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Excitation spectrum of a ^{3}He atom moving in He II at zero temperature

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The recoil spectrum $S(q,\omega)$ for a single ^{3}He moving in He II at zero temperature is calculated within a mode-coupling approximation. The effective mass of the ^{3}He particle is found to be $m^* = 2.35 m_3$. The dispersion curve for elementary excitations is shown to deviate considerably from a parabolic one yielding a higher density of states for energies near the He II roton gap. The undamped quasiparticle excitations cease to exist for a momentum about 2 Å^{-1}; their excitation strength drops to zero. The dispersion curve continues above 2 Å^{-1} as a resonance in the multiple-excitation background.

I. INTRODUCTION

In this paper the recoil function $S(q, \omega)$ measuring the probability for momentum transfer q and energy transfer ω to a single ^{3}He atom moving in He II at zero temperature will be studied. This function can, in principle, be determined by inelastic neutron scattering from dilute mixtures of ^{3}He in He II: For very small concentration x the contribution to the total scattering cross section of the mixture stemming from the ^{3}He impurity-density fluctuations is $xS(q, \omega)$. So far neutron-scattering data are available for concentrations down to 6% (Ref. 1) and at a higher temperature for a 5% dilution.[2]

For momenta smaller than some critical value q_c, $S(q, \omega)$ is expected to exhibit infinitely sharp resonances at $\omega = \epsilon_i(q)$. For frequencies $\omega > \epsilon_i(q)$ or momenta $q > q_c$ the ^{3}He motion can dissipate energy to the He II system by emitting elementary He II excitations thus causing damping. The infinitely sharp resonances at $\omega = \epsilon_i(q)$ represent undamped ^{3}He quasiparticle excitations, the basic object of investigation of the kinetic theory of dilute He II–^{3}He mixtures.[3] The quasiparticle excitations can be viewed[4] as the motion of a ^{3}He impurity surrounded by a streaming pattern of He II coupled together by the effective ^{3}He–He II interactions. Note that this "particle" is, at zero temperature, of infinite lifetime since it cannot transfer energy or momentum to the superfluid bath in which it is moving.

For small momenta the quasiparticle dispersion is of the form $\epsilon_i(q) = q^2/2m^*$ proposed by Landau and Pomeranchuk[5] with the impurity's bare mass replaced by an enlarged effective mass m^* reflecting the He II backflow. This effective mass has been calculated by Davison and Feenberg and Woo *et al.*[6] There is one direct experimental indication[1] on a deviation of $\epsilon_i(q)$ from quadratic behavior at larger wave numbers and a wealth of different interpretations[7-13] of the results of experiments[14-19] connected only indirectly with $\epsilon_i(q)$. Whereas, it is obvious that the quasiparticle-hole continuum found in neutron-scattering experiments on 6% mixtures[1] lies, for wave numbers around the He II roton momentum, below the Landau-Pomeranchuk parabola only indirect conclusions on $\epsilon_i(q)$ can be drawn from the other measurements.[15-18] Nevertheless, most authors, with the exception of Ruvalds *et al.*,[13] agree on the necessity of interpreting the measurements of the velocity of fourth sound,[15] the ion mobility,[16] the normal-fluid density,[17] and the information gained from heat-pulse techniques[18] in terms of a deviation from a parabolic dispersion producing a higher density of states at larger wave numbers. However, there are at least two hypotheses on the specific form of the dispersion. Stephen and Mittag[8] and Varma[9] as well as Sobolev and Esel'son[10] discuss a rotonlike minimum in the ^{3}He dispersion following a suggestion of Pitaevskij.[7] Esel'son *et al.*,[11] recently deduced from data on the normal fluid density another version of $\epsilon_i(q)$ with a higher density of states at large momenta due to a flat part with an endpoint near the He II roton minimum. The particle-hole excitation spectrum obtained by Ruvalds *et al.*,[13] within a generalized Bogoliubov-Zubariev theory for ^{3}He-^{4}He mixtures does not display, however, such deviations from the Landau-Pomeranchuk form.

The present work aims at a determination of $\epsilon_i(q)$ within a microscopic approach, which is a modification of the mode-coupling theory applied earlier to an evaluation of the liquid He II excitation spectrum.[20] The recoil function $S(q, \omega)$ is written as the absorptive part of the dynamical-impurity-density fluctuation susceptibility $\chi_i(q, z)$. This function is expressed in terms of a frequency $\Omega_0(q)$ given by the restoring force towards static density changes and by a polarization kernel $M(q, z)$.

The imaginary part of the latter describes decay of ^{3}He motion by generation of He II excitations and the real part, representing virtual-mode excitations, describes the backflow.

II. THEORY

A. ^{3}He response function

Let $\rho_i(\vec{q}) = \exp(i\vec{q}\cdot\vec{r}_i)$ denote the ^{3}He impurity-density fluctuation operator. The information on propagation of such impurity-density fluctuations is contained in the dynamical-density response function

$$\chi_i(q,z) = i\int_0^\infty dt\, e^{izt}\langle[\rho_i^\dagger(\vec{q},t),\rho_i(\vec{q})]\rangle\,. \tag{2.1}$$

Equation (21) can be represented[21] in terms of a characteristic frequency $\Omega_0(q)$ and a relaxation kernel $M(q,z)$,

$$\chi_i(q,z) = \frac{-q^2/m_i}{z^2-\Omega_0^2(q)+zM(q,z)}\,. \tag{2.2}$$

Here $\Omega_0^2(q) = q^2/m_i\,\chi_i(q,z=0)$ is obviously connected with the static impurity response towards density fluctuations. Both functions $\chi_i(q,z)$ and $M(q,z)$ have the usual analytic properties[21] leading to the representation of the absorptive part $\chi_i''(q,\omega)$ of the susceptibility [Eq. (2.2)]

$$\chi_i''(q,\omega) = \frac{q^2}{m_i}\,\frac{\omega M''(q,\omega)}{[\omega^2-\Omega_0^2(q)+\omega M'(q,\omega)]^2+[\omega M''(q,\omega)]^2} \tag{2.3}$$

in terms of the real part $M'(q,\omega)$ and the absorptive part $M''(q,\omega)$ of the relaxation kernel

$$M(q,\omega\pm i0) = M'(q,\omega)\pm iM''(q,\omega)\,.$$

A Kramers-Kronig relation

$$M'(q,\omega) = \frac{2\omega}{\pi}\,\mathrm{P}\int_0^\infty d\epsilon\,\frac{M''(q,\epsilon)}{\epsilon^2-\omega^2} \tag{2.4}$$

connects M' and the imaginary part M''. Note that $M''(q,\omega)$ is an even, positive function.

Because of the analytic properties mentioned the compressibility sum rule of the spectral function $\chi_i''(q,\omega)$ [Eq. (2.3)] reads

$$\int_0^\infty \frac{d\omega}{\pi}\,\frac{\chi_i''(q,\omega)}{\omega} = \frac{q^2/2m_i}{\Omega_0^2(q)} \tag{2.5}$$

and the f sum rule follows to be

$$\int_0^\infty \frac{d\omega}{\pi}\,\omega\chi_i''(q,\omega) = \frac{q^2}{2m_i}\,. \tag{2.6}$$

Relations (2.5) and (2.6) are not affected by the choice of a special approximation to $M(q,z)$. Another integral restriction on the form of the density fluctuation spectrum $\chi_i''(q,\omega)$ follows from the fluctuation-dissipation theorem.[22] At zero temperature the relation between the response function and van Hove's function $S(q,\omega)$[23] is

$$\chi_i''(q,\omega)\,\Theta(\omega) = \tfrac{1}{2}S(q,\omega)\,. \tag{2.7}$$

Integration of Eq. (2.7) over all frequencies yields

$$\int_0^\infty \frac{d\omega}{\pi}\,\chi_i''(q,\omega) = 1\,, \tag{2.8}$$

since in the one impurity problem $\langle\rho_i^\dagger(\vec{q})\rho_i(\vec{q})\rangle = 1$. For a given approximation to the kernel $M(q,z)$ Eq. (2.8) will be used to determine $\Omega_0(q)$ and with it the static susceptibility $\chi_i(q,z=0)$.

We consider the relaxation kernel $M(q,z)$ to be the basic quantity of the present theory which aims at its approximation. The polarization kernel $M(q,z)$ describes, in analogy, to the case of the photon self-energy in quantum electrodynamics, the effect of the impurity–He II interaction: For $M(q,z)\equiv 0$ one recovers the free-impurity response function with the free-particle dispersion $\Omega_0^0(q) = q^2/2m_i$ obtained from Eq. (2.8). The relaxation spectrum $M''(q,\omega)$ describes dissipation of impurity density fluctuations into other degrees of freedom. This decay of the coherent impurity motion is due to interaction with the He II. The real part $M'(q,\omega)$ of the relaxation kernel represents virtual excitations of modes which can be viewed as backflow. They renormalize the ^{3}He excitation energies.

B. Undamped quasiparticle excitations

As will be shown later, $M(q,z)$ is such that the density response $\chi_i(q,z)$ [Eq. (2.2)] has poles on the real axis at frequencies $\epsilon_i(q)$ which simultaneously solve

$$\omega^2-\Omega_0^2(q)+\omega M'(q,\omega) = 0\,, \tag{2.9a}$$

$$M''(q,\omega) = 0\,. \tag{2.9b}$$

The dispersion $\epsilon_i(q)$ of these undamped quasiparticle excitations differs from the free-dispersion since $M'(q,\omega)$ is nonzero except for some isolated points. That, in turn, is a consequence of the existence of real decay channels, $M''(q,\omega)>0$, over extended frequency ranges. From Eq. (2.2) one easily determines the residuum of the poles in Eq. (2.9), i.e., the excitation strength $f(q)$ of the quasiparticles

$$f(q) = \frac{q^2/m_i}{\epsilon_i(q)}\left|1+\frac{\Omega_0^2(q)}{\omega^2}+\frac{\partial M'(q,\omega)}{\partial\omega}\right|^{-1}_{\omega=\epsilon_i(q)}\,. \tag{2.10}$$

Note that the partial frequency derivative of

$M'(q,\omega)$ enters into the denominator of Eq. (2.10). Whereas, for the free-impurity motion with energy $\epsilon_i^0(q)=\Omega_0^0(q)=q^2/2m_i$ the excitation strength is unity, here the quasiparticle excitations exhaust only a portion $f(q)<1$ of the total spectral weight of $\chi_i''(q,\omega)$. So one can write

$$\chi_i''(q,\omega)=\pi f(q)\,\delta(\omega-\epsilon_i(q))+\chi_i''(q,\omega)\big|_{\text{continuum}}\,. \quad (2.11)$$

Sufficient conditions for the appearance of resonances in the spectrum $\chi_i''(q,\omega)$ at frequencies $\Omega_R(q)$ are (a) the left side of Eq. (2.9a) vanishes, (b) $M''(q,\Omega_R(q))\ll\Omega_R(q)$ and, (c) $\partial M'(q,\omega)/\partial\omega>0$ at $\omega=\Omega_R(q)$.[20] Conditions (b) and (c) are somewhat interrelated via the Kramers-Kronig relation.

C. Mode-coupling approximation for $M(q,z)$

The quantity to be approximated is the spectral function $M''(q,\omega)$. It has the physical meaning of a generalized friction and describes processes whereby a ^{3}He excitation with energy ω and wave number q can lose energy and momentum to the He II bath. It is reasonable to take into account as dominant contributions processes in which a ^{3}He mode transfers energy and momentum in a decay to an uncorrelated two-mode excitation consisting of a He II density fluctuation and a recoiling ^{3}He wave. The decay probability will then be calculated within a lowest-order correlation approximation. These ideas have been worked out earlier[20] [the formulas of the present theory are obtained essentially by replacing in products $\rho(\vec{k}_1)\rho(\vec{k}_2)$ of He II density fluctuation operators appearing in Secs. II A and II D of Ref. 20, one operator by a ^{3}He density fluctuation operator. Here the two decay channels contain a He II and a ^{3}He excitation, respectively].

Within the general Mori-Zwanzig theory[24] one finds[25] $M(q,z)$ to be determined by the correlation function of the fluctuating force $\tau_i(\vec{q})=-\ddot{\rho}_i(\vec{q})-\Omega_0^2(q)\rho_i(\vec{q})$. Taking into account only the overlap of $\tau_i(\vec{q})$ with the pair mode excitations $\rho(\vec{p})\rho_i(\vec{q}-\vec{p})$, where $\rho(\vec{p})$ denote the He II density fluctuations, one gets[25] upon factorizing time-dependent correlations

$$M''(q,\omega)=\frac{m_i}{q^2\omega}\int\frac{d\vec{p}}{n(2\pi)^3}\int\frac{d\epsilon}{\pi}\varphi(\vec{q},\vec{p})^2\,\tfrac{1}{2}\left[\operatorname{sgn}(\epsilon)+\operatorname{sgn}(\omega-\epsilon)\right]\chi''(p,\epsilon)\,\chi_i''(|\vec{q}-\vec{p}|,\omega-\epsilon)\,. \quad (2.12)$$

Here $\chi''(p,\epsilon)$ is the density fluctuation spectrum and n the particle density of He II. The function $\varphi(\vec{q},\vec{p})$ has the physical meaning of a decay vertex. It is given by mode-normalization denominators[26] and by static correlations of $\tau_i(\vec{q})$ with the pair-mode operators $\rho(\vec{p})\rho_i(\vec{q}-\vec{p})$. The latter correlation function can be estimated using a pole ansatz for its spectrum and determining the pole strength with sum rules. In this way one can express φ in terms of the He II structure factor $S(q)$ and the ^{3}He–He II structure factor $S_{34}(q)$,[25]

$$\varphi(\vec{q},\vec{p})=-\frac{\vec{q}\cdot\vec{p}}{2m_i}\left[\epsilon_i^0(q)+\epsilon_i^0(\vec{q}-\vec{p})+\epsilon_F(p)\right]\frac{S_{34}(p)}{S(p)}\,. \quad (2.13)$$

Here $\epsilon_F(q)=q^2/2mS(q)$ is the Feynman-Bijl dispersion of He II. Equation (2.12) describes the decay rate of the coherent impurity motion due to emission of He II density fluctuations with momentum $\vec{p}$ and energy ϵ. From Eq. (2.12) one immediately deduces the impossibility of an undamped ^{3}He quasiparticle excitation with momentum q and an energy $\epsilon_i(q)$ being larger than the elementary He II excitation energy $\epsilon(q)$; energy transfer into the lower-lying He II excitations would yield in such a case a nonzero M'', i.e., damping. Momentum and energy conservation restrict the phase space for decay in Eq. (2.12) and causes $M''(q,\omega)$ to vanish for $\omega\leq\epsilon_i(q)$, i.e., $\chi_i''(q,\omega<\epsilon_i(q))=0$. Hence, the ^{3}He quasiparticles with energy $\epsilon_i(q)$ defined by the lowest-lying solution of Eqs. (2.9) are the lowest-lying excitations of the system. The existence of undamped ^{3}He quasiparticles, which necessarily are the lowest-energy levels of the system, are a consequence of the superfluidity of He II: Since there are no He II density excitations below the elementary excitation spectrum $\epsilon(q)$, a ^{3}He quasiparticle with energy $\epsilon_i(q)$ cannot transfer energy to He II. In other words, energy and momentum conservation in Eq. (2.12) enforce $M''(q,\omega)=0$ for $\omega\leq\epsilon_i(q)<\epsilon(q)$, for the kind of dispersion $\epsilon_i(q)$ obtained in Sec. III.

The crucial approximation for the relaxation kernel $M(q,z)$ was to restrict the ^{3}He atom's energy and momentum transfer only to excitation states $\rho(\vec{p})\rho_i(\vec{q}-\vec{p})$. Since it is clear that transfer will be most efficient into the lowest-lying excitations of the He II system, i.e., into single He II density excitations, one could promote a simplicity argument in favor of the combinations $\rho(\vec{p})\rho_i(\vec{q}-\vec{p})$. Further support for our approximation can be deduced from the observation of Miller *et al.*[4] that virtual excitation of pairs of density fluctuations constitute the leading contribution to the backflow.

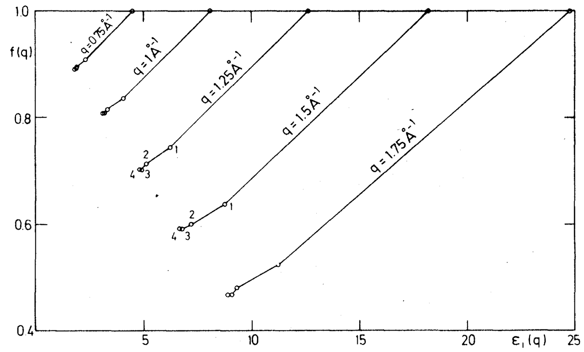

FIG. 1. Values for the quasiparticle excitation strength $f(q)$ and for the quasiparticle energy $\epsilon_i(q)$ after n iterations ($n=0,\cdots,4$) for various wave numbers. The lines are guides to the eye.

III. RESULTS

A. Technical details

Equations (2.3), (2.4), (2.8), and (2.12) are a closed set of equations to determine the impurity recoil spectrum $\chi_i''(q,\omega)$. The following input information is required to solve them: (a) the bare ^{3}He mass and the He II particle density, (b) the He II excitation spectrum, which was taken from our previous theory,[20] (c) the structure factors $S(q)$ (Ref. 27) and $S_{34}(q)$. The latter was determined from the pair distribution function $g_{34}(r)$ evaluated[28] for a mixture of bosons with mass ratio $\frac{3}{4}$. The solution has been obtained by straightforward iteration starting with the free-impurity approximation $M(q,z)\equiv 0$. To demonstrate the convergence of the iteration after four steps Fig. 1 shows for some representative values of q the quasiparticle excitation energies $\epsilon_i(q)$ and excitation strengths $f(q)$ after n iteration steps ($n=0,\ldots,4$). For a given relaxation kernel in the nth iteration the quasiparticle energy as a function of $\Omega_0(q)$ was determined graphically from Eqs. (2.9). Then one could obtain $f(q)$ from Eq. (2.10) as a function of $\Omega_0(q)$ and fix the latter via Eq. (2.8). It is, however, numerically much simpler to determine $\Omega_0(q)$, $\epsilon_i(q)$, and $f(q)$, which fulfill the sum rules of Eqs. (2.5), (2.6), and (2.8) with the use of Eq. (2.11) in the integrands.[25]

B. Relaxation kernel

Since both spectra χ'' as well as χ_i'' show δ-function peaks Eq. (2.12) involves a momentum integration over $\delta(\omega-\epsilon(p)-\epsilon_i(|\vec{q}-\vec{p}|))$, which was done numerically with a method described in Ref. 20. These contributions from the elementary excitations to the relaxation kernel [Eq. (2.12)] are by far greater than those where one of the convolution partners in Eq. (2.12) or both represent a continuous excitation spectrum. Hence fluctuations with frequency ω and wave number q are more effectively damped by creating one elementary excitation in He II than by generating a multiple-density excitation in the continuum part of χ''. The latter process is relevant only for large frequencies.

In Fig. 2 we show the relaxation kernels stemming from all combinations in the convolution integral of Eq. (2.12). Because of the above argumentation one can explain, however, the spectral structure in $M''(q,\omega)$ by merely investigating the kinematics of closing and opening of scattering channels into one ^{3}He quasiparticle and into one elementary He II excitation. The various decay thresholds can be analyzed in analogy to Pitaevskij's work.[29]

As a representative example we show in Fig. 3 for $q=2\ \text{Å}^{-1}$ the contributions to the damping function from emissions of He II phonons, maxons,[30] and rotons. The vertex [Eq. (2.13)] for decay into He II phonons with wave numbers $p\to 0$ approaches zero, so $M''(q,\omega)$ remains very small just above the threshold energy $\epsilon_i(q)$ for phonon emission. Then, however, the phonon contribution to $M''(q,\omega)$ increases rapidly, since with higher frequencies the phase space for He II phonons with larger momentum p as well as the vertex [Eq. (2.13)] increases.

The dominant contribution to M comes from maxon excitations causing the peak in M'' at $\omega\simeq 17$–18 °K for $q=2\ \text{Å}^{-1}$, (cf. Figs. 2 and 3). The phase space for maxon emission is large and so is the vertex Eq. (2.13) for maxon momenta $p\simeq 1\ \text{Å}^{-1}$. Both effects enhance the ^{3}He quasiparticle hybridization with He II maxons.

The decay of a ^{3}He excitation of frequency ω and wave number q into a long-wavelength ^{3}He quasiparticle by emitting a He II roton is possible above a threshold frequency $W(q)$. The damping function $M''(q,\omega)$ shows for ω near $W(q)$ a square-root dependence

$$\omega M''_{\text{roton}}(q,\omega)=A(q)[\omega-W(q)]^{1/2}\Theta(\omega-W(q)) \quad (3.1)$$

to be seen in the roton part of Fig. 3. If the roton dispersion is approximated by

$$\epsilon_{\text{roton}}(q)=\Delta+(q-q_0)^2/2\mu_{\text{roton}}$$

and the long-wavelength ^{3}He quasiparticle energy by $\epsilon_i(q)=q^2/2m^*$ one finds

$$W(q)=\Delta+\tfrac{1}{2}(q-q_0)^2/(\mu_{\text{roton}}+m^*)\,. \quad (3.2)$$

The threshold position $W(q)$ lies below the roton dispersion except for the momentum q_0, i.e., the minimum of the roton dispersion. Note that there cannot exist undamped ^{3}He quasiparticles with en-

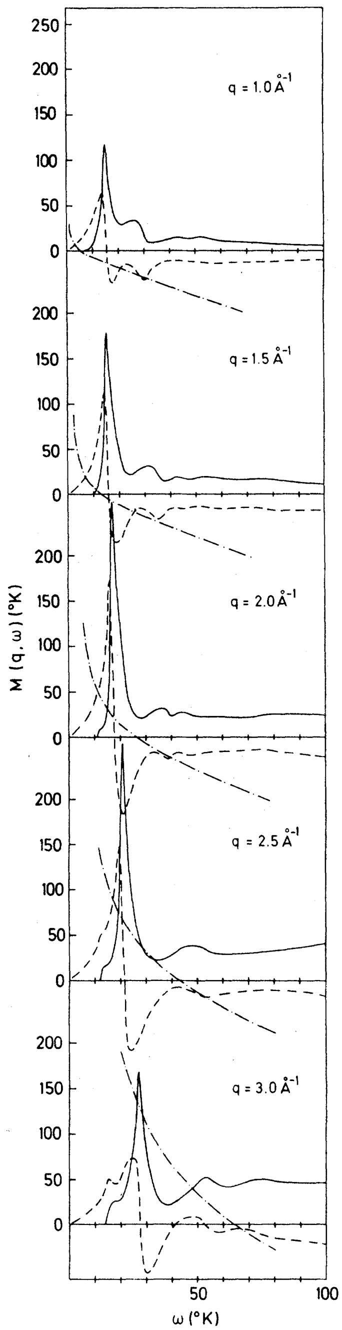

FIG. 2. Imaginary part $M''(q,\omega)$ (full curves) and real part $M'(q,\omega)$ (dashed curves) of the relaxation kernel as a function of frequency ω for various values of wave number q. The dash-dotted curve represents $\Omega_0^2(q)/\omega-\omega$.

ergy $\epsilon_i(q)>W(q)$ since M'' is nonzero above $W(q)$. That means in particular that the dispersion $\epsilon_i(q)$ can possibly merge with the He II dispersion at one point only, namely the roton minimum $q=q_0$.

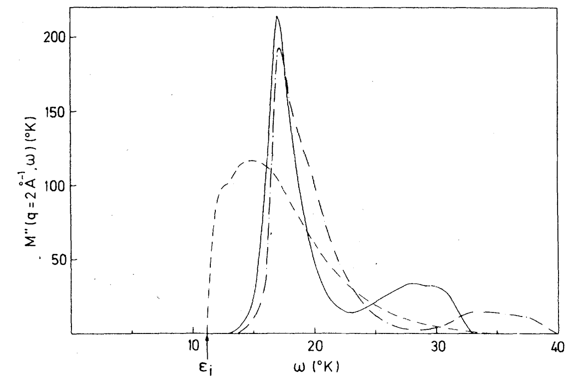

FIG. 3. Contributions to the damping function $M'(q,\omega)$ [Eq. (2.12)] for $q=2$ Å^{-1} caused by exciting a ^{3}He quasiparticle and an elementary He II excitation. Full curve denotes $4M''(q,\omega)$ due to emission of He II phonons with momentum less than 0.75 Å^{-1}. Dash-dotted curve is due to generation of He II maxons with wave numbers $0.75\leq p\leq 1.75$ Å^{-1}. Dashed curve represents $10M''(q,\omega)$ coming from excitations of rotons with momentum $1.75\leq p\leq 2.25$ Å^{-1}.

The weight $A(q)$ of the threshold [Eq. (3.1)] turns out to be rather small. This is partly due to the structure factor $S_{34}(p)$ in Eq. (2.13) being small for momenta $p\simeq q_0$.

C. Density-fluctuation spectrum

The real part of the relaxation kernel $M'(q,\omega)$ shows for low-frequencies normal dispersion. Then there is, due to the maxon peak in $M''(q,\omega)$, the steep fall off with a following increasing behavior. The high-frequency two-mode structure in $M''(q,\omega)$ causes $M'(q,\omega)$ again to switch between normal and anomalous dispersion. Consequently, there are several intersections of $M'(q,\omega)$ with the dash dotted curve $\Omega_0^2(q)/\omega-\omega$ in Fig. 2. This gives, according to Eq. (2.9a), rise to the resonance structure in the spectrum $\chi_i''(q,\omega)$ shown in Fig. 4. The high-frequency resonances in the continuum of $\chi_i''(q,\omega)$ can thus be identified via $M'(q,\omega)$ as hybridizations with two-mode excitations of M''.

For wave numbers less than a critical one $q_c\simeq 2$ Å^{-1} the relaxation kernels shown in Fig. 2 display obvious solutions to Eqs. (2.9) marked by the intersection of the dash dotted curve with M' where M'' vanishes. This implies the existence of undamped ^{3}He quasiparticle excitations with a dispersion law $\epsilon_i(q)$ shown in Fig. 5. Also shown is the dispersion $\epsilon(q)$ of elementary He II excitations that we used in this work and which was obtained earlier by us.[20] The peak positions of the resonances in the continuum part of $\chi_i''(q,\omega)$ and their half-width extensions are included in Fig. 5 as well.

For small wave numbers the dispersion $\epsilon_i(q)$ is

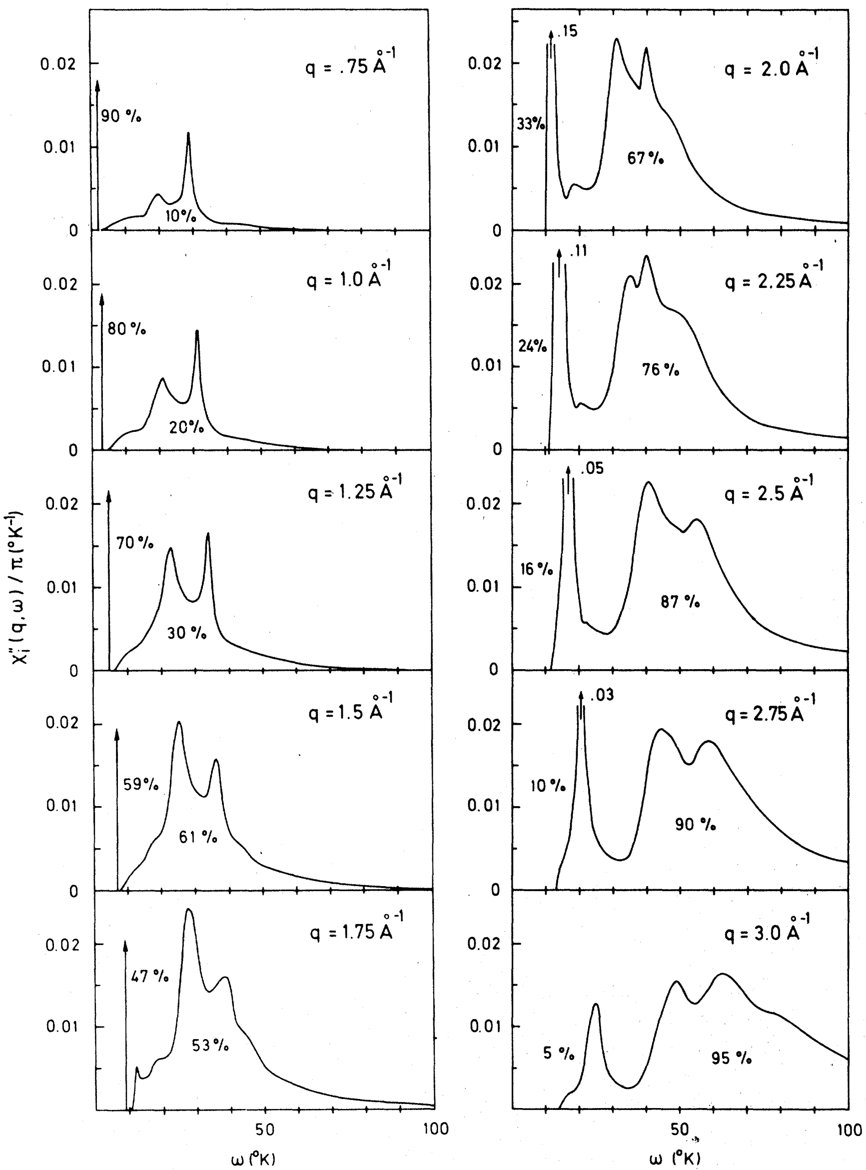

FIG. 4. Normalized-density fluctuation spectrum $\chi_i''(q,\omega)$ of ^{3}He in He II. The arrows mark the positions of undamped quasiparticle excitations.

parabolic determined by the effective mass $m^* = 2.35\, m_i$ being quite close to the experimental numbers.[14] With increasing wave numbers the level repulsion between the coherent ^{3}He excitation state of energy $\epsilon_i(q)$ and the pair continuum in $M''(q,\omega)$ on the high-frequency side becomes stronger and stronger: The large real part M' renormalizes via Eq. (2.9a) the quasiparticle energies $\epsilon_i(q)$ strongly and forces them below the parabola $q^2/2m^*$, an effect which can be visualized directly in Fig. 2. One can parametrize the resulting dispersion $\epsilon_i(q)$ of Fig. 5 by a momentum-dependent effective mass $m^*(q)$

$$\epsilon_i(q) = q^2/2m^*(q). \tag{3.3}$$

One finds $m^*(q)$ to increase almost linearly over a momentum range $0.25 \leq q \leq 2.75$ Å^{-1} with

$$m^*(q) \simeq m^*(1+aq), \quad a = 0.1\text{ Å}. \tag{3.4}$$

This implies the density of ^{3}He states to increase stronger than to be expected from a pure parabolic dispersion. It also causes the ^{3}He contribution to the normal mass to increase stronger with temperature, an effect which has been verified experimentally.[19]

Undamped quasiparticle excitations cease to exist at the critical wave vector $q_c \simeq 2$ Å^{-1} where their energy $\epsilon_i(q)$ approaches the threshold energy $W(q)$ [Eq. (3.2) and dotted curve in Fig. 5] for

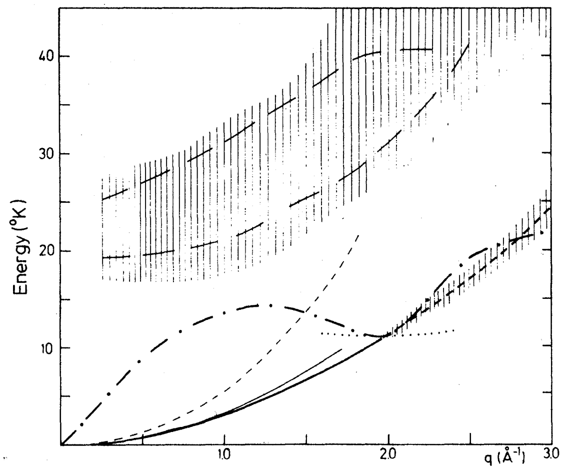

FIG. 5. Dispersion of undamped ^{3}He quasiparticle excitations $\epsilon_i(q)$ (thick full curve), dispersion of elementary He II excitations ϵ (q) (thick-dash dotted curve) as obtained earlier (Ref. 20), the long-wavelength dispersion $q^2/2m^*$ (thin curve), and the characteristic frequency $\Omega_0(q)$ (thin-dashed curve). Above $q_c \simeq 2$ Å^{-1} the position of the lowest resonance in the continuum of $\chi_i''(q,\omega)$ is indicated (thick-dashed curve) as well as its half-width extension. The dotted curve represents the threshold energy $W(q)$ [Eq. (3.2)] for roton emission. The high-frequency resonance positions of $\chi_i''(q,\omega)$ and their half-width extensions are shown in the upper part of the figure.

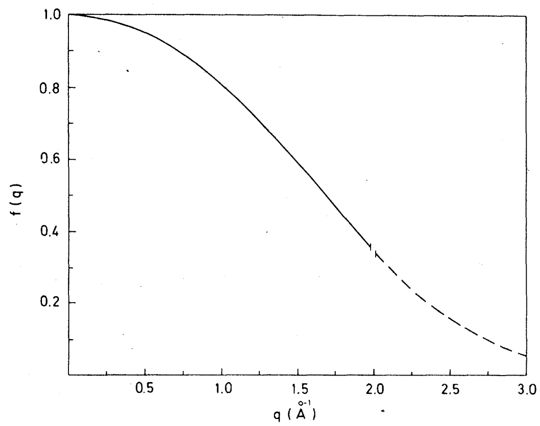

FIG. 6. Contribution $f(q)$ (full curve) of undamped ^{3}He quasiparticle excitations to the spectrum $\chi_i''(q,\omega)$. The dashed continuation for $q > q_C \simeq 2$ Å^{-1} denotes the area under the lowest-lying resonance in the continuum.

roton emission by the ^{3}He quasiparticle movement. The dispersion curve continues beyond $W(q)$ for $q>q_c$ as the lowest resonance in the continuum part of $\chi_i''(q, \omega)$. The resonance width increases with increasing q as shown in Fig. 5. The quasiparticle dispersion $\epsilon_i(q)$ is similar to the curve proposed recently by Esel'son *et al.*[11] In order that $\epsilon_i(q)$ exhibits a roton like minimum, as hypothesized earlier,[7-10] $M''(q, \omega)$ should show a strong enhancement around that wave number causing the quasiparticle level $\epsilon_i(q)$ to be pushed down. The theory in its present form does not offer the possibility for such an anomaly.

In Fig. 6 we show the contribution $f(q)$ from undamped ^{3}He quasiparticle excitations to the spectrum $\chi_i''(q, \omega)$. It is a monotonously decreasing function of momentum since the hybridization with the two-mode continuum becomes stronger and stronger the closer $\epsilon_i(q)$ approaches the continuum excitations of $M''(q, \omega)$. As explained in Sec. III D it falls off to zero at $q = q_c$ within a few hundredths of an Å^{-1}.

D. ^{3}He quasiparticle excitations near the threshold for roton emission

In this section we investigate the way $\epsilon_i(q)$ approaches the threshold $W(q)$ [Eq. (3.2)] at $q = q_c$ and how $f(q)$ drops to zero for $q \to q_c$. The behavior of $\epsilon_i(q)$ and $f(q)$ in the immediate vicinity of q_c could not be determined with the numerical work described so far since $M(q, \omega)$ is evaluated with an accuracy of 1 °K only.

According to Pitaevskij[29] the dispersion $\epsilon_i(q)$ has an endpoint at the wave vector q_c where $\epsilon_i(q)$ merges with the threshold energy $W(q)$ for roton emission: $W(q_c) = \epsilon_i(q_c)$. This is most easily understood from Eq. (2.10) for the excitation weight $f(q)$. It approaches zero at q_c since the real part of the roton contribution to $M''(q, \omega)$ [Eq. (3.1)],

$$\omega M'_{\text{roton}}(q, \omega) = -A(q)[W(q) - \omega]^{1/2}\Theta(W(q) - \omega) \quad (3.5)$$

shows a divergent derivative for $\epsilon_i(q_c) = W(q_c)$. By taking the momentum derivative of Eq. (2.9a) at $q = q_c$

$$\frac{d}{dq}[\epsilon_i^2(q) - \Omega_0^2(q) + \epsilon_i(q) M'_{\text{rest}}(q, \epsilon_i(q))]_{q_c}$$

$$= A(q_c)\frac{d}{dq}[W(q) - \epsilon_i(q)]^{1/2}_{q_c}, \quad (3.6)$$

one finds in addition that $\epsilon_i(q)$ has to merge tangentially with the threshold curve $W(q)$

$$\frac{d}{dq}[W(q) - \epsilon_i(q)]_{q_c} = 0. \quad (3.7)$$

In Eq. (3.6) the relaxation kernel was splitted into the singular roton part [Eqs. (3.1) and (3.5)] and into the nonsingular rest

$$M(q, z) = M_{\text{roton}}(q, z) + M_{\text{rest}}(q, z)$$

$$\text{for } \omega \simeq W(q),\ q \simeq q_c. \quad (3.8)$$

According to our results q_c is roughly the roton momentum q_0 so that the critical group velocity vanishes with Eqs. (3.7) and (3.2). Then one obtains from Eq. (3.6) the following equation for the second derivative of $\epsilon_i(q)$:

$$\frac{A^2(q_c)}{2}\frac{d^2[W(q)-\epsilon_i(q)]}{dq^2}\bigg|_{q_c} \simeq \left(\frac{d\Omega_0^2(q)}{dq}\right)^2_{q_c}, \qquad (3.9)$$

where the small derivative of M'_{rest} was neglected on the left side of Eq. (3.6). With the values $A(q_c) \simeq 150\ ^\circ\text{K}^{3/2}$ from Eq. (2.12) and $d\Omega_0^2(q_c)/dq_c \simeq 1590\ ^\circ\text{K}^2\ \text{Å}$ one finds the critical curvature to be $d^2\epsilon_i(q_c)/dq_c^2 \simeq -220\ ^\circ\text{K}\text{Å}^2$. That implies an energy change in $\epsilon_i(q)$ of 1 °K over a momentum interval of 0.1 Å^{-1}, too much to be resolved with our numerical method.

In order to determine how steeply $f(q)$ falls off to zero near q_c we evaluated with Eqs. (2.10), (3.5), and (3.8) the slope

$$\frac{df(q)}{dq}\bigg|_{q\to q_c-0} = -\frac{q_c^2}{m_i}\frac{2^{1/2}}{A(q_c)} \times \left(\frac{d^2}{dq^2}[W(q)-\epsilon_i(q)]\right)^{1/2}_{q_c}. \qquad (3.10)$$

If one inserts into this still exact formula the approximate relation in Eq. (3.9) one finds $f(q)$ to decrease linearly for $q \to q_c$ with a final slope of about 10 Å.

Note added in proof. Recently, Greywall[31] has inferred from his extensive experimental data of the specific heat of dilute ^{3}He–He II solution that the effective ^{3}He quasiparticle mass increases with increasing momenta giving rise to a dispersion curve practically identical in shape to ours. The excitation energies differ for $q = 2\ \text{Å}^{-1}$ by about 10%.

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