# Theory of excitations in <sup>3</sup>He-<sup>4</sup>He mixtures\*

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The elementary excitation spectrum of liquid  ${}^{3}\text{He}{}^{4}\text{He}$  mixture is calculated from first principles. The boson quasiparticles are treated by a density-variable formalism, and their interaction with the  ${}^{3}\text{He}$  excitations is explicitly derived. Using the liquid-structure factor for pure  ${}^{4}\text{He}$ , we calculate the  ${}^{3}\text{He}$  excitation dispersion over a wide momentum range; renormalization of the phonon-roton (boson) spectrum due to the presence of  ${}^{3}\text{He}$ ; lifetime of the roton excitations as a function of momentum and  ${}^{3}\text{He}$  concentration; and we estimate the possibility of resonances formed by rotons and  ${}^{3}\text{He}$  quasiparticles. The results are in contrast to previous speculations regarding the existence of a  ${}^{3}\text{He}$  roton excitation. However, our calculations provide good agreement with available experimental data. The sensitivity of the roton linewidth to the  ${}^{3}\text{He}$  quasiparticle interactions indicates that future light and neutron scattering experiments may provide insight into the microscopic nature of the interatomic helium potential.

### I. INTRODUCTION

The excitation spectrum of dilute <sup>3</sup>He-<sup>4</sup>He mixture poses an interesting challenge from the theoretical point of view. First of all, the original microscopic analysis of the Bose gas is limited to weakly interacting models whose validity is suspect at liquid-helium densities.<sup>1</sup> Thus various alternate approaches, relying in part on semiphenomenological application of physical insight, have been developed<sup>2</sup> to analyze excitations in these quantum liquids. Secondly, <sup>3</sup>He impurities in superfluid <sup>4</sup>He provide a system wherein fermion quasiparticles with variable density interact strongly with a Bose field, in analogy to the wellknown polaron problem in condensed matter.

On the basis of the low-temperature thermodynamic properties of <sup>3</sup>He-<sup>4</sup>He mixtures, Landau and Pomeranchuk<sup>3</sup> originally proposed an excitation spectrum of the form shown in Fig. 1: the Boson branch of pure <sup>4</sup>He exhibits phonon excitations E = ck at low momenta, rotons with energy  $E \simeq \Delta_4 + (k - k_0)^2/2\mu_4$  at intermediate momenta, and free-particle modes at large momenta. The proposed fermion branch at low momenta,  $\epsilon \simeq k^2/2m^*$ , has been extensively verified by various measurements which give ar estimated  $m^* \simeq 2.4m_1$ .<sup>4</sup>

Recently considerable attention has been focused on the excitation spectrum at intermediate momenta,

 $k \simeq 1$  Å<sup>-1</sup>, where strong interactions of the boson and <sup>3</sup>He quasiparticles may be expected as a result of their possible degeneracy in energy and momentum. A number of speculations have been advanced regarding the excitations in the above region: (i) Existence of



FIG. 1. Excitation spectrum  $\omega(q)$  vs momentum q. The dispersion of the region near the "roton minium" is described by  $\omega(q) \simeq \Delta_4 + (q - q_0)^2/2\mu_4$ , where  $\Delta_4 = 8.65$  °K,  $q_0 = 1.91$  Å<sup>-1</sup>, and  $\mu_4 = 0.16m_4$  ( $m_4$  is the mass of the <sup>4</sup>He atom). The lower-lying shaded curve shows the Landau-Pomeranchuk (LP) approximation to the <sup>3</sup>He spectrum.

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an energy minimum in the <sup>3</sup>He quasiparticle spectrum with a dispersion similar to the roton part of the boson branch.<sup>5</sup> (ii) Formation of a bound state of a <sup>3</sup>He quasiparticle with a roton.<sup>6</sup> (iii) Substantial shift of the roton energy  $\Delta_4$  with <sup>3</sup>He concentration.<sup>7</sup> (iv) Strong hybridization of the <sup>3</sup>He and boson branches.<sup>8</sup> (v) Modified Landau-Pomeranchuk model using an effective mass dispersion  $\epsilon = k^2/2m^*$  at intermediate momentum in addition to an essentially unchanged phonon-roton model for the Bose excitations.

Although a wealth of new experimental data on <sup>3</sup>He-<sup>4</sup>He mixtures has become available, the varied data reductions and subsequent interpretations yield conflicting evidence regarding the excitation spectrum. For a systematic analysis of the available experiments on specific heat, ion mobility, normal fluid density, neutron, and Raman scattering results we refer the reader to Ref. 9, where it is demonstrated that the modified Landau-Pomeranchuk model (v) yields quite good fits to the available raw data, in contrast to other models such as (i), (ii), and (iii) with parameters quoted in the literature. Nevertheless, very interesting details of the spectrum, for example the region where the <sup>3</sup>He quasiparticle branch intersects the phonon-roton spectrum, are now being probed by various experiments and pose a theoretical challenge.

The purpose of the present work is to develop a first-principles theory which may be applied to calculate the excitation spectrum of <sup>3</sup>He-<sup>4</sup>He mixtures and provide insight into the quasiparticle interactions in these quantum liquids. Our approach is based on a density fluctuation variable method originally discussed by Bogoliubov and Zubarev.<sup>10</sup> By analogy with recent theories of excitations in superfluid <sup>4</sup>He, we express the excitation spectrum and the quasiparticle interaction in terms of the liquid structure factor  $S_k$ , thus eliminating any adjustable parameters. To lowest order, this method reproduces the well-known Feynman-Cohen<sup>11</sup> result for the <sup>4</sup>He excitation energy  $\epsilon_k = k^2/2m_4S_k$ . In the boson case of pure <sup>4</sup>He, selfenergy corrections to the energy have been calculated using only  $S_k$  as input, and yield remarkable agreement with the measured energy values.<sup>12, 13</sup> The method also demonstrates the sensitivity of the roton-roton coupling to the details of the structure factor and in the latter case requires a self-consistent treatment.<sup>13</sup> The new formalism for mixtures is discussed in Sec. II.

First we calculate the renormalized <sup>3</sup>He quasiparticle energy considering the interactions with the phonons and rotons: We emphasize the relative sensitivity of the results to details of the liquid structure factor and compare these to the work of Davison and Feenberg<sup>14</sup> in Sec. III.

A novel result of the present theory is a calculation of the roton damping as a consequence of possible decay into a <sup>3</sup>He quasiparticle-hole pair in the degeneracy region. This feature, together with the associated roton energy shift, has a direct bearing on neutron scattering experiments and may elucidate details of the structure factor in this sensitive region of momentum as described in Sec. III.

In the case of pure <sup>4</sup>He, the existence of bound states of two rotons has been proposed<sup>15</sup> and verified by highly accurate light scattering measurements.<sup>16</sup> The binding is strongly favored by the vanishing group velocity of a roton which yields a singular behavior of the density of states and therefore a bound state of two rotons for arbitrarily weak attractive coupling.<sup>15</sup> Pitaevskii<sup>6</sup> has suggested that the scattering of a roton with a <sup>3</sup>He quasiparticle may also result in a bound state. We examine this question in Sec. IV with two goals in mind. First we calculate the criterion for the binding and thus obtain the required strength of the <sup>3</sup>He-roton coupling. Then we estimate the interaction strength from the microscopic theory and note its sensitivity to the structure factor and other variables.

Finally, in Sec. V we note the conclusions of our study and propose some directions for future research.

### **II. FORMALISM**

A system of  ${}^{3}$ He- ${}^{4}$ He atoms may be represented by the Hamiltonian

$$H = H_B + H_F + H_{int} , \qquad (2.1a)$$

$$H_B = \sum_{k} \frac{k^2}{2m_4} a_k^{\dagger} a_k + \sum_{kpq} V_{44}(q) a_{k+q}^{\dagger} a_{p-q}^{\dagger} a_p a_k \quad , \qquad (2.1b)$$

$$H_F = \sum_{p} \frac{p^2}{2m_3} C_p^{\dagger} C_p + \sum_{kpq} V_{33}(q) C_{k+q}^{\dagger} C_{p-q}^{\dagger} C_p C_k \quad , \quad (2.1c)$$

$$H_{\rm int} = \sum_{kpq} V_{34}(q) a_{k+q}^{\dagger} a_k C_{p-q}^{\dagger} C_p \quad , \tag{2.1d}$$

where  $a^{\dagger}(a)$  are Bose creation (destruction) operators for <sup>4</sup>He particles with mass  $m_4$  and  $C^{\dagger}(C)$  operators refer to the <sup>3</sup>He particles with mass  $m_3$  and obey fermion commutation relations (the spin indices have been suppressed for convenience). To a good approximation the interatomic potentials obey  $V_{33} \approx V_{44} \approx V_{34}$ , and these may be represented by a single pseudopotential  $V_q = V_{44}$  of pure liquid <sup>4</sup>He. Since the formalism will rely on the structure factor as input, the  $V_q$  represents an empirical pseudopotential in the liquid state.

For the dilute <sup>3</sup>He concentrations of interest, the <sup>3</sup>He atoms may be regarded as fermion particles interacting with the Bose excitations in a self-consistent manner. A rigorous solution for the excitations of a Bose gas at liquid-helium densities has not yet been successful; in part because of the strong quasiparticle interactions which are very sensitive to the interatomic pseudopotential. For example, calculations using the correlated basis function (CBF) technique by Davison and Feenberg<sup>14</sup> yield a substantial change of the <sup>3</sup>He quasiparticle effective mass  $m_3^*$ . In the limit of long wavelengths they find  $m_3^*$  values ranging from  $1.8m_3$ to  $2.2m_3$ , depending on their choice of interatomic helium potentials. In view of the experimental evidence<sup>4</sup> for  $m_3^* = 2.4m_3$ , the agreement is good, but the comparison cannot discern details of the potential.

We adopt the formalism using density fluctuation variables  $\rho_k$  which has been relatively successful in the study of pure <sup>4</sup>He.<sup>12,13</sup> The boson excitations are obtained by a Bogoliubov-Zubarev transformation<sup>10</sup>

$$\rho_{k} = \sum_{q} a_{k+q}^{\dagger} a_{q} = \lambda_{k}^{1/2} (b_{k} + b_{-k}^{\dagger}) \quad , \qquad (2.2)$$

which relates the density fluctuation operator  $\rho_k$  to the excitation creation (destruction) operators  $b_k^{\dagger}(b_k)$ , and is chosen to bring the original Boson Hamiltonian of Eq. (2.1b) into the form

$$H_B = \sum_{k} E_B(k) b_k^{\dagger} b_k + \cdots , \qquad (2.3)$$

where the residual phonon interaction terms have not been displayed. In Sec. III we shall examine the importance of these phonon and roton interaction terms insofar as they relate to the excitations in the mixtures. Thus to lowest order, the energy of the phonon-roton branch is

$$E_B(k) = \frac{k^2}{2m_4\lambda_k} = \frac{k}{2m_4} \left( k^2 + 4m_4 \frac{N_4}{\Omega} V_k \right)^{1/2} \quad (2.4)$$

This result follows from the theory of Bogoliubov and Zubarev<sup>10</sup> and enables us to replace the *unknown* pseudopotential  $V_k$  by a function involving  $\lambda_k$ , which approximates the liquid structure factor to lowest order. This replacement then recovers the Feynman-Cohen result  $E_B(k) \cong k^2/2m_4S_k$ . In the present work we use the relationship of Eq. (2.4) to generate an interaction Hamiltonian for the <sup>3</sup>He-<sup>4</sup>He mixtures.

As we are primarily concerned with the fermionboson field interactions we consider an effective <sup>3</sup>He Hamiltonian

$$H_F = \sum_p \epsilon_3(p) C_p^{\dagger} C_p \quad , \tag{2.5}$$

where  $\epsilon_3(p) \cong p^2/2m_3$ , at low concentrations.

Finally the effective interaction of the  ${}^{3}$ He quasiparticle and the boson field follows from Eqs. (2.1d) and (2.4) and becomes

$$H_{\rm int} = \sum_{kp} V_k \lambda_k^{1/2} (b_k + b_{-k}^{\dagger}) C_{p+k}^{\dagger} C_p \quad ; \tag{2.6}$$

it should be noted that the pseudopotential  $V_k$  can be expressed in terms of the structure factor  $\lambda_k$  using Eq. (2.4).

At the dilute <sup>3</sup>He concentrations under consideration, it is reasonable to neglect <sup>3</sup>He-<sup>3</sup>He scattering terms in the original Hamiltonian of Eq. (2).

Now the formalism enables us to calculate various features of the quasiparticle interactions over a wide range of momentum without the use of any adjustable parameters.

### **III. EXCITATION SPECTRUM**

The interaction of the fermion <sup>3</sup>He impurity with the boson field of <sup>4</sup>He excitations may be treated by perturbation theory in the low-momentum regime. On physical grounds we expect the respective <sup>3</sup>He and phonon branches to be repelled in this region of nondegenerate energies. The result is a strong renormalization of the <sup>3</sup>He effective mass<sup>4</sup> and a shift of the sound velocity<sup>17</sup> in the mixtures.

We consider the interactions over a wide range of momentum with particular attention on the roton region of  $k \sim 2$  Å<sup>-1</sup> where the <sup>3</sup>He branch may intersect the phonon-roton excitation spectrum. First we focus on the <sup>3</sup>He quasiparticles and then proceed to a study of the phonons.

# A. <sup>3</sup>He quasiparticles

The energy of a <sup>3</sup>He impurity coupled to the phonon excitations in the mixtures may be obtained from the interaction Hamiltonian Eq. (2.6) by applying the standard rules of perturbation theory. The first corrections to the <sup>3</sup>He energy are shown in Fig. 2(a), which yield a renormalized energy

$$\epsilon_3^*(p) = \epsilon_3(p) + \sum_q \frac{\lambda_q V_q^2}{\epsilon_3(p) - \epsilon_3(p-q) - E_B(q)} \quad , \quad (3.1)$$

where  $\epsilon_3(p) = p^2/2m_3$  denotes the renormalized <sup>3</sup>He particle energy and  $E_B(q)$  is the phonon-roton energy curve. An alternate possibility in the spirit of Brillouin-Wigner perturbation theory would involve using renormalized <sup>3</sup>He energies  $\epsilon_3^*$  in the energy denominator of Eq. (3.1), and solving the resulting integral equation. We shall examine this self-consistent approach as well. Our method bears formal similarities to the work of Miller, Pines, and Nozieres,<sup>18</sup> although it relies on the liquid structure factor as sole input.

The angular integration in Eq. (3.1) is trivial and yields a one-dimensional integral over momentum which must be done numerically, since the structure factor  $\lambda_k$  is obtained from experiment.<sup>19</sup> To facilitate the computation we introduce a functional form of  $V_k$ which yields a good fit to the structure factor using Eq. (2.3) as shown in Fig. 3: Surprisingly this fit can be achieved by a simple square well "potential" of height U and range a in real space which gives

$$V_k = 4\pi a^3 U(ka)^{-2} [\sin(ka)/ka - \cos(ka)] \quad (3.2)$$

Although this soft-core model gives a good description of the structure factor  $S_k$  it does not necessarily





FIG. 2. (a) Self-energy diagram for a <sup>3</sup>He quasiparticle moving in the <sup>4</sup>He background. The solid lines represent the <sup>3</sup>He mode with energy  $\epsilon_3$  and wave vector *q*. The dashed line represents the interacting <sup>4</sup>He mode with energy  $E_B$  and wave vector *k*. The  $\gamma$  represents the interaction vertex which is  $\lambda_k V_k^2$ . (b) Polarization diagram corresponding to a renormalization of the <sup>4</sup>He excitation spectrum. The symbols have the same meaning as in (a).

represent the true interatomic helium pseudopotential in the liquid!

In the case of the self-energy correction of Eq. (3.1) the deviations of  $V_k$  from a more realistic potential cannot be resolved from other corrections such as higher-order contributions to the structure factor and the Boson energies. However, we note that the <sup>3</sup>He energy of Eq. (3.1) involves an integration over k which renders the energy relatively insensitive to the details of  $V_k$ . On the other hand, our analysis of the phonon branch in Sec. III B will emphasize the structure of  $V_k$  and will develop its relation to neutron scattering data.



FIG. 3. Experimentally determined structure factor is shown by the solid curve S(k) (Ref. 15); the dashed curve is  $\lambda(k)$  obtained from Eqs. (2.3) and (3.2) with a soft-core model of height V = 40 °K and range a = 2.6 Å.

The results of numerical calculations using Eq. (3.1)and the representation of the structure factor by Eq. (3.2) are shown in Fig. 4. There is an overall shift of the <sup>3</sup>He quasiparticle branch to lower energies as a result of level repulsion from the phonons. In the long-wavelength limit the computed results may be approximated by  $\epsilon_3(p) \cong p^2/2m_3^*$  with  $m_3^* \cong 2.2m_3$ . By comparison the experimental mass value is  $m_3^* = 2.4 m_3$ .<sup>4</sup> Of course, the calculated mass can be brought into even closer alignment with experiment by minor adjustments of  $V_k$ ; however, this would not be in the spirit of our self-consistent method. Thus the small difference between our result and the experimental value is attributed to corrections to the  $\lambda_k \cong S_k$  approximation; higher-order corrections have been attempted, but they require more accurate data for the liquid structure factor than are presently available.13

Previous theoretical calculations of the <sup>3</sup>He effective mass in the mixtures have given  $m_3$ \* values ranging from  $1.8m_3$  to  $2.2m_3$  using the CBF formalism with various interatomic potentials.<sup>14</sup> Thus a 20% deviation from the experimental value is to be expected as a result of uncertainties in the potential used in the CBF techniques<sup>14</sup> and a similar limit may be inferred from the limited data on the liquid structure factor used in our theory.

The level crossing of the <sup>3</sup>He branch in the roton region  $p \approx 1.8$  Å<sup>-1</sup> yields a relatively weak energy splitting as shown in Fig. 4. Here the effects of



FIG. 4. Renormalized <sup>3</sup>He quasiparticle spectrum found by calculating the self-energy from Eq. (3.1). The dashed curves correspond to the boundaries of the unrenormalized <sup>3</sup>He spectrum,  $\omega(a) = q^2/2m_3 \pm qk_F/m_3$ , at 0.01 mol% solution of <sup>3</sup>He in <sup>4</sup>He. This corresponds to a Fermi wave number of 0.07 Å<sup>-1</sup> and a Fermi energy of 0.02 %. The renormalized spectrum is shown by the shaded continuum. The curve in the low-momentum region exhibits  $m^* \simeq 2.2m_3$ . The calculations used the  $\lambda(k)$  of Fig. 3 which is a reasonable fit to the liquid structure factor.

short-range order dominate and the splitting is sensitive to the details near the peak in the structure factor in the roton region. From the interaction Hamiltonian Eq. (2.6) and the relations of Eq. (3.1) and (2.4) it is possible to show that the product  $V_k \lambda_k^{1/2}$  changes sign near the roton minimum, thus yielding a small branch splitting in the case of the experimental structure factor results. Previously<sup>8</sup> it was demonstrated that neglect of the k dependence in the quasiparticle interaction gives a severe bending of the <sup>3</sup>He branch to lower energies. Preliminary neutron scattering data<sup>20</sup> on <sup>3</sup>He-<sup>4</sup>He mixtures are consistent with the calculated spectrum shown in Fig. 4: We make a detailed comparison with the data in Sec. III B, where the roton linewidth as well as energy is considered as a function of <sup>3</sup>He concentration.

Additional tests of the theory were performed with the Brillouin-Wigner scheme of using renormalized modes  $E_B(k)$  and  $\epsilon_3^*(k)$  in the integration over k; the resulting spectrum was shifted to lower energies by approximately 15% with these variations which indicates the quantitative limitations of the calculations. It is interesting to note that these corrections tend to increase the effective mass  $m_3^*$ . Also this would suggest that higher-order diagrams may be neglected. The vertex corrections turn out to be of order  $P_F/k_0$  and may be neglected at low <sup>3</sup>He concentrations.<sup>9</sup>

#### **B.** Boson excitations

As a consequence of the level crossing shown in Fig. 4 the phonon-roton spectrum is expected to exhibit various interesting properties, such as Landau damping in the degeneracy region. The appropriate interaction process is the Boson decay into a <sup>3</sup>He particle-hole pair as seen in Fig. 2(b). The corresponding phonon self-energy<sup>21</sup>  $\pi(q, \omega)$  yields an energy shift due to the real part which is calculated using an averaged effective mass  $\mu$  which yields a good description of the <sup>3</sup>He branch near the crossing region. Thus

$$\operatorname{Re}\Pi(q,\omega) = \frac{\mu k_F}{2\pi^2} \left\{ -1 + \frac{1}{2x} \left[ \left( \frac{Z+x^2}{2x} \right)^2 - 1 \right] \ln \left| \frac{Z-2x+x^2}{Z+2x+x^2} \right| + \frac{1}{2x} \left[ \left( \frac{Z-x^2}{2x} \right)^2 - 1 \right] \ln \left| \frac{Z-2x-x^2}{Z+2x-x^2} \right| \right\}, \quad (3.3)$$

where  $Z = \omega/\epsilon_F$  and  $x = q/p_F$  are dimensionless energy and momentum parameters normalized to Fermi energy  $\epsilon_F$  and momentum  $p_F$ , respectively.

A new decay channel for the Bosons occurs in the degeneracy region and is described by the imaginary part of the self energy

$$\operatorname{Im}\Pi(q,\omega) = \frac{\mu p_F Z}{4\pi x} \quad \text{for} \quad 0 \le Z \le 2x - x^2 \quad (3.4a)$$

$$=\frac{p_F\mu}{2\pi x}\left[1-\left(\frac{Z-x^2}{2x}\right)^2\right]$$
(3.4b)

=0 for 
$$Z \ge 2x + x^2$$
. (3.4c)

The renormalized phonon energy follows from Fig. 2(b) and Eqs. (2.6) and (3.3),

$$E_B^*(k) = E_B(k) + \lambda_k V_k^2 \operatorname{Re}\Pi(k, E_B) \quad . \tag{3.5}$$

The calculated spectrum is shown in Fig. 4 again using the liquid structure factor. In the present case however the results are extremely sensitive to the details of  $\lambda_k V_k^2$  in the intermediate region  $k \approx 1.9$  Å<sup>-1</sup>. In fact the apparent small shift of the roton region is related to the minimum in  $V_k^2$  at  $k \approx 2.0$  Å<sup>-1</sup>. Similar results are obtained at higher <sup>3</sup>He concentrations as expected, and support the conclusions of Bagchi and Ruvalds<sup>22</sup> regarding the weak concentration dependence of the roton energy. The sensitivity of the roton energy to the model potential is shown in Fig. 5 along with preliminary neutron data.<sup>20</sup> Considering that the roton energy is  $\Delta = 8.65$  °K the shift of 0.5% is indeed small, in contrast to previous speculation.<sup>7</sup> Despite



FIG. 5. <sup>4</sup>He spectrum shift (°K) vs wave number q (Å<sup>-1</sup>) at x = 5%. The date points are those of Ref. 18. The solid line corresponds to the shift calculated using the  $\lambda_k$  of Fig. 3. The dashed line corresponds to the shift calculated using the experimentally determined values of  $E_B(k)$  (Fig. 1), and using S(k) in place of  $\lambda(k)$ . Note the data and both the curves are zero near  $q \approx 1.7$  Å<sup>-1</sup>, which is where the renormalized <sup>3</sup>He continuum crosses the <sup>4</sup>He spectrum (see Fig. 4). The data of Rowe *et al.* were taken at 1.5 °K, and reflect some effects of thermal broadening, whereas the calculations were made at T = 0.

the scatter in the data points shown in Fig. 5, it appears that the possibility of a <sup>3</sup>He "rotonlike" dip<sup>5</sup> in the quasiparticle spectrum is ruled out by the neutron scattering experiments. Furthermore, our analysis suggests that an anomalous dip of the <sup>3</sup>He branch to very low energies ( $E \sim 5^{\circ}$  K as proposed in Ref. 5) cannot be achieved, using a realistic form for the liquid structure factor.

Landau damping of the phonon-roton spectrum is also highly sensitive to the helium structure factor and may provide insight into the helium pseudopotential. The calculated roton linewidth is plotted as a function of momentum in Fig. 6; it is in rough (order of magnitude) correspondence to the neutron data. Clearly more-refined data are required to draw explicit conclusions regarding the helium pseudopotential. However future experiments promise to elucidate the structure shown in Fig. 6 and thereby lead to a detailed theoretical study of the quasiparticle interactions in the roton region. It should be noted that the relevant phonon self-energy of Eqs. (3.4) does not involve an integration over momentum and thus displays specifically the momentum dependence of the phonon-<sup>3</sup>He vertex which can be extracted from the measured lifetime.

Finally we remark on the concentration dependence of the roton lifetime  $\Gamma(k = k_0)$ . Our theory suggests a sudden increase of  $\Gamma(k = k_0)$  at a critical <sup>3</sup>He concentration x = 3% due to the onset of Landau damping as the <sup>3</sup>He particle-hole continuum envelops the roton branch. This process provides a simple physical explanation of the nonlinear concentration dependence observed in the Raman data,<sup>23</sup> even though the effect is masked somewhat by thermal broadening.

# IV. <sup>3</sup>He-ROTON SCATTERING

Following the suggestion of Pitaevskii,<sup>6</sup> we investigate the possibility of forming a bound state of a roton and a <sup>3</sup>He quasiparticle. We calculate first the required coupling strength to form a bound state, and then estimate its expected value from the above theory. For convenience in estimating the binding criterion we introduce a model interaction Hamiltonian describing the coupling of a roton to a <sup>3</sup>He quasiparticle

$$H = \gamma_4 \sum_{kpq} b_k^{\dagger} a_k C_{p-q}^{\dagger} C_p \quad , \tag{4.1}$$

where the coupling  $\gamma_4$  is taken as momentum independent to simplify the formalism. This approximation enables us to express the scattering of a <sup>3</sup>He



FIG. 6. Roton linewidth  $\Gamma$  (°K) vs wave number q (Å<sup>-1</sup>) for x = 5%. The neutron data are from Ref. 18. The solid line corresponds to the calculation made utilizing the model  $\lambda_k$  of Fig. 3. The dashed line corresponds to the calculation made using the experimentally determined values of  $E_B(k)$ , and S(k) in lieu of  $\lambda(k)$ . Again the data reflect the effects of thermal broadening, and experimental uncertainty.

quasiparticle with a roton by a geometric series which gives<sup>15</sup>

$$F(k, \omega) = F^{(0)}(k, \omega) / [1 - \gamma_4 F^{(0)}(k, \omega)] \quad , \qquad (4.2a)$$

where  $F^{(0)}(k, \omega)$  is the propagator for the roton-<sup>3</sup>He pair:

$$F^{(0)}(k,\omega) = \frac{1}{(2\pi)^3} \int \frac{d^3k'}{\omega - E_{k'} - \epsilon_{k-k'}} \quad (4.2b)$$

Formation of a bound state is manifested by a pole in the propagator for the interacting system  $F(k, \omega)$ which yields the binding criterion

$$1 - \gamma_4 F^{(0)}(k, \omega) = 0 \quad . \tag{4.3}$$

It is natural to focus on the roton region of the Boson spectrum since these excitations have vanishing group velocity and therefore high density of final scattering states. This is the physical reason why a bound pair of rotons is split off below the continuum energy  $2\Delta_4$  by arbitrarily weak attractive coupling.<sup>15</sup> In the case of <sup>3</sup>He-<sup>4</sup>He mixtures we have the roton energy  $E_k = \Delta_4 + (k - k_0)^2/2\mu_4$  and the <sup>3</sup>He branch  $\epsilon_{K-k} = (K - k)^2/2m_3^*$ . As a consequence of the <sup>3</sup>He quasiparticle dispersion the binding criterion of Eq. (4.3) will require a finite critical value of the coupling  $\gamma_4^0$  which we now obtain in the case of zero total momentum. Thus we consider the vicinity of the continuum threshold energy for the pair  $\omega_T = \Delta_4 + k_0^2/2m_3^*$ , for which

$$F(K=0,\omega_T) \cong \frac{m^* k_0}{2\pi^2} \left[ -\frac{4k_D}{k_0} \left[ 1 - \frac{\mu}{m^*} \right]^{-1} + \left( \frac{1 + \mu/m^*}{1 - \mu/m^*} \right)^2 \ln \left| \frac{2\mu/m^* + (\mu/m^* - 1)k_D/k_0}{2\mu/m^* - (\mu/m^* - 1)k_D/k_0} \right| \right],$$
(4.4)

where  $k_D$  is a cut-off momentum for the roton. Typical values are  $k_D/k_0 = 0.2$  and  $\mu/m^* = 0.1$ ; the corresponding value of the critical coupling strength is

$$\gamma_4^c \cong -4/m^* k_0 \quad , \tag{4.5}$$

which is roughly  $\gamma_4^c = -0.2 \times 10^{-38} \text{ erg cm}^3$ . By comparison estimates of  $\gamma_4 \cong 2.4 \times 10^{-38} \text{ erg cm}^3$  have been obtained from cross-section calculations<sup>22</sup> which would at first glance strongly favor a strongly bound state. However, such a comparison is highly misleading since the scattering cross section which enters into collision broadening includes contributions over several angular momentum channels whereas bound states would be found in specific channels. A similar situation exists in pure <sup>4</sup>He, where the estimates of the roton lifetime give a coupling more than an order of magnitude larger than the coupling in the l = 2 state which is observed experimentally.<sup>16</sup>

A crude theoretical estimate of this coupling can be obtained from the microscopic theory, using the interaction of Eq. (2.6), to generate the lowest-order scattering process of a roton with a <sup>3</sup>He excitation (via the exchange of a <sup>3</sup>He excitation). Thus we obtain an effective interaction

$$\gamma_4 \simeq \lambda_{k_0} V_{k_0}^2 / [\Omega - \epsilon_3(q)] \quad , \tag{4.6}$$

which may yield an attractive component, of the order  $\gamma_4 \sim -\lambda_{k_0} V_{k_0}^2 / \langle \epsilon_3(q) \rangle$ . This quantity is related to the level splitting in the roton region of Fig. 4 which gives  $\lambda_{k_0} V_{k_0}^2 / [\Delta - \epsilon_3(k_0)] = 3 \,^{\circ}$ K, corresponding to  $\gamma_4 \simeq -2 \times 10^{-38}$  erg cm<sup>3</sup>. Within our formalism another important process is the phonon mediated roton-<sup>3</sup>He scattering: this gives roughly  $\gamma_4 \simeq -g_{\rho}g_3/sq$ , where s is the sound velocity,  $g_{\rho} = V_q \lambda_q^{1/2}$  from Eq. (2.6), and the three-phonon vertex  $g_3$  can be estimated from previous work.<sup>12,13</sup> Using the experimental values for the second velocity, we estimate  $\gamma_4 \simeq -2.8 \times 10^{-38}$  erg cm<sup>3</sup>, which is *attractive* and the same order as the above "Compton" scattering contribution.

In the case of <sup>3</sup>He-<sup>3</sup>He quasiparticle scattering in <sup>3</sup>He-<sup>4</sup>He mixtures, <sup>24</sup> the attractive component of the coupling due to phonon exchange is effectively cancelled by a competing excluded volume mechanism. Here we shall estimate the excluded volume contribution to <sup>3</sup>He-roton scattering following the phenomenological approach of McMillan.<sup>25</sup> The results are similar in form to Eq. (2.6) with the replacement  $V_k \lambda_k^{1/2} \rightarrow g_\rho + g_\nu$ , where

$$g_{\rho} = \alpha m_4 s^2 (S_q/N)^{1/2} (1 - S_q)$$
(4.7)

and

$$g_{\nu} = (\vec{\mathbf{k}} \cdot \vec{\mathbf{q}}) (1 - S_q) / 2m_3 (NS_q)^{1/2}$$
 (4.8)

The excluded volume constant<sup>25</sup>  $\alpha \cong 0.28$  is obtained from experiment. With this modification, the estimate of the <sup>3</sup>He-roton coupling is reduced to  $\gamma_4 \cong -1.5 \times 10^{-38}$  erg cm<sup>3</sup>; addition of the altered phonon exchange term gives a total value  $\gamma_4 \cong -2 \times 10^{-38}$  erg cm<sup>3</sup>.

It is interesting to note that all of the above processes yield an attractive coupling, even though reduced by the excluded volume, which is an order-ofmagnitude stronger than the critical value required to form a bound state. This situation is reminiscent of the microscopic theory of roton interactions<sup>13,26</sup> in pure <sup>4</sup>He whose *bare* (or lowest-order) strength was found to be similar to the above estimates, but renormalization of the coupling by higher-order scattering processes reduces the coupling by more than an order of magnitude.<sup>13</sup> It is reasonable to anticipate that higher-order terms may dominate the <sup>3</sup>He-roton coupling, as well, although an explicit calculation of these terms is beyond the scope of the present work.

## **V. CONCLUSIONS**

The calculated <sup>3</sup>He quasiparticle spectrum resembles closely the original Landau-Pomeranchuk model and intersects the boson branch near the roton minimum. This general behavior is relatively insensitive to details of the structure factor, and it accounts for several anomalous features observed in neutron and light scattering experiments. For example, with increasing <sup>3</sup>He concentrations the fermion <sup>3</sup>He quasiparticle continuum should broaden and envelop the roton minimum at concentrations exceeding 3%. The new channel for decay of rotons into <sup>3</sup>He-quasiparticle-hole pairs should yield an extra broadening with a nonlinear concentration dependence as observed in the Raman data.<sup>23</sup>

On the basis of our results it is difficult to understand how a <sup>3</sup>He "rotonlike" excitation may occur. In the Bose liquid the acoustic phonons at low momenta should evolve to free-particle-like modes at large momenta, which naturally yields an intermediate roton region. On the other hand the Fermion <sup>3</sup>He quasiparticles obey the well-known limiting dispersion at low p,  $\epsilon_3 = p^2/2m^*$ , and presumably tend to the free-particle mode at high momenta: Since  $m^* \simeq 2m_3$ , the formation of a <sup>3</sup>He roton minimum at intermediate momenta would require an extraordinary level repulsion from the Boson branch, which is not at all evident in our theory.

Our analysis may be extended to further calculations of quasiparticle interactions providing that the details of the liquid structure may be deduced to greater accuracy, especially in the roton region. Future measurements of the roton energy and damping provide an ideal means for this purpose as shown in Sec. III.

It would be particularly interesting to extend the present analysis to calculate the scattering amplitude of two <sup>3</sup>He quasiparticles, with a view toward possible pairing and formation of an associated superfluid phase in the mixtures.

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FIG. 4. Renormalized <sup>3</sup>He quasiparticle spectrum found by calculating the self-energy from Eq. (3.1). The dashed curves correspond to the boundaries of the unrenormalized <sup>3</sup>He spectrum,  $\omega(a) = q^2/2m_3 \pm qk_F/m_3$ , at 0.01 mol% solution of <sup>3</sup>He in <sup>4</sup>He. This corresponds to a Fermi wave number of 0.07 Å<sup>-1</sup> and a Fermi energy of 0.02 %. The renormalized spectrum is shown by the shaded continuum. The curve in the low-momentum region exhibits  $m^* \simeq 2.2m_3$ . The calculations used the  $\lambda(k)$  of Fig. 3 which is a reasonable fit to the liquid structure factor.