Dynamic structure function of a Bose gas at $T = 0$

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The dynamic structure function $\mathcal{S}(k,\omega)$, as a function of wave vector k and frequency ω, is calculated rigorously for a simple Bose gas at $T = 0$. The dielectric formulation is used to satisfy general symmetry requirements for a Bose system, and the calculation is carried out in the first approximation beyond Bogoliubov taking into account the three-phonon process. An analytic solution in terms of elliptic integrals is obtained for the width of $\mathcal{S}(k,\omega)$ valid for arbitrary k and ω. Qualitatively, $\mathcal{S}(k,\omega)$ at finite but small k is found to have a square-root behavior near the threshold frequency for two-phonon production, a peak at the elementary excitation frequency, and a long power-law tail at high frequencies. Illustrative numerical results are presented for the width of $\mathcal{S}(k,\omega)$, the imaginary part of the phonon spectrum, and $\mathcal{S}(k,\omega)$ itself. Finally, the impulse approximation and the extraction of the condensate density n_0 from $\mathcal{S}(k,\omega)$ in the large-k limit are discussed.

I. INTRODUCTION

Neutron scattering measurements[1,2] of superfluid ^{4}He have provided direct observation of the elementary excitations of the system, have demonstrated the existence of a vast region of multiexcitations at higher energies, and may provide direct evidence for Bose-Einstein condensation at still higher energies near the free-particle spectrum. Many theories[2] have been constructed in order to investigate the rich and largely unexplained structure of the multiexcitations. Unfortunately, these theories do not give unambiguous descriptions of the experimental results. Furthermore, no consistent microscopic analysis of the multiexcitations in Bose systems exists to our knowledge in the literature. Since the high-energy multiexcitations may reflect more of the microscopic structure of the system than the low-energy elementary excitations, it seems desirable that a microscopic analysis be carried out. In this paper we present a rigorous microscopic calculation of the dynamic structure of a simple Bose gas at zero temperature.[3] Although the results of such a study may not be directly applicable to superfluid ^{4}He, it may offer clues for improving existing phenomenological theories and aids for more ambitious microscopic calculations.

The basic reason for the dearth of consistent microscopic theories of the multiexcitation region resides in the inability of previous approximation schemes[4–6] to go beyond the quasiparticle (Bogoliubov) model without violating several general symmetry requirements. One such requirement follows from Bose condensation and rotation-translation invariance[3]: The discrete single-particle spectrum and the discrete density spectrum coincide. A second and closely related requirement can be derived[6,7] by an application of global gauge invariance onto the Bose condensed state: The long-wavelength limit of the single-particle spectrum is gapless.[5] A third requirement, which is not restricted to Bose systems, arises from local gauge invariance: Local particle number is conserved; i.e., the continuity equation and related sum rules hold.[3] Recently, these symmetry requirements have been successfully incorporated into a microscopic theory of Bose systems in I,[3] where a dielectric formulation was used to build in the exact requirements *before* any approximation scheme was attempted.

To be more explicit, let us adopt throughout this paper the notation used in I. Consider the density response function $\mathcal{F}(k, \omega)$, which is given by

$$\mathcal{F} = F/(1 - vF) = F/\epsilon \ . \tag{1.1}$$

Here the irreducible density correlation function $F(k, \omega)$ is defined as the contributions of all diagrams with no isolated interaction line, $v(k)$ is the interparticle potential, and $\epsilon(k, \omega)$ is the dielectric function. The first general requirement is built into the theory by using a diagrammatic analysis to write the denominators of the single-particle, density, and longitudinal-current response functions (the zero-helicity response functions in I) in terms of the dielectric function $\epsilon(k, \omega)$ multiplied by nonsingular factors. This is true for Bose systems irrespective of the form of v. Hence the various discrete zero-helicity spectra coincide into the elementary excitation spectrum, which can be found by setting $\epsilon(k, \omega) = 0$. The chemical potential μ in the single-particle response function $\mathcal{G}_{\lambda\sigma}$ is determined by the Hugenholtz-Pines relation[5]; hence the second requirement is fulfilled. To incorporate local number conservation, we use the generalized

Ward identities which are derived from the continuity equation, e.g.,

$$\omega^2 F = k^2(F^{zz} + n/m) , \qquad (1.2)$$

where F^{zz} is the irreducible longitudinal-current correlation function, $\vec{k}$ is along the z axis, n is the density, and m is the particle mass. Substituting (1.2) into (1.1), we express $\mathfrak{F}$ in terms of the longitudinal-current correlation function

$$\mathfrak{F} = \frac{nk^2}{m}\left[\omega^2 \bigg/ \left(1 + \frac{m}{n}F^{zz}\right) - \frac{nv}{m}k^2\right]^{-1} . \qquad (1.3)$$

Note that (1.3) follows directly from the definition (1.1) and Eq. (1.2), which is simply a consequence of the continuity equation. Thus, (1.3) is independent of the particles' statistics. However, the following application of (1.3) is valid only for Bose statistics. One desirable feature of (1.3) in this case is that at small k the elementary excitation spectrum ω_k is seen to be linear in k for a short-ranged $v(k)$ and is given by

$$(\omega_k/k)^2 \equiv c^2 = nv/m + vF^{zz}(k, ck) . \qquad (1.4)$$

It is well known[1] that the linear response of a system to a density probe like neutron scattering can be given in terms of the dynamic structure function $\mathcal{S}(k, \omega)$ defined as

$$\mathcal{S}(k, \omega) = -(1/\pi)\mathrm{Im}\,\mathfrak{F}(k, \omega), \quad \omega \geqslant 0 . \qquad (1.5)$$

Applying (1.5) to (1.3), we obtain the exact expression

$$\mathcal{S}(k, \omega) = \frac{\omega^2 k^2 S^{zz}}{|\,\omega^2 - (nv/m)k^2 - vk^2 F^{zz}|^2} , \qquad (1.6)$$

$$S^{zz}(k, \omega) = -(1/\pi)\mathrm{Im}\,F^{zz}(k, \omega), \quad \omega \geqslant 0 , \qquad (1.7)$$

which is valid for either Bose or Fermi systems.[7]

In this paper we present a rigorous microscopic analysis of $\mathcal{S}(k, \omega)$ using (1.6) in a simple Bose gas to the first approximation in which multiexcitations appear. In Sec. II, we evaluate $\mathcal{S}(k, \omega)$ in the zeroth (Bogoliubov) approximation and develop a perturbation expansion for $\mathcal{S}(k, \omega)$. The first-order calculation beyond Bogoliubov of $\mathcal{S}(k, \omega)$ is carried out in Sec. III. The behavior of $\mathcal{S}(k, \omega)$ near the threshold and in the long-wavelength limit is examined. An analytic solution in terms of elliptic integrals is obtained for the width of $\mathcal{S}(k, \omega)$ for arbitrary k and ω. Numerical results calculated from the analytic solution are presented for the width of $\mathcal{S}(k, \omega)$, the imaginary part of the elementary excitation spectrum ω_k, and $\mathcal{S}(k, \omega)$ itself. The large-k limit of $\mathcal{S}(k, \omega)$ is examined with emphasis on the condensate contribution. Finally we discuss some of the qualitative features of $\mathcal{S}(k, \omega)$ and consider their applicability to superfluid ^{4}He.

II. PERTURBATION EXPANSION FOR $\mathcal{S}(k,\omega)$

Perturbation expansions for the response functions, e.g., $\mathfrak{F}$ and $\mathcal{G}_{\lambda\sigma}$, have been developed in I. The dynamic structure function $\mathcal{S}$ was obtained in I from the expanded $\mathfrak{F}$ by the use of (1.5). In the present work we reverse the order and take (1.5) first, resulting in the exact expression (1.6) for $\mathcal{S}$, and then develop a perturbation expansion for the irreducible F^{zz} in (1.6). The limitations of the perturbation expansion in I will, from this point of view, become evident.

A. Zeroth (Bogoliubov) approximation

It is instructive to evaluate the general form (1.6) in the zeroth approximation of a Bose system. A distinctive feature of a Bose system is that the irreducible F^{zz} in (1.6) can be written [I (2.25)] in terms of regular functions

$$F^{zz} = \Lambda^z_\mu G_{\mu\nu} \Lambda^z_\nu + F^{zzr} , \qquad (2.1)$$

where Λ^z_μ is the longitudinal-current vertex and F^{zzr} is the regular longitudinal-current correlation function. Here the irreducible Green's function $G_{\mu\nu}$ satisfies the Dyson equation $G^{-1}_{\mu\nu} = G^{(0)-1}_{\mu\nu} - M_{\mu\nu}$, where $G^{(0)}_{\mu\nu}$ is the noninteracting Green's function and $M_{\mu\nu}$ is the irreducible self-energy. The zeroth order is defined by $\Lambda^z_\mu = n_0^{1/2}(k/2m)\beta_\mu$, $F^{zzr} = 0$, and $M_{\pm\pm} - \mu = M_{\pm\mp} = 0$, where $\beta_\mu = \mathrm{sgn}\mu$ and n_0 is the condensate density. Using these relations in (2.1) and (1.7), we obtain

$$F^{zz}(k, \omega) = (n/m)\epsilon_k^2(\omega^2 - \epsilon_k^2 + i\eta)^{-1} + O(v) , \qquad (2.2)$$

where $\eta = 0_+$, and

$$S^{zz}(k, \omega) = (n/m)\epsilon_k^2 \delta(\omega^2 - \epsilon_k^2) + O(v) , \qquad (2.3)$$

where $\epsilon_k = k^2/2m$. Substituting (2.2) and (2.3) into (1.6), we find

$$\mathcal{S}(k, \omega) = \frac{1}{\pi v}(\omega^2 - \epsilon_k^2)\frac{\overline{\eta}}{(\omega^2 - \omega_k^{2(0)})^2 + \overline{\eta}^2} , \qquad (2.4)$$

where $\overline{\eta}$ is $O(v)$ and $\omega_k^{(0)}$ is the Bogoliubov spectrum

$$\omega_k^{(0)} = [(nv/m)k^2 + \epsilon_k^2]^{1/2} . \qquad (2.5)$$

In the limit $\overline{\eta} \to 0$ in (2.4), we obtain the well-known result

$$\mathcal{S}(k, \omega) = n(k^2/2m\omega_k^{(0)})\delta(\omega - \omega_k^{(0)}) . \qquad (2.6)$$

Note that to zeroth order there is no depletion, i.e., $n = n_0$, and that the highly singular nature of S^{zz} in (2.3) produces no width and no continuum multiexcitations in (2.6). In higher-order approximations, there exist depletion and a less singular $S^{zz}(k, \omega)$, which is expected to lead to a width and to multiexcitations.

To prepare for higher-order approximations, we specialize these results to a simple model of a Bose gas in which the short-range interparticle potential $v(k)$ can be summarized by the s-wave scattering length a. In zeroth order the natural units for this simple Bose gas are ($\hbar = 1$) $k_0 = ms_0 = (4\pi na)^{1/2}$ for the momentum and $T_0 = ms_0^2 = k_0^2/m$

$=4\pi na/m$ for the energy. The small dimensionless coupling constant is $g=4\pi ak_0=(4\pi a)^{3/2}n^{1/2}$. It is convenient to measure momentum and energy in units of k_0 and T_0; in these dimensionless natural units $g=4\pi a=n^{-1}$ and $k_0=T_0=m=s_0=1$. Our zeroth-order results then become

$$g\,\mathcal{S}(k,\omega)=(k^2/2\omega_k^{(0)})\delta(\omega-\omega_k^{(0)}) , \qquad (2.7a)$$

$$\omega_k^{2(0)}=k^2(1+\tfrac{1}{4}k^2) . \qquad (2.7b)$$

Hereafter we shall restrict the calculation to this model.

B. First approximation beyond Bogoliubov

To go beyond Bogoliubov, we develop a perturbation expansion for the basic quantity in the exact expression (1.6) for $\mathcal{S}$, viz., the irreducible longitudinal-current correlation F^{zz}. Since F^{zz} satisfies (2.1), we expand formally the regular functions (Λ_μ^z, $G_{\mu\nu}$, F^{zzr}) in (2.1) to first order in g, collect the $O(g)$ terms, and write the result in the form

$$gF^{zz}=F^{zz(0)}+gF^{zz(1)}+O(g^2) , \qquad (2.8)$$

where $F^{zz(0)}$ is given in (2.2). Substituting (2.8) and (2.2) into (1.6), we obtain $\mathcal{S}(k,\omega)$ in the form

$$g\,\mathcal{S}(k,\omega) =\frac{1}{\pi}k^2\frac{-g\omega^{-2}\mathfrak{N}_I^{zz(1)}}{(\omega^2-\omega_k^{2(0)}-g\omega^{-2}\mathfrak{N}_R^{zz(1)})^2+(-g\omega^{-2}\mathfrak{N}_I^{zz(1)})^2} , \qquad (2.9)$$

where $\mathfrak{N}_R^{zz}\equiv \mathrm{Re}\,\mathfrak{N}^{zz}$, $\mathfrak{N}_I^{zz}\equiv\mathrm{Im}\,\mathfrak{N}^{zz}$,

$$\mathfrak{N}^{zz(1)}\equiv(\omega^2-\epsilon_k^2)^2F^{zz(1)}+\omega^2k^2v^{(1)} , \qquad (2.10)$$

and $v^{(1)}$ is defined by the expression $v/g=1+gv^{(1)}+O(g^2)$. Loosely speaking, $g\mathfrak{N}_I^{zz(1)}$ may be referred to as the width of $\mathcal{S}(k,\omega)$. In particular, when $g\to 0$ (2.9) reduced to (2.7). Since we have included in (2.9) only the effects of the $O(g)$ term $F^{zz(1)}$, we refer to (2.9) as the $O(g)$ expression for $\mathcal{S}(k,\omega)$, even though infinite-order terms are included via the denominator.

In I, the expression (2.9) is effectively further expanded in powers of g, resulting in a separation into a discrete contribution, proportional to a δ function at $\mathrm{Re}\,\omega_k$, and a continuum contribution that forms the background. Such a separation was found to be useful in investigating the structure functions $\mathcal{S}_m(k)=\int_0^\infty d\omega\,\omega^m\,\mathcal{S}(k,\omega)$ at small k and in giving an interpretation to each contribution to $\mathcal{S}_m(k)$. Caution must be exercised, however, in the use of such a separation of $\mathcal{S}(k,\omega)$ for ω near $\omega_k^{(0)}$. For example, in the continuum contribution one finds a divergence proportional to $(\omega-\omega_k^{(0)})^{-2}$, which is clearly a result of the expansion of (2.9) in powers of g. In this paper we avoid such divergences by using directly the expression (2.9) to calculate $\mathcal{S}(k,\omega)$ for arbitrary k and ω.

As is easily seen Eqs. (1.5) and (2.9) imply that to $O(g)$ the location of the physical pole of $\mathcal{S}(k,\omega)$, i.e., the elementary excitation spectrum ω_k, is given by

$$\mathrm{Re}\,\omega_k=\omega_k^{(0)}+\tfrac{1}{2}g(\omega_k^{(0)})^{-3}\mathfrak{N}_R^{zz(1)}(k,\omega_k^{(0)}) , \qquad (2.11a)$$

$$\mathrm{Im}\,\omega_k=\tfrac{1}{2}g(\omega_k^{(0)})^{-3}\mathfrak{N}_I^{zz(1)}(k,\omega_k^{(0)}) , \qquad (2.11b)$$

which can be shown to be consistent with (1.4). For brevity's sake, we shall refer to ω_k as the phonon spectrum and the elementary excitation as a phonon. As we shall see, however, (2.11) does not imply that (2.9) is in fact, a Lorentzian; (2.11) merely gives information about the peak in $\mathcal{S}(k,\omega)$. Further information on $\mathcal{S}(k,\omega)$ must come from a detailed analysis of (2.9), in particular the width $g\omega^{-2}\mathfrak{N}_I^{zz(1)}(k,\omega)$.

The $O(g)$ diagrams that contribute to $F^{zz(1)}$ in (2.8) (see I, Fig. 6) include the process in which one phonon decays into two phonons and the inverse process in which two phonons coalesce into one. In other words, the first approximation beyond Bogoliubov takes into account the three-phonon process, but not the four-phonon process. The basic effect of the three-phonon process is to introduce a continuum contribution to $\mathcal{S}(k,\omega)$ and thus new features that cannot be described at all within the zeroth order. The four-phonon process will modify these features but is not expected to introduce qualitatively different features. Hence the present first-order calculation can be considered germane to the understanding of the qualitative features of $\mathcal{S}(k,\omega)$ of a Bose system.

III. FIRST-ORDER CALCULATION

In this section we shall evaluate $\mathcal{S}(k,\omega)$ to $O(g)$, given by (2.9). We first consider in Sec. III A the behavior of $\mathcal{S}(k,\omega)$ near the threshold for two-phonon production. In Sec. III B we investigate the behavior of $\mathcal{S}(k,\omega)$ in the long-wavelength limit. The analytic solution in terms of elliptic integrals is outlined for $\mathfrak{N}_I^{zz(1)}(k,\omega)$ in Sec. III C, and numerical results based on the analytic solution are also presented. The large-wave-vector limit of $\mathcal{S}(k,\omega)$ is examined in Sec. III D, and a discussion of the qualitative features of $\mathcal{S}(k,\omega)$ follows in Sec. III E.

A. Threshold behavior of $\mathcal{S}(k,\omega)$

Since the phonon spectrum $\omega_k^{(0)}$ possesses positive curvature, the decay of a phonon into two or more phonons is kinematically allowed. As decay processes into three or more phonons are higher than $O(g)$, within the present approximation scheme, it is obvious that $g\,\mathcal{S}(k,\omega)$ is equal to zero for $\omega<\omega_k^{\mathrm{th}}$, where the two-phonon production threshold is given by

$$\omega_k^{\mathrm{th}}=2\omega_{k/2}^{(0)}=k(1+\tfrac{1}{16}k^2)^{1/2} . \qquad (3.1)$$

We now show that $g\mathcal{S}(k,\omega)$ rises as $(\omega-\omega_k^{\rm th})^{1/2}$ as ω is increased from $\omega_k^{\rm th}$ at any fixed k.

Equation (2.9) implies that for $\omega\approx\omega_k^{\rm th}$, $\mathcal{S}(k,\omega)$ is given by

$$g\mathcal{S}(k,\omega)=-(k^2/\pi)(g/\omega^2)\mathfrak{N}_I^{zz(1)}(k,\omega)\times(\omega^2-\omega_k^{(0)2})^{-2}+O(g^2)\ . \qquad (3.2)$$

[Note that (3.2) is precisely the continuum contribution given in I (4.40).] Thus we must calculate $\mathfrak{N}_I^{zz(1)}(k,\omega)$, whose integral definition is given in Appendix A in the form

$$\mathfrak{N}_I^{zz(1)}(k,\omega)=\int d^3p\, f(\vec{p},\vec{k};\omega)\times\delta(\omega-\omega_{|\vec{p}-\vec{k}/2|}-\omega_{|\vec{p}+\vec{k}/2|})\ , \qquad (3.3)$$

where $f(\vec{p},\vec{k};\omega)$ is a complicated but smooth function of $\vec{p}$, $\vec{k}$, and ω. If we carry out the trivial angular integration and make a coordinate transformation from $(p,\vec{p}\cdot\vec{k})$ to (λ,η) defined by

$$(\lambda,\eta)=(|\vec{p}-\tfrac{1}{2}\vec{k}|,\ |\vec{p}+\tfrac{1}{2}\vec{k}|)\ , \qquad (3.4a)$$

$$(p^2,\vec{p}\cdot\vec{k})=(\tfrac{1}{2}(\lambda^2+\eta^2-\tfrac{1}{2}k^2),\ \tfrac{1}{2}(\eta^2-\lambda^2))\ , \qquad (3.4b)$$

then we have

$$\mathfrak{N}_I^{zz(1)}=\frac{2\pi}{k}\int_{\eta_-}^{\eta_+}\eta\,d\eta\int_0^\infty\lambda\,d\lambda\, f(k,\omega;\eta,\lambda)\times\delta(\omega-\omega_\lambda^{(0)}-\omega_\eta^{(0)})\ , \qquad (3.5)$$

where the limits of integration $\eta_\pm$ are given by

$$\eta_\pm=|x\pm\tfrac{1}{2}k| \qquad (3.6a)$$

and $x>0$ is a solution of

$$\omega=\omega_{x+k/2}^{(0)}+\omega_{x-k/2}^{(0)}\ . \qquad (3.6b)$$

Remarkably, (3.6b) simplifies to a third-degree equation in x^2:

$$x^6+x^4\left[4\left(1+\frac{k^2}{8}\right)-\frac{\omega^2}{k^2}\right]+4x^2\left[\left(1+\frac{k^2}{8}\right)^2-\frac{\omega^2}{k^2}\left(1+\frac{3k^2}{8}\right)\right]+\frac{\omega^2}{k^2}(\omega^2-\omega_k^{\rm th2})=0\ . \qquad (3.6c)$$

Thus far, the calculation for $\mathfrak{N}_I^{zz(1)}$ has been completely general; we now focus on $\omega\approx\omega_k^{\rm th}$, in which case the solution of Eq. (3.6c) satisfies $x\ll\frac{1}{2}k$. Thus we may neglect the first two terms of Eq. (3.6c), obtaining

$$x\approx\frac{2}{k^2}\left(\frac{2(\omega_k^{\rm th})^3}{3+\frac{1}{8}k^2}(\omega-\omega_k^{\rm th})\right)^{1/2}\ . \qquad (3.7)$$

Then after carrying out the trivial integrations in Eq. (3.5), we obtain

$$\mathfrak{N}_I^{zz(1)}\approx\frac{2\pi f(k,\omega_k^{\rm th};\frac{1}{2}k,\frac{1}{2}k)}{(1+\frac{1}{8}k^2)k^2}\left(\frac{2(\omega_k^{\rm th})^5}{3+\frac{1}{8}k^2}(\omega-\omega_k^{\rm th})\right)^{1/2}\ . \qquad (3.8)$$

Substituting (3.8) into (3.2), we see that $\mathcal{S}(k,\omega)$ is proportional to $(\omega-\omega_k^{\rm th})^{1/2}$ at any fixed k, which is confirmed by the explicit numerical calculations to be presented later.

We remark that the above square-root behavior can be obtained more generally, i.e., outside the limitations imposed by the simple model of a Bose gas. If the zeroth-order phonon spectrum $\omega_k^{(0)}$ is replaced by ω_k, an arbitrary phonon spectrum having positive curvature at momentum $\frac{1}{2}k$, then a simple expansion of Eq. (3.6b) to $O(x^2)$ allows evaluation of integrals of the type Eq. (3.3) in the form

$$\mathfrak{N}_I^{zz(1)}=\frac{\pi k f}{|\dot\omega_{k/2}|(\ddot\omega_{k/2})^{1/2}}(\omega-\omega_k^{\rm th})^{1/2}\ , \qquad (3.9)$$

where $\dot\omega_{k/2}\equiv(\partial\omega_q/\partial q)_{q=k/2}$. Thus a system with a well-defined phonon spectrum with positive curvature is expected to exhibit in $\mathcal{S}(k,\omega)$ a square-root dependence on ω near the two-phonon threshold at any fixed k.

B. Long-wavelength behavior of $\mathcal{S}(k,\omega)$

Another region in which it is comparatively simple to find an analytic solution for $\mathcal{S}(k,\omega)$ is the long-wavelength region $\omega_k^{(0)}\ll\omega$, where (2.9) reduces to

$$g\mathcal{S}(k,\omega)=-(k^2/\pi\omega^6)g\mathfrak{N}_I^{zz(1)}(k,\omega)+O(g^2)\ , \qquad (3.10)$$

and $\mathfrak{N}_I^{zz(1)}$ can be determined from (3.5) and (3.6). In the $k\ll\omega$ region, Eq. (3.6c) becomes

$$x^4+4x^2-\omega^2=0\ , \qquad (3.11)$$

which has a solution

$$x=[(\omega^2+4)^{1/2}-2]^{1/2}\ \text{ or }\ \omega=2\omega_x^{(0)}\ . \qquad (3.12)$$

Performing the trivial integrations of (3.5) then yields

$$\mathfrak{N}_I^{zz(1)}(k,\omega)=[2\pi\omega x/(\omega^2+4)^{1/2}]f(k,\omega;x,x)\ . \qquad (3.13)$$

Extracting the function f from the integrals of Appendix A and using (3.10), we obtain $\mathcal{S}(k,\omega)$ in the long-wavelength region, i.e., $k/\omega\ll1$, $\omega_k^{(0)}/\omega\ll1$,

$$\mathcal{S}(k,\omega)=\frac{7k^4}{120\pi^2}\frac{[(\omega^2+4)^{1/2}-2]^{5/2}}{\omega^5(\omega^2+4)^{1/2}}\ . \qquad (3.14)$$

In making the approximation $k\ll\omega$, we have lost all information about the threshold behavior of $\mathcal{S}(k,\omega)$. In fact, Eq. (3.14) taken at face value for all ω's shows a finite maximum at $\omega=0$. As ω increases, $\mathcal{S}(k,\omega)$ decreases initially as ω^2 and then at high frequencies as $\omega^{-7/2}$. Clearly, $\mathcal{S}(k,\omega)$ does not behave as a Lorentzian, and can be interpreted as the continuum contribution due to multiphonons.

The ω moments of (3.14) are easily found, and, together with the discrete δ-function contribution in I, the f sum rule is found to be satisfied. In the limit $\omega\to\infty$ Eq. (3.14) reduces to

$$\mathcal{S}(k,\omega)=(7/120\pi^2)k^4\omega^{-7/2}\ , \qquad (3.15)$$

which agrees with that found in I. In this form, the long tail of $\mathcal{S}(k, \omega)$ is conspicuous and the divergence of $\mathcal{S}_m(k)$ for $m \geq 3$ is easily seen. As mentioned in I, this divergence arises from the constant potential v assumed in our model and a large ω cutoff of the order of the inverse time of collision would arise in a more realistic model.

C. Analytic solution for $\mathfrak{N}_I^{zz(1)}(k,\omega)$ and numerical results

Here we sketch how $\mathfrak{N}_I^{zz(1)}(k, \omega)$ for arbitrary k and ω can be evaluated analytically in terms of elliptic integrals. The resulting expression is then used in a numerical calculation of $\mathfrak{N}_I^{zz(1)}(k, \omega)$, $\mathrm{Im}\,\omega_k$, and $\mathcal{S}(k, \omega)$.

In order to carry out the integration indicated in Eq. (3.5), we transform variables from (λ, η) to (ζ, ξ) given by

$$(\zeta, \xi) = (\omega_\lambda^{(0)}, \omega_\eta^{(0)}) . \tag{3.16}$$

After carrying out the (trivial) integration over ζ (involving the δ function), we are led to the following expression for $\mathfrak{N}_I^{zz(1)}(k, \omega)$:

$$\mathfrak{N}_I^{zz(1)}(k, \omega) = \frac{2\pi}{k} \int_{\xi_-}^{\xi_+} d\xi \, \frac{\xi(\omega - \xi) f((\omega - \xi), \xi; k, \omega)}{\{(1+\xi^2)[1+(\xi-\omega)^2]\}^{1/2}} , \tag{3.17}$$

where the integration limits are

$$\xi_\pm = \omega_{\eta_\pm}^{(0)} , \tag{3.18}$$

with $\eta_\pm$ given by Eq. (3.6). As f [which may be extracted from the integrands listed in Appendix A and (3.3)] is a sufficiently simple function of ξ, $(1+\xi^2)^{1/2}$, and $[1+(\xi-\omega)^2]^{1/2}$, Eq. (3.17) may be expressed exactly in terms of elliptic integrals.[8] This calculation outlined is straightforward but tedious, and the resulting expressions are listed in Appendix B.

Having obtained an analytic expression for $\mathfrak{N}_I^{zz(1)}(k, \omega)$, we proceed to evaluate numerically $\mathfrak{N}_I^{zz}(k, \omega)$, $\mathrm{Im}\,\omega_k$, and $\mathcal{S}(k, \omega)$. In Fig. 1 $\mathfrak{N}_I^{zz(1)}(k, \omega)$ is plotted at $k = 1.0$ as a function of ω extending from ω_k^{th} through $\omega_k^{(0)}$. Two prominent features are

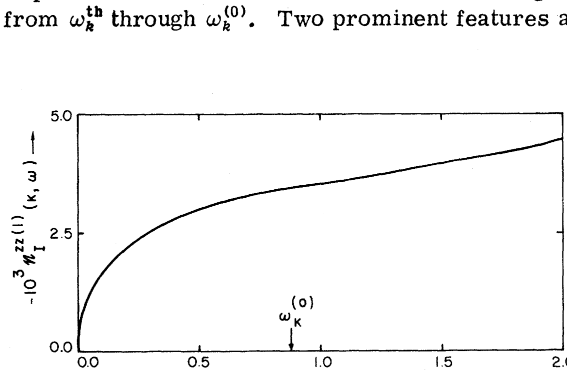

FIG. 1. Threshold behavior of $\mathfrak{N}_I^{zz(1)}(k, \omega)$ at $k=1.0$, for ω from the threshold ω_k^{th} through $\omega_k^{(0)}$.

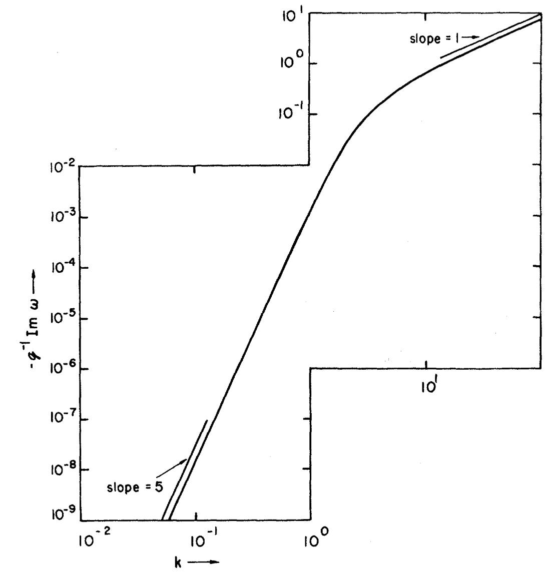

FIG. 2. Imaginary part of the spectrum $-g^{-1}\,\mathrm{Im}\,\omega_k$ as a function of k on a log-log scale.

the square-root behavior near the threshold frequency and, in contrast to I, the absence of any divergence at the zeroth-order spectrum $\omega_k^{(0)}$. This latter feature is an indication of the consistency of the present perturbation expansion.

Evaluating $\mathfrak{N}_I^{zz(1)}(k, \omega)$ at $\omega = \omega_k^{(0)}$ yields via (2.11b) the imaginary part of the phonon spectrum, which is plotted in Fig. 2. At long wavelengths, $\mathrm{Im}\,\omega_k$ displays the well-known k^5 dependence[3,4]; at short wavelengths, $\mathrm{Im}\,\omega_k$ bends over to a linear k dependence.[4] Quantitatively, the numerical result for $k<1$ verifies the long-wavelength expansion for $\mathrm{Im}\,\omega_k$ found in I, Eq. (C.5). More structure is of course expected in the model-dependent intermediate-k region if a more complicated interparticle potential is used in the calculation.

To calculate $\mathcal{S}(k, \omega)$ from (2.9), we need to know the function $\mathfrak{N}_R^{zz(1)}(k, \omega)$ as well as $\mathfrak{N}_I^{zz(1)}(k, \omega)$. Since $\mathfrak{N}_R^{zz(1)}$ appears in the denominator, it contributes significantly only for ω near the pole of $\mathcal{S}(k, \omega)$ and gives $O(g^2)$ corrections at the threshold or in the high-frequency region. Hence we can approximate $\omega^{-2}\mathfrak{N}_R^{zz(1)}(k, \omega)$ in (2.9) by $(\omega_k^{(0)})^{-2}\mathfrak{N}_R^{zz(1)}(k, \omega_k^{(0)})$ and write

$$g\mathcal{S}(k, \omega) = \frac{1}{\pi} k^2 \frac{-g\omega^{-2}\mathfrak{N}_I^{zz(1)}(k, \omega)}{[\omega^2 - (\mathrm{Re}\,\omega_k)^2]^2 + [-g\omega^{-2}\mathfrak{N}_I^{zz(1)}(k, \omega)]^2} , \tag{3.19}$$

where $\mathrm{Re}\,\omega_k$ is given by (2.11a). For small k, $\mathrm{Re}\,\omega_k$ has been evaluated in I. Using the analytic expressions for $\mathfrak{N}_I^{zz(1)}(k, \omega)$, we have evaluated numerically $\mathcal{S}(k, \omega)$ for $g = 0.1$ and $k = 0.1$ as a function of ω, which is plotted in Fig. 3. The square-

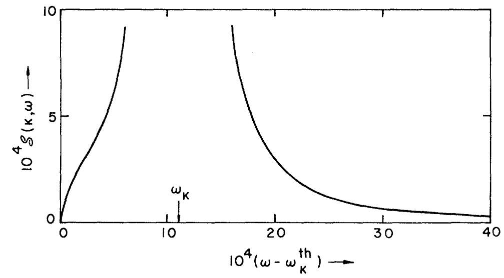

FIG. 3. Dynamic structure function $S(k,\omega)$ at $k=0.1$, $g=0.1$ for ω from the threshold ω_k^{th} through the peak at $\mathrm{Re}\,\omega_k$ into the long-tail region.

root behavior near the threshold $\omega=\omega_k^{th}$, the strong peak at $\omega=\mathrm{Re}\,\omega_k$, and the long tail at high frequencies are clearly seen. Note that the ω dependence is not Lorentzian nor even symmetrical about the peak at $\mathrm{Re}\,\omega_k$, and that the multiphonon contribution to $S(k,\omega)$ gives rise to a continuum.

D. Large-wave-vector limit of $S(k,\omega)$

The large-k limit of $S(k,\omega)$ is of interest mainly because of the possibility that the condensate density n_0 can be deduced from the measured $S(k,\omega)$ in superfluid ^{4}He. The usual impulse approximation[9] corresponds to letting $k\to\infty$, in which limit the condensate density n_0 shows up as the area under a sharp peak in $S(k,\omega)$, broadened by final-state interactions, on top of an even broader background corresponding to the noncondensate particles.

It is therefore instructive to see whether we can extract n_0 from the large-k limit of our model $S(k,\omega)$, which has a broad background as well as a peak. The difficulty inherent in this undertaking lies not only on the complexity of the expressions defining $S(k,\omega)$, but also in the ambiguity in the choice of precisely how much of the function is considered to be part of the peak. Nevertheless, we find that, at least within a specific limit, n_0 can be recovered from $S(k,\omega)$.

As we are interested in the area of the peak of $S(k,\omega)$, it will be calculationally advantageous to be able to approximate S by a δ function. As k becomes large, $\omega_k^{(0)}\to\epsilon_k$, $-\mathrm{Im}\,\omega_k\to gk/4\pi$ and $gS(k,\mathrm{Re}\,\omega_k)\to 4/gk$. Thus, in the limit $k\to\infty$, but $g\to 0$ fast enough that $gk\to 0$, (2.9) reduces cleanly to a δ function:

$$gS(k,\omega)=\zeta_k\delta(\omega-\epsilon_k)\ , \qquad (3.20)$$

where

$$\zeta_k=1+\frac{g}{2\omega_k^{(0)}}\,\frac{\partial}{\partial\omega}[\omega^{-2}\mathfrak{N}_R^{zz(1)}(k,\omega)]\omega_k^{(0)}\ . \qquad (3.21)$$

Using (A1) we can express the derivative in (3.21) in terms of the integrals defined in Appendix A:

$$\frac{1}{2}\frac{\partial}{\partial\omega}[\omega^{-2}\mathfrak{N}_R^{zz(1)}(k,\omega)]_{\epsilon_k}$$
$$=-n'^{(1)}\epsilon_k-(S^{(1)}-M_2^{(1)}-\mu^{(1)})_R+2k\Lambda_{+R}^{z(1)}$$
$$-A_R^{(1)}+k^2\frac{\partial}{\partial\omega}[A_R^{(1)}+(S^{(1)}-\mu^{(1)})_R]\ . \qquad (3.22)$$

It can be verified that for $k\gg 1$ only the first term $-n'^{(1)}\epsilon_k$ in (3.22) is important, the other terms being $O(k)$. For example, the magnitude of $A_R^{(1)}$ [Eq. (A2e)] can be estimated by transforming the integration variable from $\vec{p}$ to $\vec{q}=\vec{p}/k$ and letting $k\to\infty$ within the integrand. We obtain in this manner at $\omega=\epsilon_k$

$$A_R^{(1)}=P\int\frac{d^3q}{(2\pi)^3}\,k\left(\frac{1}{1+q^2+\vec{q}\cdot\hat{k}}-\frac{1}{q^2+\vec{q}\cdot\hat{k}}\right),$$

which is obviously $O(k)$. Thus, from (3.21) and (3.22) in the limit $k\gg 1$ we obtain to $O(g)$

$$\zeta_k=g[n_0+O(1/k)]\ . \qquad (3.23)$$

Substituting (3.23) into (3.20), we obtain the result found in the impulse approximation for $k\to\infty$.

E. Discussion

The present model calculation of $S(k,\omega)$ is, to the best of our knowledge, the first consistent microscopic analysis of a Bose system that takes into account not only all of the symmetry requirements mentioned in the Introduction but also depletion and multiexcitations. The major limitation of the present model, and also one of its simplifying elements, is that the interparticle potential is summarized by only one parameter g, which is assumed to be small. Bearing this in mind, we discuss several general features of $S(k,\omega)$ found in $O(g)$ and consider applicability to liquid ^{4}He.

The square-root behavior near the two-phonon threshold was shown to be quite general [see (3.9)] and is expected to be present in liquid ^{4}He. Because of its proximity to the one-phonon peak, such a behavior, however, would be quite difficult to observe directly by neutron scattering. Even if the one-phonon peak were displaced away from the threshold, we are not too optimistic that any threshold behavior can be resolved with the present technology.

In the model calculation the long high-ω tail for a fixed finite k [see (3.15)] arises from the three-phonon process, one phonon decaying into two or two phonons coalescing into one. Such three-phonon processes are now believed to be present in liquid ^{4}He and it is reasonable to expect a high-ω tail to be a general feature of multiexcitations. The existing neutron scattering data[1,2] displays a high-ω tail, but poor statistics and unknown counter efficiencies over the wide frequency range covered by the tail hamper any quantitative comparison. A more deliberate measurement of the high-ω tail is needed.

The extraction of n_0 in the large-k limit of $\mathcal{S}(k, \omega)$ confirms the intuitive impulse approximation for small g. In superfluid ^{4}He, however, the coupling parameter g is large and the broadening expressed in $\mathfrak{N}_I^{zz(1)}$ is expected to be significant. Thus at finite k a clean isolation[10] of condensate contribution may be difficult.

In view of the many qualitative features that have been uncovered by the model calculation, and the fact that the calculation is a consistent one, it may be useful to extend the calculation to a somewhat more reasonable form of the interparticle potential $v(k)$. Such a calculation appears to be feasible and would help sort out the effects that are dependent on the explicit form of $v(k)$ and those that are perfectly general.

APPENDIX A: INTEGRAL EXPRESSION OF $\mathfrak{N}^{zz(1)}$

For ease of reference we repeat here the explicit forms of the regular functions that contribute to $\mathfrak{N}^{zz(1)}$. For further details, the reader should consult I. $\mathfrak{N}^{zz(1)}$ is given by

$$\begin{aligned}\mathfrak{N}^{zz(1)}(k,\omega) = \epsilon_k(\omega^2-\epsilon_k^2)[&(S^{(1)}+M_2^{(1)}-\mu^{(1)})\\ &+2\omega k^{-1}\delta_\mu\Lambda_\mu^{z(1)}+k\beta_\mu\Lambda_\mu^{z(1)}-\epsilon_k n'^{(1)}]\\ &+k^2[\omega\epsilon_k A^{(1)}+\epsilon_k^2(S^{(1)}-\mu^{(1)})+\omega^2 v^{(1)}]\\ &+(\omega^2-\epsilon_k^2)^2F^{zzr(1)}\,,\end{aligned} \tag{A1}$$

where $\delta_\mu = 1$, $\beta_\mu = \mathrm{sgn}\mu$, $S = \frac{1}{2}(M_{++}+M_{--})$, $A = \frac{1}{2}(M_{++} - M_{--})$, and $M_2 = M_{+-}$. The regular functions (Λ_μ^z, $M_{\mu\nu}$, F^{zzr}) to $O(g)$ are given in terms of one-loop integrals:

$$S^{(1)}+M_2^{(1)}-\mu^{(1)} = \int\frac{d^3p}{(2\pi)^3}\lambda_p\lambda_{\vec p+\vec k}Q^+, \tag{A2a}$$

$$S^{(1)}-M_2^{(1)}-\mu^{(1)} = \frac{1}{2}\int\frac{d^3p}{(2\pi)^3}\left[\frac{1-\lambda_p^2}{\lambda_p}+\left(\frac{\lambda p}{\lambda_{\vec p+\vec k}}+1\right)Q^+\right], \tag{A2b}$$

$$\delta_\mu\Lambda_\mu^{z(1)} = \frac{1}{2}\int\frac{d^3p}{(2\pi)^3}(\lambda_p-\lambda_{\vec p+\vec k})(\vec p\cdot\hat k+\tfrac{1}{2}k)Q^-, \tag{A2c}$$

$$\beta_\mu\Lambda_\mu^{z(1)} = \frac{1}{2}\int\frac{d^3p}{(2\pi)^3}\left(\frac{\lambda p}{\lambda_{\vec p+\vec k}}-1\right)(\vec p\cdot\hat k+\tfrac{1}{2}k)Q^+, \tag{A2d}$$

$$A^{(1)} = \int\frac{d^3p}{(2\pi)^3}\lambda_pQ^-, \tag{A2e}$$

$$F^{zzr(1)} = \frac{1}{8}\int\frac{d^3p}{(2\pi)^3}\frac{(\lambda_p-\lambda_{\vec p+\vec k})^2}{\lambda_p\lambda_{\vec p+\vec k}}(\vec p\cdot\hat k+\tfrac{1}{2}k)^2Q^+, \tag{A2f}$$

$$v^{(1)} = \int\frac{d^3p}{(2\pi)^3}\frac{1}{p^2}, \tag{A2g}$$

$$gn'^{(1)} \equiv (1-gn_0)^{(1)} = g/3\pi^2, \tag{A2h}$$

where

$$\lambda_p = \tfrac{1}{2}p(1+\tfrac{1}{4}p^2)^{-1/2}, \tag{A3}$$

$$Q^\pm = (\omega+i\eta-\omega_{\vec p+\vec k}^{(0)}-\omega_p^{(0)})^{-1}\mp(\omega+i\eta+\omega_{\vec p+\vec k}^{(0)}+\omega_p^{(0)})^{-1}. \tag{A4}$$

For calculating $\mathfrak{N}_I^{zz(1)}(k,\omega)$ at $\omega > 0$ we have

$$\mathrm{Im}\,Q^\pm = -\pi\delta(\omega-\omega_{\vec p+\vec k}^{(0)}-\omega_p^{(0)}). \tag{A5}$$

From (A1)–(A5) we see that $\mathfrak{N}_I^{zz(1)}$ has the form quoted in (3.3).

Note that the integrals defined in (A2a) and (A2g) have large p divergence. However, the infinities cancel upon addition in (A1); so $\mathfrak{N}^{zz(1)}$ is well defined for all k and ω. This is easily proved as follows. The divergent terms of (A1) contribute D to $\mathfrak{N}^{zz(1)}$, where

$$D = \omega^2\epsilon_k[(S^{(1)}+M_2^{(1)}-\mu^{(1)})+2v^{(1)}].$$

As $p\to\infty$, the integrand of $(S^{(1)}+M_2^{(1)}-\mu^{(1)})$ (A2a) approaches $Q^+\to 2/p^2$, which cancels the integrand of $2v^{(1)}$ (A2g).

APPENDIX B: $\mathfrak{N}_I^{zz(1)}(k,\omega)$ IN TERMS OF ELLIPTIC INTEGRALS

We here list the results of the integration outlined in Sec. III C:

$$-\frac{1}{\pi}(S^{(1)}+M_2^{(1)}-\mu^{(1)})_I = \frac{1}{(2\pi)^2k}\left[-\left(\frac{\alpha_-}{\alpha_+}\right)^{1/2}u+\xi-\ln([\xi+(1+\xi^2)^{1/2}]\{\xi-\omega+[1+(\xi-\omega)^2]^{1/2}\})\right]_{\xi_-}^{\xi_+}, \tag{B1}$$

$$\begin{aligned}-\frac{1}{\pi}(S^{(1)}-\mu^{(1)})_I = \frac{1}{4(2\pi)^2k}\Bigg[&-\left(\frac{\alpha_-}{\alpha_+}\right)^{1/2}u+3\xi-\ln[\xi+(1+\xi^2)^{1/2}]-3\ln\{\xi-\omega+[1+(\xi-\omega)^2]^{1/2}\}\\ &-\xi\left(\frac{1+(\xi-\omega)^2}{1+\xi^2}\right)^{1/2}-\left(\frac{\alpha_+}{\alpha_-}\right)^{1/2}E(u)\Bigg]_{\xi_-}^{\xi_+},\end{aligned} \tag{B2}$$

$$\begin{aligned}-\frac{1}{\pi}\delta_\mu\Lambda_{\mu I}^{z(1)} = \frac{1}{2(2\pi)^2k^2}\Bigg[&\omega\xi+2(1+\xi^2)^{1/2}-2[1+(\xi-\omega)^2]^{1/2}-\omega\ln([\xi+(1+\xi^2)^{1/2}]\{\xi-\omega+[1+(\xi-\omega)^2]^{1/2}\})\\ &+\omega\left(\frac{\alpha_-}{\alpha_+}\right)^{1/2}u+\omega\xi\left(\frac{1+(\xi-\omega)^2}{1+\xi^2}\right)^{1/2}+\omega\left(\frac{\alpha_+}{\alpha_-}\right)^{1/2}E(u)\Bigg]_{\xi_-}^{\xi_+},\end{aligned} \tag{B3}$$

$$-\frac{1}{\pi}\beta_\mu\Lambda_{\mu I}^{z(1)} = \frac{1}{2(2\pi)^2k^2}\left[2\ln\left(\frac{\xi+(1+\xi^2)^{1/2}}{(\xi-\omega)+[1+(\xi-\omega)^2]^{1/2}}\right)+2\xi+\omega(1+\xi^2)^{1/2}+\omega[1+(\xi-\omega)^2]^{1/2}\right.$$

$$+(2+\omega^2)\left(\frac{\alpha_-}{\alpha_+}\right)^{1/2} u - 2\xi\left(\frac{1+(\xi-\omega)^2}{1+\xi^2}\right)^{1/2} - 2\left(\frac{\alpha_+}{\alpha_-}\right)^{1/2} E(u)\Bigg]_{\xi_-}^{\xi_+} , \tag{B4}$$

$$-\frac{1}{\pi}A_I^{(1)} = \frac{1}{(2\pi)^2 k}\Bigg[(1+\xi^2)^{1/2} - \tfrac{1}{2}\ln\left(\frac{(1+\xi^2)^{1/2}+[1+(\xi-\omega)^2]^{1/2}}{(1+\xi^2)^{1/2}-[1+(\xi-\omega)^2]^{1/2}}\right)$$
$$-\frac{(\omega^2+4)^{1/2}(\alpha_-/\alpha_+)^{3/2}}{[1-(\alpha_-/\alpha_+)^2]\,\mathrm{sn}(a)\,\mathrm{dn}(a)\,\mathrm{cn}(a)}\Pi(u,a) - \alpha_-\left(\frac{\alpha_-}{\alpha_+}\right)^{1/2} u\Bigg]_{\xi_-}^{\xi_+} , \tag{B5}$$

$$-\frac{1}{\pi}F_I^{zzr(1)} = \frac{1}{8(2\pi)^2 k^3}\Bigg[2(\omega^2+4)\xi + (8+6\omega^2)\left(\frac{\alpha_-}{\alpha_+}\right)^{1/2} u$$
$$+2(\omega^2-4)\xi\left(\frac{1+(\xi-\omega)^2}{1+\xi^2}\right)^{1/2} + 2(\omega^2-4)\left(\frac{\alpha_+}{\alpha_-}\right)^{1/2} E(u)\Bigg]_{\xi_-}^{\xi_+} , \tag{B6}$$

where

$$\alpha_\pm = \tfrac{1}{2}[\pm\omega + (\omega^2+4)^{1/2}] . \tag{B7}$$

Here u is the elliptic integral[8] of the first kind given by

$$u = \mathrm{cs}^{-1}[(\xi\sqrt{\alpha_-} - \sqrt{\alpha_+})/(\xi\sqrt{\alpha_+} + \sqrt{\alpha_-})], \tag{B8}$$

and $E(u)$ and $\Pi(u, a)$ are the Jacobi elliptic integrals[8] of the second and third kind, respectively, where a is defined by

$$[1-(\alpha_-/\alpha_+)^2]\,\mathrm{sn}^2(a) = 1 + \alpha_-/\alpha_+ , \tag{B9}$$

and where the modulus β of the elliptic functions employed here is given by

$$\beta = [1-(\alpha_-/\alpha_+)^2]^{1/2} . \tag{B10}$$

We caution that the integration limits $\xi_\pm$ [given by Eq. (3.17)] are such that $\Pi(u, a)$ is the Cauchy principal value of the integral.

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