) bound states. Taking full account of those states we might see that more distinct structures would appear at (or near)  $E=E_3^c$  and  $E_4^c$ . We feel that not only theoretical but also experimental efforts may be required to clarify the situation.

#### V. SUMMARY

With an appropriate form (1) for the attractive roton-roton interaction we have solved the three-roton Schrödinger equation to find that three-roton bound states are formed in the *s*- and *d*-wave channels and numerically obtained the relation between the three-roton binding energies and the strength of the attractive interaction. We have found that for both *s*- and *d*-wave states the three-roton binding energies of around 1 K follow from assuming the large values of the strength of the attractive interaction, e.g., those obtained by BPZ.<sup>20</sup> On the other hand, if we can determine the binding energies from experiment such as Raman scattering, we can directly estimate the strength of the attractive interaction.

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