Excitations in normal liquid ^{3}He

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The dynamical density and spin-density response functions are expressed within a dispersion-relation representation in terms of the corresponding static susceptibilities and relaxation kernels. The kernels are approximated by two-mode decay processes. The resulting coupled integral equations are solved to get self-consistent spectral functions of the density and spin-density response. It is found that a density mode can decay into two density modes and two spin-fluctuation excitations whereas a spin-density fluctuation decays only into a density mode and a spin-density excitation. The theory predicts a well-defined zero-sound mode. The calculated excitation spectra of zero sound and spin-fluctuation excitations and their strengths are compared with neutron-scattering results.

I. INTRODUCTION

Some time ago Pines[1] argued that the Landau zero-sound mode should be expected to exist in normal liquid ^{3}He for wave numbers $q \sim q_F$. Recently, neutron inelastic scattering experiments[2,3] done at temperatures in the mK range have demonstrated that the scattering function contains two peaks for wave numbers up to 1.2 Å^{-1}. The peak at lower energy is due to collective spin-density fluctuations in the particle-hole regimes whereas the peak at higher energies is identified as a zero-sound mode of collective particle-number fluctuations.

The neutron scattering results have been interpreted[3-8] within the framework of generalized random-phase approximation (RPA) theories. The emphasis in these approaches is on the extension of Landau's Fermi-liquid theory to finite q,ω. That requires the introduction of various parameters, for which at present, it does not seem to be possible to provide derivations and justifications. Therefore our aim in this paper is to develop a parameter-free theory of collective excitations in normal liquid ^{3}He. Other attempts in this direction along different lines of approach have been reported by Valls *et al.*[9]

In Sec. II we describe the formalism we used to calculate dynamical susceptibilities, correlation functions, and relaxation functions. We also include relevant results concerning their analytical behavior and their spectral properties. In Sec. III we review the generalized RPA theories and give a brief outline of the polarization-potential approach of Aldrich *et al.* Then we present our alternative: a self-consistent mode-coupling approximation for the relaxation kernels appearing in the dispersion-relation representation of the dynamical susceptibilities. A description of the evaluation of their spectra and a discussion of the results of our theory are given in Sec. IV. Section V contains a summary and our conclusions.

II. GENERAL FORMALISM

We are interested in the fluctuation dynamics of the particle-number density

$$\rho(\vec{q})=\frac{1}{\sqrt{N}}\sum_n e^{-i\vec{q}\cdot\vec{r}_n}=\rho_\uparrow(\vec{q})+\rho_\downarrow(\vec{q}) \tag{2.1}$$

and of the spin density

$$\sigma(\vec{q})=\frac{1}{\sqrt{N}}\sum_n \sigma_z(\vec{r}_n)e^{-i\vec{q}\cdot\vec{r}_n}=\rho_\uparrow(\vec{q})-\rho_\downarrow(\vec{q}) \tag{2.2}$$

of normal liquid ^{3}He in a paramagnetic state described by the Hamiltonian

$$H=\sum_n \frac{p_n^2}{2m}+\tfrac{1}{2}\sum_{n,m}{}' v(|\vec{r}_n-\vec{r}_m|) \;. \tag{2.3}$$

In (2.2), $\sigma_z(\vec{r}_n)$ has eigenvalues ± 1, i.e., $\sigma_z^2(\vec{r}_n)=1$. The ^{3}He particles of bare mass m move in a spin-independent central symmetric potential $v(r)$ acting between pairs.

A. Susceptibilities, correlations, and relaxation functions

The fluctuation dynamics of the two densities ρ and σ are most conveniently described in terms of two complex dynamical susceptibilities[10] ($A=\rho$ or σ),

$$\chi_A(q,z)=\pm i\int_{-\infty}^{\infty} dt\, \Theta(\pm t)e^{izt}\langle [A(-\vec{q},t),A(\vec{q})]\rangle \quad \text{for } \mathrm{Im}z \gtrless 0 \;, \tag{2.4}$$

measuring the response of variable A to a perturbation coupling to A. We do not have to consider cross susceptibilities between ρ and σ—they vanish due to spin-rotation invariance of ρ and H. Furthermore, spatial isotropy implies χ_A to depend only on the modulus $q=|\vec{q}|$. In (2.4) Θ is the unit step function. The angular brackets denote an ensemble average appropriate to the Hamiltonian (2.3).

The time evolution of variables is determined by

$$\frac{dA(t)}{dt}=i[H,A(t)]=i\mathscr{L}A(t) \;. \tag{2.5}$$

With the above definition of the Liouville operator $\mathscr{L}$, one obtains the time dependence of variables in the form

$$A(t)=e^{i\mathscr{L}t}A \tag{2.6}$$

to be used later on.

The response functions (2.4) are analytic in the complex z plane off the real axis and decay sufficiently fast for large z to allow for the Cauchy representation

$$\chi_A(q,z)=\int_{-\infty}^{\infty}\frac{d\omega}{\pi}\frac{\chi_A''(q,\omega)}{\omega-z}\ . \quad (2.7)$$

The spectral function $\chi_A''(q,\omega)$ being the discontinuity of $\chi_A(q,z)$ across the real axis

$$\chi_A(q,\omega\pm i0)=\chi_A'(q,\omega)\pm i\chi_A''(q,\omega) \quad (2.8)$$

is the frequency Fourier spectrum of the response function

$$\chi_A''(q,\omega)=\tfrac{1}{2}\int_{-\infty}^{\infty}dt\,e^{i\omega t}\langle[A(-\vec{q},t),A(\vec{q})]\rangle\ . \quad (2.9)$$

The even real part $\chi_A'(q,\omega)$ and the odd imaginary part $\chi_A''(q,\omega)$ of $\chi_A(q,\omega+i0)$ are connected via Kramers-Kronig relations.

Furthermore, the response spectra $\chi_A''(q,\omega)$ are related to the correlation spectra

$$S_A(q,\omega)=\int_{-\infty}^{\infty}dt\,e^{i\omega t}\langle\delta A(-\vec{q},t)\delta A(\vec{q})\rangle \quad (2.10a)$$

$$=2\Theta(\omega)\chi_A''(q,\omega) \quad (2.10b)$$

via the fluctuation-dissipation theorem (2.10b) written down here in its zero-temperature limit version. Note that, e.g., in a scattering experiment with unpolarized neutrons, one can measure the dynamic structure factor

$$S(q,\omega)=S_\rho(q,\omega)+0.245S_\sigma(q,\omega)\ , \quad (2.11)$$

which is given by the sum of the density correlation spectrum $S_\rho(q,\omega)$ and the spin-density correlation spectrum $S_\sigma(q,\omega)$ weighted by the ratio 1.2/4.9 of incoherent and coherent scattering cross sections.

We consider the response functions (2.4) to be the basic quantities. To investigate them we will employ a dispersion-relation representation

$$\chi_A(q,z)=\frac{-q^2/m}{z^2-\Omega_A^2(q)+zM_A(q,z)} \quad (2.12)$$

in terms of a characteristic frequency $\Omega_A(q)$

$$\Omega_A^2(q)=\frac{q^2/m}{\chi_A(q,z=0)} \quad (2.13)$$

and of a complex polarization—or relaxation kernel $M_A(q,z)$. In Appendix A we derive (2.12) together with the explicit expression for M_A within Mori's projector formalism.[11] To that end we introduce yet another complex function,

$$\phi_A(q,z)=\frac{\chi_A(q,z)-\chi_A(q,z=0)}{z}\ , \quad (2.14)$$

i.e., Kubo's relaxation function.[12] Obviously ϕ_A has similar analytical properties as the susceptibility χ_A and, moreover, the spectra are intimately related to each other,

$$\phi_A''(q,\omega)=\chi_A''(q,\omega)/\omega\ . \quad (2.15)$$

It is very convenient to write the relaxation function as a resolvent matrix element

$$\phi_A(q,z)=(A(\vec{q})\,|\,(\mathscr{L}-z)^{-1}\,|\,A(\vec{q}))\ . \quad (2.16)$$

That is achieved by introducing the scalar product

$$(A_i\,|\,A_j)=\chi_{ij}(z=0)=\phi_{ij}(t=0) \quad (2.17)$$

in the vector space of dynamic variables $\{A_i\}$ via the static susceptibility

$$\chi_{ij}(z=0)=i\int_0^{\infty}dt\langle[A_i^*(t),A_j]\rangle$$

$$=\int_{-\infty}^{\infty}\frac{d\omega}{\pi}\frac{\chi_{ij}''(\omega)}{\omega}\ . \quad (2.18)$$

In Appendix A it is shown that the relaxation kernel $M_A(q,z)$ has the same analytical properties as $\phi_A(q,z)$. The spectrum $M_A''(q,\omega)$ is even in ω and positive semidefinite. Therefore, the real part

$$M_A'(q,\omega)=2\omega\mathscr{P}\int_0^{\infty}\frac{d\omega'}{\pi}\frac{M_A''(q,\omega')}{\omega'^2-\omega^2}\ , \quad (2.19)$$

being connected to $M_A''(q,\omega)$ via the Kramers-Kronig relation (2.19), is odd in ω and varies linearly in ω for small frequencies.

B. Frequency moments

For completeness and later use we list here some of the frequency-sum rules,

$$C_{2n}(q)=\int_{-\infty}^{\infty}\frac{d\omega}{\pi}\omega^{2n}\phi_A''(q,\omega)$$

$$=\int_{-\infty}^{\infty}\frac{d\omega}{\pi}\omega^{2n-1}\chi_A''(q,\omega)$$

$$=\int_0^{\infty}\frac{d\omega}{\pi}\omega^{2n-1}S_A(q,\omega) \quad (2.20)$$

of the relaxation, response, and correlation spectra. They appear in the $1/z$ expansion of, e.g., the relaxation function

$$\phi_A(q,z)=\int_{-\infty}^{\infty}\frac{d\omega}{\pi}\frac{\phi_A''(q,\omega)}{\omega-z}=-\frac{1}{z}\sum_{n=0}C_{2n}(q)\frac{1}{z^{2n}}\ . \quad (2.21)$$

The expansion coefficients are easily identified as matrix elements

$$C_{2n}(q)=(A(\vec{q})\,|\,\mathscr{L}^{2n}\,|\,A(\vec{q})) \quad (2.22)$$

if one uses the fact that

$$\phi_A''(q,\omega)=\pi(A(\vec{q})\,|\,\delta(\omega-\mathscr{L})\,|\,A(\vec{q}))\ . \quad (2.23)$$

Hence the $n=0$ moment is the static susceptibility

$$(A(\vec{q})\,|\,A(\vec{q}))=\chi_A(q)=\chi_A(q,z=0)\ , \quad (2.24)$$

which yields in the long-wavelength limit either the isothermal compressibility

$$\lim_{q\to 0}\chi_\rho(q)=nK_T=(nC_T^2)^{-1} \quad (2.25)$$

or the Pauli paramagnetic susceptibility[14]

$$\lim_{q\to 0}\chi_\sigma(q)=\chi_{\text{Pauli}}/n\mu^2\ . \quad (2.26)$$

Here n is the equilibrium particle-number density, C_T is the isothermal sound velocity, and μ is the spin magnetic moment of the ^{3}He nucleus. The f-sum rule $C_2(q)$ yields for both $A=\rho$ and $A=\sigma$,

$$(A(\vec{q})\,|\,\mathscr{L}^2\,|\,A(\vec{q}))=q^2/m\ , \tag{2.27}$$

upon using the general relation

$$(A\,|\,\mathscr{L}\,|\,B)=\langle [A^\dagger,B]\rangle\ . \tag{2.28}$$

Thus the characteristic frequency $\Omega_A(q)$ entering (2.12) is determined by the ratio C_2/C_0,

$$\Omega_A^2(q)=\frac{(A(\vec{q})\,|\,\mathscr{L}^2\,|\,A(\vec{q}))}{(A(\vec{q})\,|\,A(\vec{q}))}\ . \tag{2.29}$$

Of course, one can form combinations of other moments with the dimension of a frequency, e.g., $(C_4/C_2)^{1/2}$ which has been discussed in the literature.[8,15] We do not add to this discussion[16] here since only $\Omega_A(q)$ enters explicitly into the dispersion-relation representation of the susceptibilities at the level displayed in (2.12).

The last moments we need are the total spectral intensities of the scattering laws

$$S_A(q)=\int_{-\infty}^{\infty}\frac{d\omega}{2\pi}S_A(q,\omega)=\int_0^{\infty}\frac{d\omega}{\pi}\chi_A''(q,\omega)\ . \tag{2.30}$$

Here $S_\rho(q)$ is the density structure factor

$$S_\rho(q)=1+n\int d\vec{r}\,e^{-i\vec{q}\cdot\vec{r}}[g(r)-1]\ , \tag{2.31}$$

which can also be measured by x-ray diffraction while $S_\sigma(q)$ is the spin or magnetic structure factor

$$S_\sigma(q)=1+n\int d\vec{r}\,e^{-i\vec{q}\cdot\vec{r}}g_\sigma(r)\ . \tag{2.32}$$

The correlation functions

$$g(r)=g_l(r)+g_u(r) \tag{2.33a}$$

and

$$g_\sigma(r)=g_l(r)-g_u(r) \tag{2.33b}$$

are given as combinations of pair correlation functions for particles with like spins, $g_l(r)$, and unlike spins, $g_u(r)$. The latter are normalized such that $g_{l,u}(r\to\infty)=\frac{1}{2}$. While there is at present sufficient information available[17,18] about $S_\rho(q)$, little is known about $S_\sigma(q)$. Ceperley *et al.*[19] have performed Monte Carlo calculations of static correlations for Fermi liquids, but how close they are to actual liquid ^{3}He is not yet known.

C. Other representations of the dynamic susceptibilities

It is useful to make contact with general representations of the susceptibilities $\chi_A(q,z)$ obtained within other theoretical frameworks. To that end we introduce a reference response function $\widetilde{\chi}_A(q,z)$ in terms of which the susceptibility $\chi_A(q,z)$ can be written as

$$\chi_A(q,z)=\frac{\widetilde{\chi}_A(q,z)}{1+\psi_A(q,z)\widetilde{\chi}_A(q,z)}\ . \tag{2.34}$$

Hence

$$\psi_A(q,z)=\chi_A^{-1}(q,z)-\widetilde{\chi}_A^{-1}(q,z) \tag{2.35}$$

is given by the difference of the inverse susceptibilities which makes it most suited for approximations. The reference susceptibility so far is arbitrary. It can be the response function of free particles as discussed by Takeno and Yoshida[8,20] or a quasiparticle or a screened response function[7] or something else. If one employs the dispersion-relation representation of the reference susceptibility

$$\widetilde{\chi}_A(q,z)=\frac{-q^2/m}{z^2-\widetilde{\Omega}_A^2(q)+z\widetilde{M}_A(q,z)}\ , \tag{2.36}$$

one can express[21] the "polarization potential"

$$\psi_A(q,z)=\psi_A(q)+\frac{m}{q^2}z[\widetilde{M}_A(q,z)-M_A(q,z)] \tag{2.37}$$

in terms of a frequency-dependent part given by the difference of the relaxation kernels and a static part

$$\psi_A(q)=\psi_A(q,z=0)=\chi_A^{-1}(q)-\widetilde{\chi}_A^{-1}(q) \tag{2.38}$$

given by the difference of the inverse static susceptibilities.

III. APPROXIMATIONS

A. Generalized RPA theories

The starting point of all mean-field type calculations is the representation (2.34). The standard RPA, for example, is obtained by using for $\widetilde{\chi}_A(q,z)$ the Lindhard response function $\chi_0(q,z)$ of an ideal Fermi gas of quasiparticles of effective mass m^* (number-density and spin-density susceptibilities of an ideal Fermi gas are the same). Furthermore, the frequency dependence of $\psi_A(q,z)$ is ignored, i.e., $\widetilde{M}_A(q,z)-M_A(q,z)=0$, and the mean field $\psi_A(q)$ is fixed by the experimental structure factor via the fluctuation-dissipation theorem. This was done by Stirling *et al.*[4] to interpret their experimental data. Later Glyde and Khanna,[5] Aldrich *et al.*,[6,7] and Yoshida and Takeno[8] have tried to extend the Landau theory to finite q,ω.

In the approach of Aldrich and Pines[7] commonly known as the polarization-potential model, it is assumed that

$$m[\widetilde{M}_A(q,\omega)-M_A(q,\omega)]=\omega f_1^A(q) \tag{3.1}$$

is purely real which violates causality. Furthermore, the real part depends only linearly on frequency. That is reasonable for small ω in view of (2.19) but obviously wrong for larger ω. For the static part of the polarization potential, the authors use $\psi_A(q)=f_0^A(q)$ with $f_0^A(q)$, $f_1^A(q)$ denoting four q-dependent generalized Landau parameters discussed below. Then the susceptibilities have the form

$$\chi_A(q,z)=\frac{\widetilde{\chi}_A(q,z)}{1+\left[f_0^A(q)+\dfrac{z^2}{q^2}f_1^A(g)\right]\widetilde{\chi}_A(q,z)}\ , \tag{3.2}$$

where the reference response functions $\widetilde{\chi}_A(q,z)$ are given further below. The static polarization functions $f_0^\rho(q)$ $[f_0^\sigma(q)]$ are taken as the Fourier transform of the sum (difference) of the effective interactions $f^{\uparrow\uparrow}(r)$ between particles of parallel spin and $f^{\uparrow\downarrow}(r)$ between particles of antiparallel spin. These interactions being unknown, the authors give arguments for a parameterization of

$$f^{\uparrow\uparrow}(r)=a^{\uparrow\uparrow}\left[1-\left[\frac{r}{r^{\uparrow\uparrow}}\right]^8\right]\quad\text{for } r<r_c^{\uparrow\uparrow} \tag{3.3}$$

and similarly of $f^{\uparrow\downarrow}(r)$, and the assumption that for

$r > r_c = 3$ Å an attractive van der Waals interaction can be used. Also

$$f_0^\rho(r) = [f^{\uparrow\uparrow}(r) + f^{\uparrow\downarrow}(r)]/2$$

was assumed to have the same form as (3.3), namely

$$f_0^\rho(r) = a_\rho[1 - (r/r_\rho)^8]$$

for $r \le r_\rho$. The latter was fitted to large-q neutron scattering experiments and a_ρ was taken from the experimentally determined Landau parameter $f_0^\rho(q=0)$. The options for the choices of the parameters determining $f^{\uparrow\downarrow}(r)$ and $f_0^\sigma(r)$ are even less unique and the authors discuss various values and their implications.

The function $f_1^\sigma(q)$ was set equal to zero while $f_1^\rho(q)$ is determined according to $m^*(q) = m + f_1^\rho(q)$ by the wave-number-dependent effective mass $m^*(q)$ of ^{3}He which was extracted from neutron scattering experiments. For the reference susceptibility, the authors take

$$\tilde{\chi}_A(q,z) = \alpha_A(q)\chi_0^*(q,z) + \chi_A^{\text{mult}}(q) , \tag{3.4}$$

a combination of a weighted Lindhard function $\chi_0^*(q,z)$, wherein the mass is replaced by the effective one, $m^*(q)$, and a real part $\chi_A^{\text{mult}}(q)$ reflecting multiparticle excitations in a frequency-independent approximation.

The results of the polarization-potential theory give a fair description of the experimental neutron scattering data. That applies also to the approach of Yoshida and Takeno.[8] Therein the Lindhard response was taken as the reference susceptibility, and for the difference of the relaxation kernels $\Delta M_\rho(q,t)$ entering the polarization potential, the authors used a phenomenological Gaussian ansatz while the potential for spin-density fluctuations was taken to be static. Lastly, we mention that Beal-Monod,[22] upon using a paramagnon model for spin-density fluctuations, found the neutron scattering data to be consistent with a Stoner enhancement factor of 0.9. From this finding, which seems to be in agreement with what one obtains from the static spin susceptibility, one concludes that liquid ^{3}He at low temperatures $T \ll T_F$ is nearly ferromagnetic.

B. Mode-coupling theory

While the polarization-potential approach describes the experiments fairly well, it does not seem to be possible at present to provide a microscopic picture for the various parameters in the theory. Therefore, we develop in this section a semimicroscopic theory of excitation in normal liquid ^{3}He which is free of fit parameters. To that end we use the exact dispersion-relation representation of the two susceptibilities $\chi_A(q,z)$ in terms of the relaxation kernels $M_A(q,z)$ (A7). The latter we evaluated self-consistently within a two-mode decay approximation.[23,24]

The two-mode excitations considered are described by products

$$B(\vec{q},\vec{k}) = \delta A(\vec{k})\delta A'(\vec{q}-\vec{k}) \tag{3.5}$$

of two density modes, two spin-density modes, and one density and one spin-density mode. Therefore A and A' stand for ρ or σ. Spin-rotation invariance of ρ and H allows decay of a density mode into two density modes and into two spin-density excitations but not into a spin-density mode and a density mode. Similarly, a spin-density mode can decay into another spin-density mode only by emitting a density fluctuation. The various kernels due to the decays $\rho \to \rho\rho$, $\rho \to \sigma\sigma$, and $\sigma \to \sigma\rho$ can be written[23,24] approximately as

$$M_A(q,z)\,|_{\text{two mode}} \simeq \sum_{\vec{k},\vec{k}'} \varphi_{A\leftrightarrow B}(\vec{q},\vec{k})\phi_B(\vec{q},z;\vec{k},\vec{k}') \times \varphi_{A\leftrightarrow B}(\vec{q},z;\vec{k},\vec{k}') , \tag{3.6}$$

where the two-mode relaxation function

$$\phi_B(\vec{q},z;\vec{k},\vec{k}') = (B(\vec{q},\vec{k})\,|\,(\mathcal{L}-z)^{-1}\,|\,B(\vec{q},\vec{k}')) \tag{3.7}$$

is evaluated by factorizing four-point correlations $\langle \delta A(t)\delta A'(t)\delta A\delta A' \rangle$ into products of two-point correlations. The vertices are given by

$$\varphi_{A\leftrightarrow B}(\vec{q},\vec{k}) = \sum_{\vec{k}'} (Q\mathcal{L}^2 A(\vec{q})\,|\,B(\vec{q},\vec{k}'))[(B\,|\,B)^{-1}]_{\vec{k}',\vec{k}} . \tag{3.8}$$

The normalization matrix

$$(B(\vec{q},\vec{k})\,|\,B(\vec{q},\vec{k}')) = \int_{-\infty}^{\infty} \frac{d\omega}{\pi}\phi_B''(\vec{q},\omega;\vec{k},\vec{k}') \tag{3.9}$$

is determined by the relaxation spectrum obtained with the above factorization approximation. Since the frequency integral is somewhat insensitive to the detailed spectral distribution, we calculate the above moment for undamped two-mode fluctuations.

We now demonstrate the evaluation of the remaining first matrix element in (3.8) for

$$\begin{aligned}(Q\mathcal{L}^2\rho(\vec{q})\,|\,\sigma(\vec{k})\sigma(\vec{q}-\vec{k})) &= \frac{\vec{q}\cdot\vec{k}}{m}S_\sigma(k) + \frac{\vec{q}\cdot(\vec{q}-\vec{k})}{m}S_\sigma(\vec{q}-\vec{k}) \\ &\quad - \Omega_\rho^2(q)(\rho(\vec{q})\,|\,\sigma(\vec{k})\sigma(\vec{q}-\vec{k}))\end{aligned} \tag{3.10}$$

as an example. The other cases are similar. The static three-point susceptibility

$$(\rho(\vec{q})\,|\,\sigma(\vec{k})\sigma(\vec{q}-\vec{k})) = \int_{-\infty}^{\infty} \frac{d\omega}{\pi}\frac{1}{\omega}\chi_{\rho,\sigma\sigma}''(\vec{q},\omega;\vec{k}) \tag{3.11}$$

is evaluated by using a two-pole approximation[23] for the above spectrum,

$$\begin{aligned}\frac{1}{\pi}\chi_{\rho'\sigma\sigma}''(\vec{q},\omega;\vec{k}) &= C\delta[\omega-\Omega_\rho(q)] \\ &\quad + D\delta[\omega-\Omega_\sigma(k)-\Omega_\sigma(\vec{q}-\vec{k})] \\ &\quad -(\omega\to-\omega) .\end{aligned} \tag{3.12}$$

The constants C,D are determined by two spectral moments of $\chi_{\rho'\sigma\sigma'}''$, namely

$$2C\Omega_\rho(q)+2D[\Omega_\sigma(k)+\Omega_\sigma(\vec{q}-\vec{k})]$$
$$=(\mathscr{L}^2\rho(\vec{q})\,|\,\sigma(\vec{k})\sigma(\vec{q}-\vec{k}))$$
$$=\frac{\vec{q}\cdot\vec{k}}{m}S_\sigma(\vec{k})+\frac{\vec{q}\cdot(\vec{q}-\vec{k})}{m}S_\sigma(\vec{q}-\vec{k}) \tag{3.13}$$

and

$$C+D=\langle\rho^*(\vec{q})\sigma(\vec{k})\sigma(\vec{q}-\vec{k})\rangle$$
$$\simeq S_\rho(q)S_\sigma(k)S_\sigma(\vec{q}-\vec{k})\;. \tag{3.14}$$

In the last line we used the convolution approximation[25] for the equal-time three-point correlation function. We also replaced in the vertices the characteristic frequencies $\Omega_A(q)$ by their zeroth-order approximation

$$\epsilon_A^0(q)=\frac{q^2}{2mS_A(q)}\;. \tag{3.15}$$

Combining everything, we find that the spectrum of the density relaxation kernel in the mode-coupling approximation is given by the sum of two contributions,

$$M_\rho''(q,\omega)=M_{\rho_1}''(q,\omega)+M_{\rho_2}''(q,\omega)\;, \tag{3.16}$$

$$M_{\rho_i}''(q,\omega)=\frac{1}{32\pi^3nq\omega}\int_0^\infty dp\,p\int_{|q-p|}^{q+p}dk\,kV_i^2(k,p,q)\int_0^\omega\frac{d\omega'}{\pi}\chi_i''(p,\omega')\chi_i''(k,\omega-\omega')\;, \tag{3.17}$$

where the first, $i=1$, is due to decay into two density modes ($\chi_1=\chi_\rho$) while the second, $i=2$, reflects decay into two spin-density excitations ($\chi_2=\chi_\sigma$). On the other hand, the spectrum of the spin-density relaxation kernel is determined in mode-coupling approximation by the decay channel $\sigma\to\rho\sigma$, allowed by spin-rotation invariance

$$M_\sigma''(q,\omega)=\frac{1}{16\pi^3nq\omega}\int_0^\infty dp\,p\int_{|q-p|}^{q+p}dk\,kV_3^2(k,p,q)\int_0^\omega\frac{d\omega'}{\pi}\chi_\rho''(p,\omega')\chi_\sigma''(k,\omega-\omega')\;. \tag{3.18}$$

The vertex functions are

$$V_1=[\epsilon_\rho^0(q)+\epsilon_\rho^0(p)+\epsilon_\rho^0(k)]\times\left[\frac{q^2+p^2-k^2}{2q^2S_\rho(p)}+\frac{q^2+k^2-p^2}{2q^2S_\rho(k)}-1\right], \tag{3.19a}$$

$$V_2=[\epsilon_\rho^0(q)+\epsilon_\sigma^0(p)+\epsilon_\sigma^0(k)]\times\left[\frac{q^2+p^2-k^2}{2q^2S_\sigma(p)}+\frac{q^2+k^2-p^2}{2q^2S_\sigma(k)}-1\right], \tag{3.19b}$$

$$V_3=[\epsilon_\sigma^0(q)+\epsilon_\rho^0(p)+\epsilon_\sigma^0(k)]\times\left[\frac{q^2+p^2-k^2}{2q^2S_\rho(p)}+\frac{q^2+k^2-p^2}{2q^2S_\sigma(k)}-1\right]. \tag{3.19c}$$

The set of equations (2.12), (2.19), and (3.16)–(3.19) is a closed system of nonlinear coupled integral equations. Its self-consistent solution is described below.

IV. CALCULATION AND RESULTS

In an iterative procedure,[23,24] we evaluate the new spectra of the density ($A=\rho$) and the spin-density ($A=\sigma$) response functions

$$\chi_A''(q,\omega)=\frac{\omega M_A''(q,\omega)q^2/m}{[\omega^2-\Omega_A^2(q)+\omega M_a'(q,\omega)]^2+[\omega M_A''(q,\omega)]^2} \tag{4.1}$$

with the relaxation spectra $M_A''(q,\omega)$ [(3.16)–(3.18)] [obtained from the $\chi_A''(q,\omega)$ of the previous iteration] and the real parts $M_A'(q,\omega)$ obtained via the Kramers-Kronig relation (2.19). Instead of determining $\Omega_A^2(q)$ (2.13) from the old spectra $\chi_A''(q,\omega)$, we found it more convenient to choose $\Omega_A^2(q)$ at each iteration step such that the experimental equal-time structure factors $S_A(q)$ (2.30) were guaranteed by (4.1).

For $S_\rho(q)$ we used the experimental result of Achter and Meyer[17] and Hallock[18] while for $S_\sigma(q)$ we used the Monte Carlo result of Ceperely *et al.*[19] Note that besides the two functions $S_\rho(q)$ and $S_\sigma(q)$ shown in Fig. 1, the only other input into our theory is the density $n=1.634\times10^{22}\ \text{cm}^{-3}$ and the bare mass m of ^{3}He atoms.

The integrations were done using the standard Simpson method. We started the iteration procedure for solving the above-described set of nonlinearly coupled integral equations with $M_\rho(q,z)=0=M_\sigma(q,z)$. Then the spectral functions $\chi_A''(q,\omega)$ of the fifth iteration agreed with those of the fourth iteration within less than 5%. At this stage we added to the mode-coupling relaxation kernels [(3.16)–(3.18)] that one of an ideal Fermi gas of mass $m^*=3m$ to account for the free-gas relaxation of collective fluctuations. With the new kernels

$$M(q,z)=M(q,z)\,|_{\text{mode coupling}}+M_0(q,z)\;,$$

the iteration procedure was continued. While the density

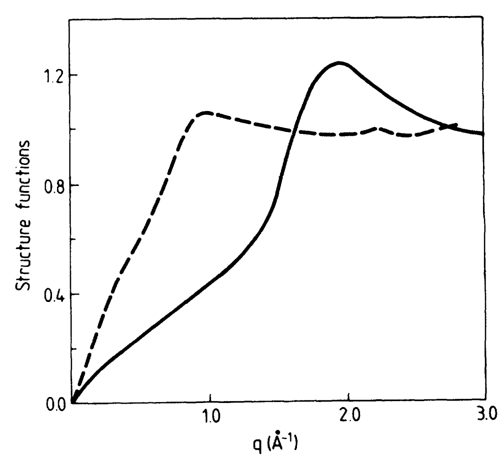

FIG. 1. Static structure factors of the particle-number density $S_\rho(q)$ (solid line) and of the spin density $S_\sigma(q)$ (dashed line).

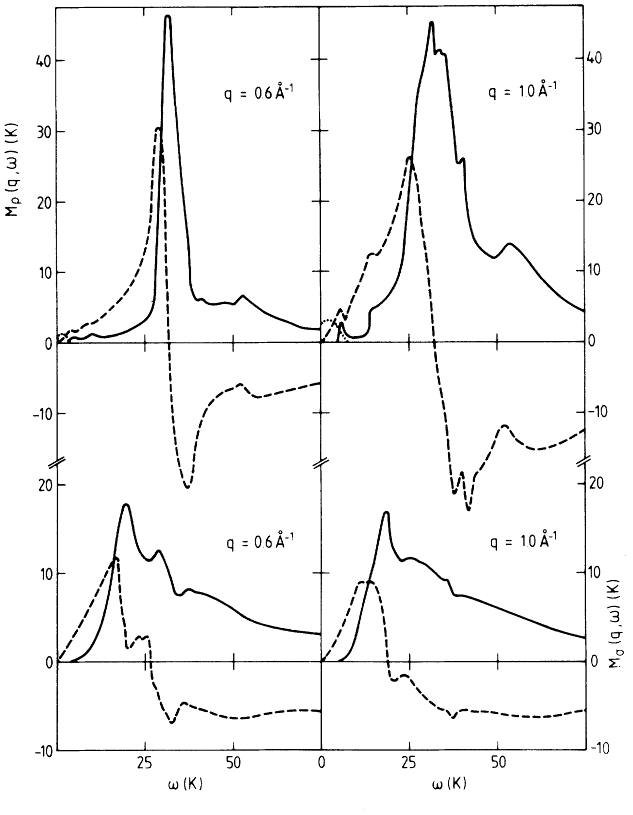

FIG. 2. Relaxation kernels of particle-number-density fluctuations $M_\rho(q,\omega)$ and of spin-density fluctuations $M_\sigma(q,\omega)$ for two representative wave numbers. Solid lines denote imaginary parts and dashed lines denote real parts of the mode-coupling contributions to $M_A(q,\omega)$ resulting from the last iteration. The relaxation spectra $M_0''(q,\omega)$ of the ideal Fermi gas of mass $m^*=3m$ are shown by dots.

fluctuation spectrum remained unchanged, another iteration was necessary to stabilize also the spin-density fluctuation spectrum to within an accuracy of better 5%.

The calculated mode-coupling contributions to the relaxation kernels $M_A(q,\omega)$ resulting from the last iteration are plotted in Fig. 2 for two representative wave numbers as functions of ω. The free-particle contributions to the relaxation kernels which are shown there as well are obviously very small compared to the mode-coupling part. The spectra of both kernels, $M_\rho''(q,\omega)$ and $M_\sigma''(q,\omega)$, increase first, attain a maximum, and finally fall off to zero for large ω with some minor superimposed structure. This behavior is dictated by the two-mode decay kinematics. The maximum in $M_\rho''(q,\omega)$, e.g., around $\omega\simeq 30$ K is due to decay into two density fluctuations of which each is localized in the ω-q plane in the region of maximal density of states around the maximum of the dispersion (at $\omega\simeq 15$ K, c.f. further below) where the slope of the dispersion vanishes.

Similarly, the maximum in the spin-density damping spectrum $M_\sigma''(q,\omega)$ at $\omega\simeq 20$ K is produced by decay into density fluctuations of energy $\omega\simeq 15$ K for which the available phase space is maximal, and into a spin-density fluctuation near $\omega\to 0$ for which also the density of states is maximal. Note that the decay spectrum $M_\sigma''(q,\omega)$ is overall smaller than $M_\rho''(q,\omega)$ since the $\rho\rho$ decay channels are not available for spin-density fluctuations.

As an aside we remark that one gains an easy, qualitative insight into the structure of the two-mode decay spectra [(3.17) and (3.18)] by replacing the spectra $\chi_A''(q,\omega)$ in the convolution integrals by δ functions centered at the corresponding dispersion $\chi_A''(q,\omega)\sim\delta[\omega-\epsilon_A(q)]$. Then, leaving the vertices aside, the decay spectra [(3.17) and (3.18)] measure two-mode density of states whose size is determined by one-mode density of states $[\partial\epsilon_A(k)/\partial k]^{-1}$ and phase-space kinematics due to momentum and energy conservation for the decay partners.

We found numerically that the decay of density fluctuations into two spin-density fluctuations, i.e., $M_{\rho_2}''(q,\omega)$, is negligible compared to the decay into two density fluctuations, i.e., $M_{\rho_1}''(q,\omega)$. The main reasons are that the vertex V_2 (3.19b) is small compared to the vertex V_1 (3.19a), and, in addition, the phase space for two density excitations is for the considered frequencies larger than that for two spin-density fluctuations. This blocking of the decay channel $\rho\to\sigma\sigma$ implies that number-density fluctuations are almost decoupled from spin-density fluctuations (but *not* vice versa).

Let us discuss now the spectral functions $\chi_\rho''(q,\omega)$ and $\chi_\sigma''(q,\omega)$ for number-density and spin-density fluctuations. They were obtained self-consistently within the mode-coupling approximation to the relaxation kernels $M_A(q,\omega)$ by the above-described iteration procedure. Figure 3 shows $\chi_\rho''(q,\omega)$ (solid curve) and $\chi_\sigma''(q,\omega)$ (dashed curve) for two representative wave numbers $q=0.6$ and 1.0 Å^{-1}. The sharp resonances denote zero-sound and spin-fluctuation excitations, respectively, with relative spectral strengths shown by precentages in the figure. In Fig. 3(b), $\chi_\rho''(q=1.0$ Å$^{-1},\omega)$ shows a peak below the zero-sound mode at the spin-density frequency $\omega=\epsilon_\sigma(q)$, but the associated spectral weight is negligible. For $q=0.6$ Å^{-1}, there is a shoulder at $\omega=\epsilon_\sigma(1)\simeq 4$ K.

The energy of the zero-sound mode is plotted in Fig. 4. In this figure the continuous curve marked 1 is the plot of $\epsilon_\rho^0(q)=q^2/[2mS_\rho(q)]$ obtained from the structure function given in Fig. 1. The solid curve at lower energy is the self-consistent result of the mode-coupling theory. The neutron scattering experimental data as reported by Sköld and Pelizzari[2] are shown by closed circles if the spin-fluctuation peak in the total cross section is fitted by a paramagnon model, and by closed squares if the spin-fluctuation peak is fitted by a free-Fermi-gas model. Open circles show the result obtained if the peak positions are estimated by eye.[2] The maximum difference between experimental peak position and our calculated values is less than 20%. Whereas the experimental dispersion of the zero-sound mode saturates around 0.7 Å^{-1}, the theoretical curve flattens at larger-q values. The relative spectral weight $f_\rho(q)$ of the zero-sound mode is shown in Fig. 4. The experimental values of $f_\rho(q)$ depend whether the spin-fluctuation peak is fitted by a paramagnon model (closed circle) or by the free-Fermi-gas model (closed square). Our theoretical results (solid curve) are closer to the latter.

The energy of the spin-fluctuation excitation $\epsilon_\sigma(q)$ and its spectral strength $f_\sigma(q)$ are plotted in Fig. 5. The values of $\epsilon_\sigma(q)$ as reported by Sköld and Pelizzari[2] are also shown by closed circles. Neutron scattering results for $f_\sigma(q)$ are

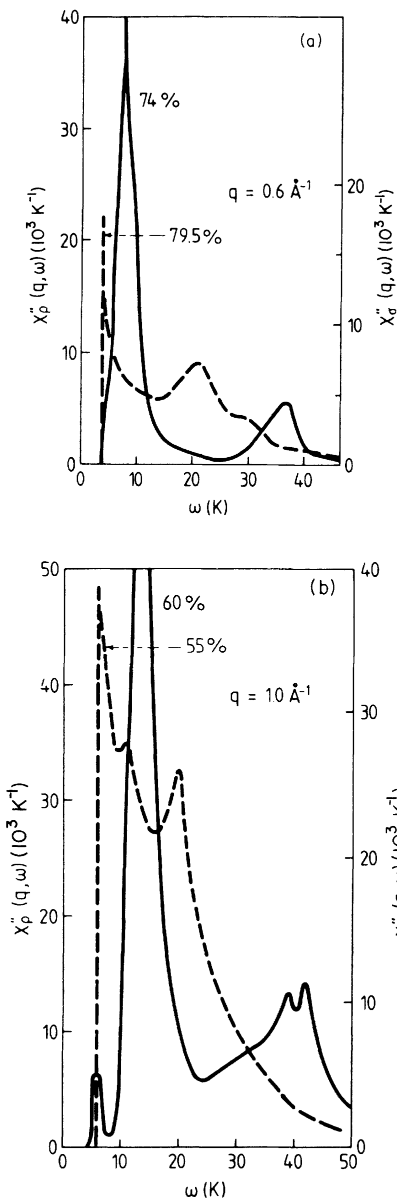

FIG. 3. Dynamic number-density and spin-density susceptibilities vs frequency for two representative wave numbers. Solid lines denote $\chi'_\rho(q,\omega)$, dashed lines denote $\chi''_\sigma(q,\omega)$. Percentages show the spectral strength of zero-sound and spin-fluctuation excitations.

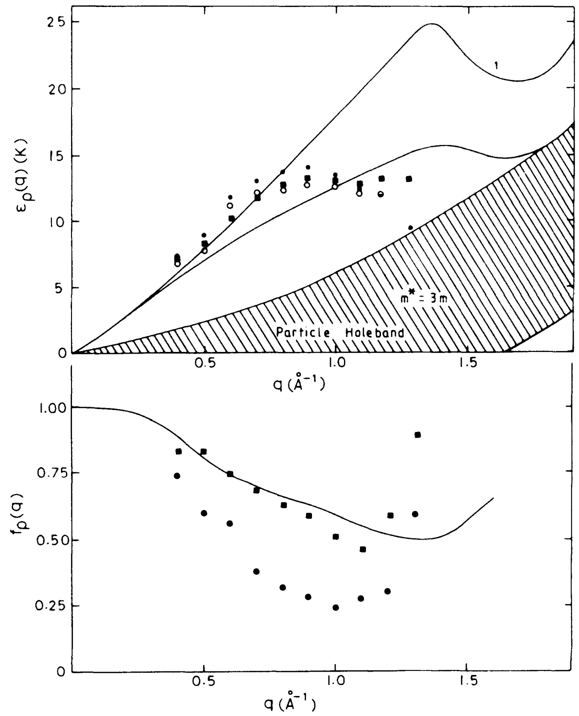

FIG. 4. Zero-sound energy $\epsilon_\rho(q)$ and its spectral strength $f_\rho(q)$ vs wave number. The upper curve marked 1 denotes $\epsilon_\rho^0(q)=q^2/(2mS_\rho(q))$. Experimental results as described in the text are shown by circles and squares.

not available for comparison.

Finally, the characteristic restoring forces $\Omega_A(q)$ (2.13) are plotted in Fig. 6. Note that so far no information was available about the static susceptibilities

$$\chi_A(q,z=0)=q^2/[m\Omega_A^2(q)] .$$

V. SUMMARY AND CONCLUSIONS

We have expressed the dynamic density and spin-density response functions for liquid ^{3}He within a dispersion-relation representation in terms of their static

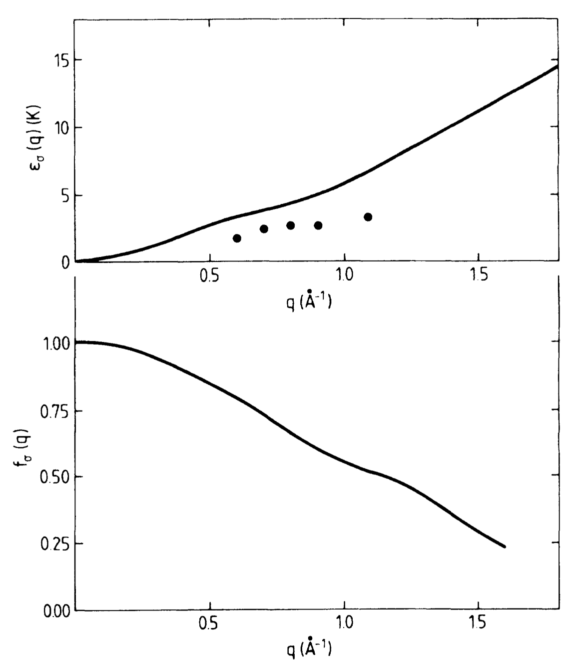

FIG. 5. Spin-fluctuation excitation energy $\epsilon_\sigma(q)$ and its strength $f_\sigma(q)$ vs wave number.

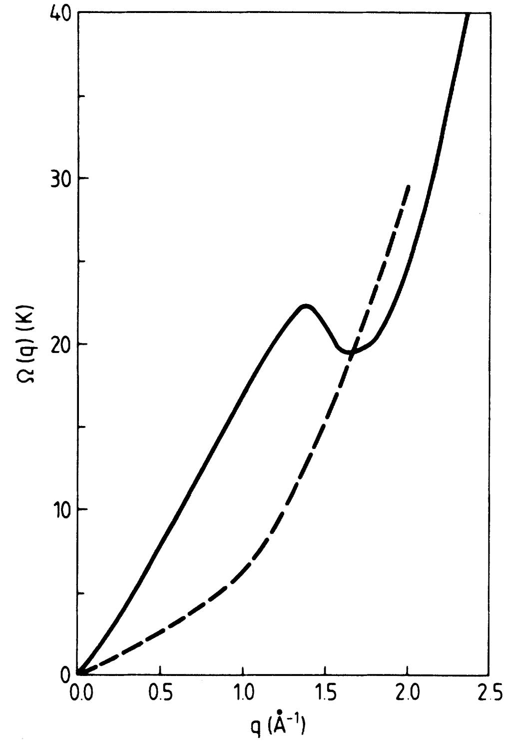

FIG. 6. Characteristic frequencies $\Omega_A(q)$ (2.13) corresponding to static susceptibilities $\chi_\rho(q)$ and $\chi_\sigma(q)$ vs wave number.

susceptibilities and two relaxation kernels. The dissipative parts of the complex kernels depending on frequency and wave number are approximated by two-mode decay processes, and the decay vertices are expressed in terms of structure functions. The real parts are evaluated via Kramers-Kronig relations.

It is found that density excitations can decay into two density modes and into two spin-fluctuation excitations. A spin-density fluctuation, on the other hand, is allowed by spin-rotation symmetry to decay only into a combination involving a density mode and a spin-fluctuation mode. The above approximation leads to two coupled nonlinear integral equations which have been solved by iteration and which determine in a self-consistent way the two dynamic susceptibilities. Owing to a small vertex decay of density fluctuations into two spin-fluctuation modes is negligible compared to decay into two density modes. Therefore, number-density fluctuations are practically decoupled from spin-density fluctuations. The relaxation mechanism of the latter, however, is determined by the decay coupling to two-mode excitations involving number-density fluctuations and spin-density fluctuations.

Our theory goes certainly beyond RPA. It needs as input only the static structure factors. In view of this fact, we consider the agreement with neutron scattering results to be good. In particular, we obtain well-defined density excitations for not too large wave numbers. Since an explicit coupling of zero-sound modes to multiparticle-hole excitations is not contained in our present framework, e.g., via a separate decay channel, we conclude that this coupling is small.

ACKNOWLEDGMENTS

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APPENDIX: DISPERSION-RELATION REPRESENTATION OF $\chi_A(q,z)$

Here we generate the dispersion-relation representation (2.12) of the dynamical susceptibilities $\chi_A(q,z)$ with Mori's projector formalism.[11] Taking matrix elements of the general resolvent identity

$$P(\mathscr{L}-z)^{-1}P[z-\mathscr{L}+Q(Q\mathscr{L}Q-z)^{-1}Q]P=-P \tag{A1}$$

between the "states" $A(\vec{q})$ (in our case $A=\rho$ or $A=\sigma$) onto which the projector

$$P=|A(\vec{q}))\frac{1}{\chi_A(q)}(A(\vec{q})| \tag{A2}$$

projects, we obtain

$$\phi_A(q,z)\left[z+\frac{1}{\chi_A(q)}(\mathscr{L}A(\vec{q})|(Q\mathscr{L}Q-z)^{-1}|\mathscr{L}A(\vec{q}))\right.$$
$$=-\chi_A(q)\ . \tag{A3}$$

Here $Q=1-P$ projects onto the orthogonal complement of $A(\vec{q})$ and

$$\chi_A(q)=\chi_A(q,z=0)=(A(\vec{q})|A(\vec{q})) \tag{A4}$$

normalizes $P=P^2$. In (A3) we made use of the orthogonality of $\mathscr{L}|A)$ and $|A)$.

Repeating the analogous procedure for the reduced resolvent $(Q\mathscr{L}Q-z)^{-1}$, one arrives at the formula

$$\phi_A(q,z)=-\chi_A(q)\left[z-\frac{\Omega_A^2(q)}{z+M_A(q,z)}\right]^{-1}. \tag{A5}$$

The characteristic frequency $\Omega_A(q)$ for fluctuations of the density $A(\vec{q})$ is given by

$$\Omega_A^2(q)=\frac{(A(\vec{q})|\mathscr{L}^2|A(\vec{q}))}{(A(\vec{q})|A(\vec{q}))}=\frac{q^2/m}{\chi_A(q)}, \tag{A6}$$

and the kernel

$$M_A(q,z)=\frac{m}{q^2}(Q\mathscr{L}^2A(q)|(\mathscr{L}'-z)^{-1}|Q\mathscr{L}^2A(\vec{q})) \tag{A7}$$

is the relaxation function of the anharmonic part of the generalized force $\mathscr{L}^2A(\vec{q})$ acting upon the density $A(\vec{q})$—the harmonic part being proportional to A itself is projected out by Q. The dynamics of the above force in (A7) is generated by the operator $\mathscr{L}'=Q'\mathscr{L}Q'$ which is restricted via the projector Q' to the subspace containing neither single-mode density fluctuations $\vec{A}(q)$ nor single-mode current fluctuations $\mathscr{L}A(\vec{q})$. From (A5) or even more directly from a comparison of (A7) with (2.16), one concludes that the relaxation kernel $M_A(q,z)$ has the same analytical properties as the relaxation function $\phi_A(q,z)$.

That leads, e.g., to a Cauchy representation

$$M_A(q,z)=\int_{-\infty}^{\infty}\frac{d\omega}{\pi}\frac{M_A''(q,\omega)}{\omega-z} \quad \text{(A8)}$$

with the spectral function

$$M_A''(q,\omega)=\pi\frac{m}{q^2}(Q\mathscr{L}^2A(\vec{q})\,|\,\delta(\omega-\mathscr{L}')\,|\,Q\mathscr{L}^2A(\vec{q})), \quad \text{(A9)}$$

which is even in ω and positive semidefinite as $\phi_A''(q,\omega)$ (2.23). The dispersion-relation representation (2.12) of the susceptibility $\chi_A(q,z)$ follows directly from (A5) and the definition (2.14) of Kubo's relaxation function $\phi_A(q,z)$.

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[1]D. Pines, in *Quantum Fluids,* edited by D. Brewer (North-Holland, Amsterdam, 1966), p. 257.

[2]K. Sköld, C. A. Pelizzari, R. Kleb, and G. E. Ostrowski, Phys. Rev. Lett. 37, 541 (1976); K. Sköld and C. A. Pelizzari, J. Phys. C 11, L589 (1978), and contribution to Roy. Soc. Discuss. Meeting Neutr. Scatt. in Biology, Chemistry, and Physics, London (unpublished).

[3]P. A. Hilton, R. A. Cowley, R. Scherm, and W. G. Stirling, J. Phys. C 13, L295 (1980).

[4]W. G. Stirling, R. Scherm, P. A. Hilton, and R. A. Cowley, J. Phys. C 9, 1643 (1976).

[5]H. R. Glyde and F. C. Khanna, Phys. Rev. Lett. 37, 1692 (1976); Can. J. Phys. 56, 1906 (1977).

[6]C. H. Aldrich III, C. J. Pethick, and D. Pines, Phys. Rev. Lett. 37, 845 (1976).

[7]C. H. Aldrich III and D. Pines, J. Low. Temp. Phys. 32, 689 (1979).

[8]F. Yoshida and F. Takeno, Prog. Theor. Phys. 62, 37 (1979).

[9]O. T. Valls, G. F. Mazenko, and H. Gould, Phys. Rev. B 18, 264 (1978); 25, 1663 (1982).

[10]D. N. Zubarev, Usp. Fiz. Nauk. 71, 71 (1960); [Sov. Phys.—Usp. 3, 320 (1960); P. C. Martin, in *Problème à N Corps,* edited by C. deWitt and R. Balin (Gordon and Breach, New York, 1968).

[11]H. Mori, Prog. Theor. Phys. 33, 423 (1965); 34, 399 (1965); R. Zwanzig, Phys. Rev. 124, 983 (1961).

[12]One may verify (Ref. 13) that (2.14) is the Laplace transform

$$\phi_A(q,z)=\pm i\int_{-\infty}^{\infty}dt\,\Theta(\pm t)e^{izt}\phi_A(q,t) \quad \text{for Im}z\gtrless 0$$

of

$$\phi_A(q,t)=\int_0^{\beta}d\lambda\langle\delta A^*(q,t)\delta A(q,i\lambda)\rangle\ .$$

[13]D. Forster, *Hydrodynamic Fluctuations, Broken Symmetry, and Correlation Functions* (Benjamin, Reading, Massachusetts, 1975).

[14]J. C. Wheatly, Rev. Mod. Phys. 47, 415 (1975).

[15]R. D. Puff, Phys. Rev. A 137, 423 (1965); E. Satir and A. Widom, J. Low Temp. Phys. 6, 397 (1972).

[16]N. Mihara and R. D. Puff, Phys. Rev. 174, 221 (1968); H. B. Singh, and K. N. Pathak, Phys. Rev. B 10, 2764 (1974).

[17]E. K. Achter and L. Meyer, Phys. Rev. 188, 291 (1969).

[18]R. Hallock, J. Low Temp. Phys. 9, 109 (1972).

[19]D. Ceperley, G. V. Chester, and M. H. Kalos, Phys. Rev. B 16, 3081 (1977).

[20]S. Takeno and F. Yoshida, Prog. Theor. Phys. 60, 1304 (1978).

[21]K. N. Pathak and V. K. Jindal, *Proceedings of the Nuclear Physics and Solid State Physics Symposium* (Bhabha Atomic Research Centre, Trambay, Bombay, India, 1979).

[22]M. T. Beal-Monod, J. Low. Temp. Phys. 37, 123 (1979).

[23]W. Götze and M. Lücke, Phys. Rev. B 13, 3825 (1976).

[24]M. Lücke, *Lecture Notes in Physics,* edited by A. Pekalski and J. Przystawa (Springer, Berlin, 1980), p. 74, Vol. 115.

[25]H. W. Jackson and E. Feenberg, Rev. Mod. Phys. 34, 686 (1962).