Theoretical study of the dynamic structure factor of superfluid $^4$He

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We study the dynamic structure factor $S(q, \omega)$ of superfluid $^4$He at zero temperature in the roton momentum region and beyond using field-theoretical Green’s function techniques. We start from the Gavoret-Nozières two-particle propagator and introduce the concept of quasiparticles. We treat the residual (weak) interaction between quasiparticles as being local in coordinate space and weakly energy dependent. Our quasiparticle model explicitly incorporates the Bose-Einstein condensate. A complete formula for the dynamic susceptibility, which is related to $S(q, \omega)$, is derived. The structure factor is numerically calculated in a self-consistent way in the special case of a momentum independent interaction between quasiparticles. Results are compared with experiment and other theoretical approaches.

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I. INTRODUCTION

The dynamic structure factor $S(q, \omega)$ observed in inelastic neutron scattering experiments on superfluid $^4$He consists of a sharp peak at the Landau phonon-maxon-roton energy and a structured continuum at higher energies. While there is general agreement that the phonon part of the excitation spectrum is due to a collective mode of the $^4$He superfluid (zero sound), the character of the observed sharp structure at higher momentum transfers has been the subject of considerable debate. This debate is reviewed in some detail in the books by Griffin[7] and Glyde and Griffin[8]. In particular, the analysis of the temperature dependence of the dynamic structure factor suggests that the roton excitation may be a single particle excitation from the condensate, while the excitations at intermediate momenta are described as a mixture of collective and single particle processes (Glyde-Griffin scenario).

As was pointed out by Gavoret and Nozières (GN)[9], in the presence of a Bose condensate, the time-ordered density-density correlation function $\chi^T(q, \omega)$ of a Bose system splits into two parts,

$$\chi^T(q, \omega) = \Lambda^a(q, \omega)G^a(q, \omega)\Lambda^b(q, \omega) + \chi^T_R(q, \omega).$$

(1)

The second term $\chi^T_R$ describes density-density fluctuations of non-condensed particles, while the first term explicitly contains the single particle Green’s functions $G^a(q, \omega)$. This term is unique to a Bose-condensed liquid and vanishes in the absence of a condensate. In simple physical terms, one may interpret this condensate term as a density fluctuation due to the excitation of single atoms out of the condensate. According to the Glyde-Griffin scenario, this interpretation may be useful in the roton region. For small energies and momenta, however, GN showed that both terms in Eq. (1) share the same poles, which are due to compressional sound waves.

Systematic attempts to describe the excitations of superfluid $^4$He in the momentum region at and above the roton minimum within a phenomenological field-theory began with the work of Pitaevskii[10] who showed that the phonon-maxon-roton curve terminates at twice the roton energy due to quasiparticle decay. His elegant ideas were developed further by Zawadowski, Ruvalds and Solana (ZRS)[11]. Starting from a phenomenological Hamiltonian written in terms of quasiparticle operators, ZRS found a continuum in the one-particle spectral density of states lying above the sharp single-quasiparticle peak. In contrast to other approaches the work of ZRS is grounded in a field-theoretical analysis similar to the GN theory. However, since the density operator in terms of quasiparticle descriptions to $S(q, \omega)$. Their pessimistic view about ZRS-like models may stem from the incomplete density operators used in their calculations. A more general expression for the density operator was proposed by Pistolesi[12], however without a clear connection to the basic GN theory. As in the ZRS approach, the role of the Bose broken symmetry remains unclear, because the condensate does not appear explicitly within that model.

The goal of our work is three-fold: (a) to find a quasiparticle model for $S(q, \omega)$, which is based on the general formalism of GN and applicable in the roton region and beyond, (b) to find a connection between this model and the phenomenological field theory of Pitaevskii and ZRS and (c) to calculate $S(q, \omega)$ consistently (i.e. under consideration of all terms in Eq. (1)) within the model. This entails a consistent calculation of the sharp roton peak together with the multi-particle continuum.

In Sec. II we discuss the general formalism of GN introducing our notation and sign convention. In Sec. III, we introduce the concept of quasiparticles into the microscopic theory of GN. Treating the interaction between quasiparticles as being local in coordinate space, we ar-
rive at a model of ZRS-type, but with an explicit consideration of the Bose condensate and with an expression for $\chi^T$, which includes both terms in Eq. (3). We study qualitative properties of the model in Sec. III. Thereafter, we present the iteration scheme used in our numerical calculations of $S(\vec{q}, \omega)$ (Sec. IV). The results of the calculation are presented in Sec. V together with comparisons to experiment as well as to other theoretical calculations. Finally, in Sec. VI, we discuss our conclusions and give an outlook for a further refinement of our calculations.

II. THEORETICAL FOUNDATION

In this section we review the GN formalism defining our notation and sign conventions. As is known from Belaev's work, the presence of a Bose condensate introduces "anomalous" propagators. Gavoret and Nozières systematically extended Belaev's theory to the two-body propagator. For the structure factor, in particular, this leads to the first term in Eq. (4).

A. Response function

The dynamic structure factor $S(\vec{q}, \omega)$, which is measured in neutron scattering experiments, is given at zero temperature by

$$S(\vec{q}, \omega) = \frac{1}{n} \text{Im} \chi^T(\vec{q}, \omega) \theta(\omega);$$

(2)

the $\theta$-function cuts off negative frequency contributions and $n$ denotes the density of the Bose fluid. $\chi^T(\vec{q}, \omega)$ is the Fourier transform of the time-ordered density-density correlation function

$$\chi^T(\vec{q}, \omega) = \frac{1}{2\pi} \int_{-\infty}^{\infty} dt e^{i\omega t} \chi^T(\vec{q}, t),$$

(3)

which is defined as

$$\chi^T(\vec{q}, t) = -i \langle T \rho_\vec{q}(t) \rho_{-\vec{q}}(0) \rangle$$

$$= -i \sum_{\vec{p}, \vec{p}'} \langle T a^\dagger_{\vec{p}+\vec{q}/2}(t) a_{\vec{p}'}(t) a^\dagger_{\vec{p}'-\vec{q}/2}(0) a_{\vec{p}-\vec{q}}(0) \rangle.$$  

(4)

Here, $\rho_\vec{q}(t) = \sum_{\vec{p}} a^\dagger_{\vec{p}-\vec{q}/2}(t) a_{\vec{p}+\vec{q}/2}(t)$ is the density operator in the Heisenberg picture and $T$ the time-ordering operator.

B. Two-particle Green's function

Following Gavoret-Nozières, we now consider the two-particle Green's function,

$$K^\alpha_\beta(\vec{p}, \vec{p}', \vec{q}, \omega) = \langle T a^\dagger_{\vec{p}+\vec{q}/2}(t_1) a^\dagger_{\vec{p}'+\vec{q}/2}(t_2) a_{\vec{p}'+\vec{q}/2}(t_3) a_{\vec{p}-\vec{q}/2}(t_4) \rangle.$$  

(5)

The Greek indices take the values 1 or 2 and distinguish between creation and destruction operators, i.e., $a^\dagger_\vec{q}(t)$ destructs a Boson ($^4$He atom) with momentum $\vec{q}$ at time $t$ and $a_{-\vec{q}}(t) = a^\dagger_{-\vec{q}}(t)$ is a corresponding creation operator. Greek subscripts and superscripts on the left hand side of Eq. (5) label incoming and outgoing particles.

It is convenient to work with the Fourier transform of $\chi^T$ with respect to the time variables:

$$(2\pi)^3 \delta(\omega_3 + \omega_4 - \omega_1 - \omega_2) K^{\alpha_2}_{\alpha_1}(p, p', q) =$$

$$\int dt_1 dt_2 dt_3 dt_4 e^{i(\omega_1 t_1 + \omega_2 t_2 - \omega_3 t_3 - \omega_4 t_4)} K^{\alpha_3}_{\alpha_4}(\vec{p}, \vec{p}', \vec{q}, \omega).$$

(6)

Here, $p = (\vec{p}, \epsilon = (\omega_4 - \omega_3)/2), p' = (\vec{p}', \epsilon' = (\omega_2 - \omega_1)/2)$ are the relative momenta and energies of the particle pair in the initial and final states, respectively, and $q = (\vec{q}, \omega = \omega_3 + \omega_4)$ is the total momentum and energy of that pair.

It should be obvious from Eqs. (4) and (5) that the dynamic susceptibility can be written as

$$\chi^T(q) = -i \sum_{p, p'} K^{2\dagger}_{21}(p, p', q),$$

(7)

where we have used the abbreviation $\sum_p = \int \frac{d^3 p}{(2\pi)^3} \int \frac{d\epsilon}{2\pi}$.

In their diagrammatic analysis of $K^{\alpha}_{\beta}(\vec{q})$ (see Fig. 1), GN have shown that the dynamic susceptibility may be separated into two terms, a singular and a regular part,

$$\chi^T(q) = \chi^{\text{S}}_T(q) + \chi^{\text{R}}_T(q).$$

(8)

As was already alluded to in the introduction, the singular susceptibility $\chi^{\text{S}}_T(q)$ arises due to the Bose condensate and is given by

$$\chi^{\text{S}}_T(q) = \Lambda^\alpha(q) G^\beta_\alpha(q) \Lambda^\beta(q).$$

(9)

In Eq. (4) and elsewhere in this paper, summation over repeated indices is implied. The singular part of $\chi^T$ contains the Belaev single particle Green’s functions $G^\beta_\alpha(q)$. Consequently, any structure in $G^\beta_\alpha(q)$ will show up directly in the dynamic susceptibility. This is an interesting physical feature of a partly condensed Bose liquid: excitations of single particles out of the condensate determine partly the density fluctuations of the liquid. The Belaev Green’s functions obey the Dyson-Beliaev equation.

$$G^\beta_\alpha(q) = G^{\beta}_{\alpha_0}(q) + G^{\gamma}_{\alpha}(q) \Sigma^{\gamma}_{\alpha}(q) G^\beta_\gamma(q),$$

(10)

with the free Green’s functions

$$G^{1}_{01}(q) = G^{2}_{02}(-q) = (\omega - \epsilon_\vec{q} + \mu + i\eta)^{-1},$$

$$G^{2}_{01}(q) = G^{1}_{02}(q) = 0,$$

(11)

and the self energies $\Sigma^{\xi}_{\alpha}(q)$’s. The free-atom kinetic energy is denoted by $\epsilon_\vec{q}$ and the chemical potential by $\mu$. 

...
The Bose vertex functions $\Lambda^\alpha(q)$ determine how strongly single particle excitations contribute to the dynamic susceptibility,

$$\Lambda^\alpha(q) = n_0^{1/2}(\delta_{2\alpha} + \delta_{1\alpha}) + i \sum_p F^{\delta\gamma}_{\alpha\beta}(p, q) P^{\gamma\delta}_{\alpha\beta}(p, q). \tag{12}$$

Here, $n_0$ denotes the density of condensed bosons. These functions vanish in the absence of the condensate. The interaction vertex (full three point function) $P$ will be discussed in more detail below. Here and elsewhere in this paper, a boldfaced symbol stands for matrix functions. The product of two Belaev single particle propagators $G$ with total momentum $q$ is abbreviated as

$$F^{\gamma\delta}_{\alpha\beta}(p, q, q') = -(2\pi)^4 \left[ F^{\delta\gamma}_{\alpha\beta}(p, q) \delta(p - p') + F^{\delta\gamma}_{\beta\alpha}(p, q) \delta(p + p') \right] - i F^{\delta\gamma}_{\alpha\beta}(p, q) \Gamma^{\gamma\delta}_{\alpha\beta}(p, p', q) F^{\delta\gamma}_{\alpha\beta}(p', q). \tag{15}$$

The regular two-body propagator is determined by the single particle propagator $G$ and the (full) two-body interaction kernel $\Gamma$. Terms where the condensate does not contribute will be called `regular’ in this paper. $\chi^T_R$ represents the full response function of a Bose liquid in the absence of the condensate.

Following GN we separate out processes with intermediate two particle states in the interaction kernel $\Gamma$, so that it fulfills the following (coupled) Bethe-Salpeter equations. The product of two Belaev single particle propagators $R$ with total momentum $q$ is given by

$$R^{\gamma\delta}_{\alpha\beta}(p, q) = G^{\gamma\delta}_{\alpha\beta}(-p + \frac{q}{2}) G^{\gamma\delta}_{\alpha\beta}(p + \frac{q}{2}). \tag{13}$$

The regular susceptibility $\chi^T_R$ is given by

$$\chi^T_R(q) = -i \sum_{p,p'} F^{21}_{\beta\alpha}(p, p', q), \tag{14}$$

in terms of the regular two-body propagator

$$\Gamma^{\gamma\delta}_{\beta\alpha}(p, p', q) F^{\delta\gamma}_{\alpha\beta}(p', q). \tag{16}$$

FIG. 1: Diagrammatic representation of the two-particle Green’s function $K^{\delta\gamma}_{\alpha\beta}$ in energy-momentum space. The solid lines represent the single-particle Green’s functions $G^{\delta\gamma}_{\alpha\beta}$. The dashed lines indicate condensate particles. $\Gamma$ and $P$ stand for the four- and three-point vertex function, respectively. The three diagrams without any condensate line are the regular two-body propagator $F^{\delta\gamma}_{\alpha\beta}$ given by Eq. (15). They are the only contribution to $K^{\delta\gamma}_{\alpha\beta}$ in the absence of the condensate. All the other diagrams are unique to a Bose-condensed liquid and lead to the singular part of the dynamic susceptibility (see Eq. (1)).
function $\mathbf{P}$ is given by
\[
P_{\xi\nu}^\alpha(p, q) = J_{\xi\nu}^\alpha(p, q) + \frac{1}{2} \sum_{p'} \Gamma_{\xi\nu}^{\mu\nu}(p, p', q) F_{0\mu}\eta_{\mu}(p', q) J_{\eta\nu}^\alpha(p', q),
\]
and the self energy by
\[
\Sigma_\alpha^\beta(q) = \tilde{\Sigma}_\alpha^\beta(q) + \Sigma_{*\alpha}^\beta(q)
\]
with
\[
\Sigma_{*\alpha}^\beta(q) = \frac{1}{2} \sum_p J_{\xi\rho}^\alpha(p, q) F_{0\rho}\eta_{\mu}(p, q) P_{\mu}^\beta(p, q).
\]
$\mathbf{J}$ and $\tilde{\Sigma}$ are again two-particle irreducible functions and contain all diagrams without intermediate two-particle states. As is obvious from these equations, the various terms $\mathbf{G}$, $\mathbf{P}$, and $\Gamma$, which determine the structure of the susceptibility, are not independent, but are linked in a complicated way. For instance, any singularity (i.e. structure) in $\Gamma$ will show up in all terms, and care must be taken to treat them consistently.

In order to put the general formalism outlined above to work, the two-particle irreducible functions $\tilde{\Sigma}$, $\mathbf{J}$ and $\mathbf{I}$ must be determined. GN have done this in the hydrodynamic limit $\vec{q}, \omega \to 0$. But in general, this is a most formidable task. Therefore, the formalism is only useful if $\tilde{\Sigma}$, $\mathbf{J}$ and $\mathbf{I}$ can be approximated in a simple way.

### III. QUASIPARTICLE MODEL

In the following we will introduce the approximations appropriate for the momentum regime we are interested in. We are guided by the the pioneering work of Pitaevskii\[1\] as well as the ZRS phenomenological field theory\[5\].

#### A. Quasiparticles

Starting from Eq. (18) we transform the Beliaev-Dyson matrix equation (19) into the form
\[
G_{\alpha}^\beta(q) = g_{\alpha}^\beta(q) + g_{\alpha}^\gamma(q) \Sigma_{*\alpha}^\gamma(q) G_{\xi}^\beta(q)
\]
with
\[
g_{\alpha}^\beta(q) = G_{0\alpha}^\beta(q) + G_{0\alpha}^\gamma(q) \tilde{\Sigma}_{\alpha}^\gamma(q) g_{\xi}^\beta(q).
\]
At this point it is convenient to introduce the concept of quasiparticles. Eq. (20) is nothing but an expression for Green’s functions describing the propagation of particles with ‘bare’ propagators given by the $g_{\alpha}^\beta(q)$’s. Thus, we assert that, in fact, $g_{\alpha}^\beta(q)$ describe stable quasiparticles, which are helium atoms renormalized by the two-particle reducible part of the self energy. If this interpretation is at all useful, then the residual interaction of the quasiparticles must be weak. We will exploit this interpretation in the following: All the strong atomic interactions are contained in $\tilde{\Sigma}$ generating the ‘bare’ quasiparticle spectrum, which, of course, is not at all parabolic as for a free He atom.

Eq. (20) with the self energy (13) precisely corresponds to the Dyson equation used by Pitaevskii\[1\] as the basis of his evaluation of quasiparticle spectrum near its endpoint. Moreover, the ZRS phenomenological field theory is built on a similar basis. Thus one can identify Pitaevskii-ZRS quasiparticles with helium atoms renormalized by $\tilde{\Sigma}(q)$.

In order to further specify the quasiparticle we have to define the $\Sigma_{\alpha}^\beta$ or alternatively $g_{\alpha}^\beta$. In this work, we will take
\[
g_{\alpha}^\beta(q) = \frac{A_{\alpha}^\beta(q)}{\omega - \omega_{\alpha}^\beta + i\eta}.
\]
This kind of propagator characterizes a stable quasiparticle with the ‘bare’ spectrum $\omega_{\alpha}^\beta$ and normalization factor (residue) $A_{\alpha}^\beta(q)$. In general, such a Green’s function should have a second pole at negative energies, but it contributes only a small correction at high energies if $kT \ll \omega_{\alpha}^\beta$ and therefore, it can be neglected in our context.

Furthermore, we assume that the residues $A_{\alpha}^\beta$ fulfill the relation
\[
A_{1}^\alpha(\vec{q}) A_{2}^\alpha(\vec{q}) - A_{2}^\alpha(\vec{q}) A_{1}^\alpha(\vec{q}) = 0.
\]
The same relation holds in the Bogoliubov model\[10\] of a dilute weakly interacting Bose gas. It simplifies a formal algebraic solution of the Beliaev-Dyson equation (20) significantly and leads to a ZRS-like expression for $G_{\alpha}(q)$,
\[
G_{\alpha}^\beta(q) = \frac{A_{\alpha}^\beta(q)}{\omega - \omega_{\alpha}^\beta - A \Sigma^\alpha(q)}
\]
with
\[
A \Sigma^\alpha(q) = A^\alpha(\vec{q}) \Sigma^\alpha_{*}(q).
\]
In order to make contact with the original ZRS expressions, which contain only one Green’s function, we have to make some specific choices for the renormalization functions $A_{\alpha}^\beta$ in Eq. (24). Typically, one assumes that the ZRS calculation scheme corresponds to keeping only the diagonal element $G_{1}^\alpha$ of the Beliaev-Green’s matrix (see e.g. Chap. 10 of Ref.\[1\]) and takes $A_{1}^\alpha = A_{2}^\alpha = A_{3}^\alpha = 0$ and $A_{1}^\alpha = 1$. This choice is also inspired by the Bogoliubov approximation. One may argue that at large wavevectors the anomalous propagators are much smaller than the diagonal ones because the Bose coherence factors become unimportant as in the Bogoliubov model. However, since we do not know the explicit form of these factors in our model, we will keep the anomalous Green’s functions in the following. At the beginning of the Sec. \[7\].
we will present an alternative choice of the parameters \( A_0^\delta \), which is also consistent with ZRS scheme.

Finally, we suppose that the ‘bare’ quasiparticle spectrum is already characterized by a roton minimum and the residual interaction does not modify the spectrum qualitatively in the momentum region up to the roton minimum. This assumption is in the spirit of our approach assuming weakly interacting quasiparticles. Since an unambiguous determination of the ‘bare’ spectrum is impossible, we will study two models with different spectra (see Fig. 2): (i) Landau spectrum 6,11 which was originally chosen in order to explain the specific heat data and (ii) Bijl-Feynman spectrum 12, proposed first by Bijl and then derived by Feynman. Both spectra are qualitatively similar, but differ in the roton and maxon energies.

**B. Response function**

If the concept of quasiparticles is at all useful, the residual interaction of the quasiparticles must be weak. Thus, the interaction energy in the momentum region of interest should be much smaller than the kinetic energy of quasiparticles and the interaction vertices can be treated as being essentially local in coordinate space and weakly energy dependent. The Fourier transform of a local interaction vertex is a function of only the total momentum transfer, i.e.

\[
J(p, q) \simeq J(\tilde{q}), \quad I(p, p', q) \simeq I(\tilde{q}). \tag{26}
\]

As we shall see, this corresponds to an RPA-like approximation.

In order to determine the dynamic susceptibility in line

\[
W_{\alpha\beta}(p, p', q) = F_{\alpha\beta}^\delta(p, p', q) - iG^{\xi}_\alpha(-p + \frac{q}{2})G^{\xi}_\beta(p + \frac{q}{2})P^{\rho}_\xi(p, q)G^{\rho}_\delta(p', q)G^{\xi}_\eta(-p' + \frac{q}{2})G^{\eta}_\xi(p' + \frac{q}{2]); \tag{30}
\]

\[
\Sigma^{\delta\gamma}_\alpha(q) = \frac{1}{4} f^{\mu\nu}_\alpha(q) f^{\rho\nu}_\gamma(q) f^{\beta\rho}_\alpha(q). \tag{29}
\]

The separation of the dynamic susceptibility \( \Sigma \) into a singular and a regular part is very useful, since it emphasizes the role of the Bose-Einstein condensate, which couples the single-quasiparticle propagator \( G \) into the density-density correlation function \( \chi^T(q) \). However, for practical calculations it is sometimes more convenient to sort the diagrams for \( K_{\alpha\beta}^{\delta\gamma}(p, p', q) \) differently: Let \( W_{\alpha\beta}^\delta(p, p', q) \) be made up of all diagrams with momenta of the external lines different from zero (see Fig. 3).

\[
W_{\alpha\beta}(p, p', q) = F_{\alpha\beta}^\delta(p, p', q) - iG^{\xi}_\alpha(-p + \frac{q}{2})G^{\xi}_\beta(p + \frac{q}{2})P^{\rho}_\xi(p, q)G^{\rho}_\delta(p', q)G^{\xi}_\eta(-p' + \frac{q}{2})G^{\eta}_\xi(p' + \frac{q}{2}); \tag{30}
\]
\( W \) precisely corresponds to the two-particle Green’s functions introduced by Fukushima and Iseki. Apart from the regular two-particle propagator \( F \) it contains a term, which renormalizes \( F \) by taking into account the possibility that two quasiparticles interact via the three point vertex \( P \) and propagate as one quasiparticle in an intermediate step. It follows from Eq. (12) that this second term belongs to \( \chi(q) \) in Eq. (6).

With Eq. (30) we can write the dynamic susceptibility in the form

\[
\chi^T(q) = n_0 \sum_{\alpha \beta} G_{\alpha \beta}^2(q) + n_0^{1/2} \left[ G_{\alpha}^2(q) + G_{\beta}^2(q) \right] J_{\alpha \beta}^\xi(q) F_{\eta \xi}^{21}(q) + w_{21}^2(q),
\]

where the function \( w_{21}^2(q) \) is given by

\[
w_{21}^2(q) = -i \sum_{p, p'} W_{21}^2(p, p', q).
\]

A brief discussion of expression (31) is in order: The first term describes one-quasiparticle excitations and vanishes in the absence of the condensate. The second term corresponds to the direct excitation of two quasiparticles. Since in the absence of the condensate \( W_{\alpha \beta}^2 \) reduces to the regular two-particle propagator, this term goes over into the full response function above \( T_\lambda \). The term describes an interference between the one- and two-particle channel and it disappears as well in the absence of the condensate. Eq. (31) shows how these three terms must be combined in order to calculate the susceptibility.

In earlier literature, the dynamic structure factor was either calculated from the imaginary part of the single particle propagator (first term in Eq. (31), see e.g. Ref. 7) or from the imaginary part of the two-body propagator \( w_{21}^2 \) (e.g. Ref. 13). The interference term was neglected. Juge and Griffin emphasized that all terms may be important, however they did not combine them in order to calculate \( S(q, \omega) \).

It is possible to express the susceptibility entirely in terms of \( g_0^2(q) \) and \( f_{\alpha \beta}^\gamma(q) \). To this end, we transform first the expressions (28) and (32) by using of (16) and (17),

\[
f_{\alpha \beta}^\gamma(q) = f_{\alpha \beta}^{\gamma}(q) + \frac{1}{\rho_\mu \nu_\rho} I_{\mu \nu}^{(p)}(q) J_{\eta \xi}^{(q)} w_{21}^{(q)}(q),
\]

\[
w_{21}^2(q) = f_{21}^{(q)}(q) + \frac{1}{\rho_\mu \nu_\rho} I_{\mu \nu}^{(p)}(q) J_{\eta \xi}^{(q)} w_{21}^{(q)}(q).
\]

Obviously, we have found a set of algebraic equations for \( f_{\alpha \beta}^\gamma(q) \) and \( w_{21}^2(q) \), which are similar to the Dyson-Belavie equation (29) for \( G_{\alpha \beta}^0(q) \). We can solve them formally to obtain

\[
\chi^T(q) = n_0 \sum_{\alpha \beta} \left[ \left( 1 - \frac{1}{4} J_{\alpha \beta}^q(q) f_{\alpha \beta}^q(q) J_{\alpha \beta}^q(q) \right)^{-1} \right]^{\rho_\mu \nu_\rho} g_0^2(q) + n_0^{1/2} \sum_{\alpha} \left[ \left( 1 - \frac{1}{4} J_{\alpha \beta}^q(q) f_{\alpha \beta}^q(q) J_{\alpha \beta}^q(q) \right)^{-1} \right]^{\rho_\mu \nu_\rho} g_0^2(q) J_{\alpha \beta}^{\xi}(q) f_{\eta \xi}^{21}(q) + \sum_{\rho \sigma} \left[ \left( 1 - \frac{1}{4} f_{\rho \sigma}^{(q)} J_{\rho \sigma}^{(q)} g_0^2(q) J_{\rho \sigma}^{(q)} \right)^{-1} \right]^{\rho_\mu \nu_\rho} f_{\alpha \beta}^{\gamma}(q)
\]

with \( f_{\rho \sigma}^{\gamma}(q) \) given in terms of \( f_{\alpha \beta}^{\gamma}(q) \)

\[
f_{\rho \sigma}^{\gamma}(q) = \left[ \left( 1 - \frac{1}{2} f_0(q) I(q) \right)^{-1} \right]^{\rho_\mu \nu_\rho} f_{\alpha \beta}^{\gamma}(q) + f_{\alpha \beta}^{\gamma}(q);
\]

obvious matrix notation is employed. The denominators in (29) clearly show the RPA character of the approximation applied here. Note, that all terms in \( \chi^T(q) \) have the same pole structure. Thus both the sharp peak and the continuum observed in \( S(q, \omega) \) receive contributions from all three terms. It may be useful to stress, that up to this point, no approximations are involved in the derivation of (35) apart from Eq. (28). However, in order to explicitly evaluate \( \chi^T(q) \) we will need the approximations for \( g_0^2 \) made in Sec. IIIA.

We want to end this section by noting that an expression similar to Eq. (31) was proposed by Pistolesi as an extension of the Zawadowski-Ruvalds-Solana work. His Eq. (4) corresponds term by term to our Eq. (31). But there are also some differences between both calculations. First of all, the Bose-Einstein condensate does not appear explicitly in Pistolesi’s expression. Instead he introduces two fitting parameters. Secondly, he deals with only one Green’s function and the connection to the general formalism of Gavoret-Nozières remains unclear. To evaluate \( \chi^T(q) \) Pistolesi extracts the regular part of the two-quasiparticle propagator from experimental data. In our calculation (see Sec. III), we will calculate it within an iteration scheme.
IV. QUALITATIVE CONSIDERATIONS

In this section, we will qualitatively study two specific kinematical regions, which deserve special attention: the endpoint region and quasidegree scattering at high energy and momentum transfers.

A. Endpoint of the spectrum

As has been shown by Pitaevskii, the renormalized single-quasiparticle spectrum of a Bose liquid has an endpoint, i.e. at zero temperature undamped excitations cannot exist at momenta larger than some threshold value, provided the ‘bare’ quasiparticle spectrum is characterized by a minimum. Pitaevskii has clarified the character of the spectrum near its endpoint in a quite general way by analyzing the singularities of the single-quasiparticle propagator.

Pitaevskii started from the following expression for the self energy (written in our notation):

\[
\Sigma^* (q) = \frac{i}{(2\pi)^4} \int d^4p P(p,q)G(p)G(q-p)J(p,q)
\]

which is similar to our Eq. (13). The only difference is that Pitaevskii did not consider all Beliaev-Green functions as we do. However, since all these functions have the same pole structure (see e.g. Ref. [11]), near the singularities our expression should lead to the same results except for some coefficients and/or regular contributions, which are not of interest for the analytical behavior of the propagators. Thus Pitaevskii’s prediction about the endpoint of the renormalized spectrum due to the decay of quasiparticles holds within our model.

Pitaevskii distinguished three kinds of decay processes into two excitations: (i) phonon creation, (ii) decay into excitations with finite momenta propagating in the same direction with the same velocity and (iii) decay into two rotons.

Since we are only interested in the momentum region \(10 \leq \tilde{q} \leq 40 \text{ nm}^{-1}\) and do not take phonons into account, the emission of two rotons is the only possible decay channel. Thus, the spectrum should have an endpoint of the third kind, which is characterized by a logarithmic singularity. This endpoint leads to a threshold at twice the roton energy in the imaginary part of the self energy, i.e. to

\[
\text{Im} \Sigma^* (q, \omega < 2\Delta) = 0. \tag{38}
\]

Here, \(\Delta\) denotes the roton (minimum) energy.

Using Eq. (13) in conjunction with Eq. (12) we find that the imaginary part of the one-quasiparticle Green’s function consists of a sharp peak below and a continuum above twice the roton energy,

\[
\text{Im} G^\beta_\alpha (q) = -\pi A^\beta_\alpha (q) \delta (\omega - \omega^0_\tilde{q} - \text{ARe} \Sigma^* (q)) \theta (2\Delta - \omega) + \text{Im} M^\beta_\alpha (q), \tag{39}
\]

where

\[
\text{Im} M^\beta_\alpha (q) = \begin{cases} 0 & \omega < 2\Delta \\ \frac{A^\beta_\alpha (q) \text{Im} \Sigma^* (q)}{(\omega - \omega^0_\tilde{q} - \text{ARe} \Sigma^* (q))} & \omega \geq 2\Delta. \end{cases} \tag{40}
\]

To proceed further we use \(\delta (f(x)) = \sum_i \delta (x - x_i) / f'(x_i)\) with \(f(x_i) = 0\) and assume that the equation

\[
\omega - \omega^0_{\tilde{q}} - \text{ARe} \Sigma^* (q) = 0 \tag{41}
\]

has only one solution \(\omega_{\tilde{q}}\) below \(2\Delta\). We then arrive at

\[
\text{Im} G^\beta_\alpha (q) = -\pi Z^\beta_\alpha (q) \delta (\omega - \omega_{\tilde{q}}) \theta (2\Delta - \omega) + \text{Im} M^\beta_\alpha (q) \tag{42}
\]

with a renormalization factor given by

\[
Z^\beta_\alpha (q) = \frac{A^\beta_\alpha (q)}{|1 - \frac{\partial \text{ARe} \Sigma^* (q, \omega)}{\partial \omega}|} \bigg|_{\omega = \omega_{\tilde{q}}}. \tag{43}
\]

We see that in fact, the sharp component of the one-particle propagator can only exist below the threshold energy \(2\Delta\) as predicted by Pitaevskii. Furthermore, the only effect of quasiparticle renormalization below the threshold is a modification of the excitation energy and peak strength due to the real part of the self energy. There is no mechanism in a model without phonons, which could change the width of the peak below the threshold.

It is interesting to analyze the behaviour of the peak strength \(Z^\beta_\alpha\) near the endpoint. To this end we first need to determine some properties of the real part of the self energy \(\text{ARe} \Sigma^* (q)\) in the vicinity of the threshold energy. Since the real and imaginary part of the self energy are related by

\[
\text{ARe} \Sigma^* (q, \omega) = -\frac{1}{\pi} \int d\epsilon \frac{\text{ARe} \Sigma^* (q, \omega)}{\omega - \epsilon}, \tag{44}
\]

one can show that the threshold in \(\text{AIm} \Sigma^* (q)\) leads to a logarithmic singularity in \(\text{ARe} \Sigma^* (q)\), schematically shown in Fig. 3. At the threshold energy the function is finite but its left and right derivatives are infinite:

\[
\bigg| \frac{\partial \text{ARe} \Sigma^* (q, \omega)}{\partial \omega} \bigg| \rightarrow \infty \quad \text{if} \quad \omega \rightarrow 2\Delta. \tag{45}
\]

It follows immediately from Eq. (13), that the peak strength vanishes at the endpoint energy,

\[
Z^\beta_\alpha (q) \rightarrow 0 \quad \omega_{\tilde{q}} \rightarrow 2\Delta. \tag{46}
\]

Recall that the dynamic susceptibility \(\chi_T (q)\) shares poles with the single-particle Green’s function. Thus we can expect, that the strength of the sharp peak in the imaginary part of \(\chi_T (q)\) (i.e. in the dynamic structure \(S(q)\)) vanishes at the threshold as well. Such a behavior is in qualitative agreement with the standard interpretation of the experimental data.
B. High-momentum scattering

In the high-momentum region, $S(q,\omega)$ can be increasingly well described within the impulse approximation. In the following we will discuss the mechanism leading to this approximation within the framework of our model. For a more general consideration we refer to Refs. 1, 2 and 3.

We start by noting that if the momentum is high enough the kinetic energy of the quasiparticles must be very large relative to the potential energy of their interactions. Thus interaction effects (i.e. all terms containing $I$ and $J$) can be neglected and we obtain from Eq. (33) a simplified expression for the dynamic susceptibility,

$$
\chi^T(q,\omega) = n_0 \sum_{\alpha\beta} g_{\alpha\beta}(q,\omega) + f_{021}(q,\omega) + f_{012}(q,\omega)
$$

and $g_{\alpha\beta}^\delta$ given by Eq. (23). Here, we have only two contributions to $\chi^T$. The first term proportional to $n_0$ introduces single-quasiparticle excitations into the density fluctuations and produces a sharp peak in $S(q,\omega)$. The regular part $\chi^T_R$ leads to a continuum in $S(q,\omega)$. It is due to simultaneous excitation of two non-interacting particles. Unlike in Eq. (35), the terms contributing to $\chi^T$ do not have the same pole structure. In Ref. 1, a result similar to Eq. (47), however with different ‘bare’ Green’s functions, has been called an improved form of the Bogoliubov approximation.

In Eq. (48), we carry out the integration over $\epsilon$ analytically using the theorem of residues. After that the dynamic susceptibility can be written as

$$
\chi^T(q,\omega) = n_0 \sum_{\alpha\beta} g_{\alpha\beta}(q,\omega) + \int \frac{d^3p}{(2\pi)^3} \frac{A^2_2(\vec{p})A^1_1(q-\vec{p}) + A^2_1(\vec{p})A^1_2(q-\vec{p})}{\omega - \omega^0 - \omega^0_{q-p} + i\eta}. \tag{49}
$$

Finally, we find that

$$
S(q,\omega) = n_0 \sum_{\alpha\beta} A^\alpha_\alpha(q)\delta(\omega - \omega^0) + \frac{1}{n} \int \frac{d^3p}{(2\pi)^3} \left[A^2_2(\vec{p})A^1_1(q-\vec{p}) + A^2_1(\vec{p})A^1_2(q-\vec{p})\right] \delta(\omega - \omega^0 + \omega^0_{q-p}). \tag{50}
$$

If the dominant contribution to the integration over $\vec{p}$ in Eq. (50) is from momenta much less than $q$, we can use $\int d^3p \simeq \int_{D} d^3p$, where $D = \{\vec{p}: |\vec{p}| \ll |\vec{q}|\}$. In this region, we have $\omega^0 + \omega^0_{q-p} \simeq \omega^0_{q-p}$. At large enough momenta, renormalization effects coming from the irreducible part of the self energy $\Sigma(q,\omega)$ are negligible in comparison with the kinetic energy of the particles and we can use the approximation

$$
\omega^0_{q-p} \simeq \frac{(q-\vec{p})^2}{2m} \simeq \frac{q^2}{2m} - \frac{\vec{p} \cdot \vec{q}}{m}. \tag{51}
$$

Here, $m$ is the free $^4$He mass. We arrive at

$$
S^{simp}(q,\omega) \simeq n_0 \sum_{\alpha\beta} A^\alpha_\alpha(q)\delta(\omega - \frac{q^2}{2m}) + \frac{1}{n} \int \frac{d^3p}{(2\pi)^3} \left[A^2_2(\vec{p})A^1_1(q-\vec{p}) + A^2_1(\vec{p})A^1_2(q-\vec{p})\right] \delta(\omega - \frac{q^2}{2m} + \frac{\vec{p} \cdot \vec{q}}{m}). \tag{52}
$$

It follows from the second line of Eq. (23), that in the high momentum region the continuum part of $S(q,\omega)$
FIG. 5: Experimental results for \( S(q, \omega) \) at \( q = 32 \text{ nm}^{-1} \). The solid vertical line shows the position of the peak interpreted as a quasifree peak. The dashed line indicates the corresponding free-atom energy.

consists of a Doppler-broadened peak centered at the energy \( q^2 / 2m \). In other words, at very high momenta the continuum is dominated by the free atom properties of the system. Eq. (52) is in line with the Green’s function reformulation of the impulse approximation presented by Griffin. Some differences are due to specific assumptions about the form of \( g^{\alpha \beta} \) made within our approach.

For wavevectors \( |\vec{q}| \geq 32 \text{ nm}^{-1} \), one observes a peak centered close to the free-atom energy (see Fig. 5). The larger the momentum transfer the smaller the shift between the peak position and the free-atom energy. Therefore, in \(^4\text{He} \), the impulse approximation becomes valid already at moderately large momentum transfers. Since a small shift in the energy of the observed ‘quasifree’ peak indicates that the difference between \( \omega_0^\alpha \) and \( q^2 / 2m \) is small as well, the approximation provides a criterion for choosing a spectrum of ‘bare’ quasiparticles. We will exploit this in Sec. VIB.

V. PREPARATION OF THE NUMERICAL ANALYSIS

The formulas of Sec. III provide a set of equations enabling a numerical calculation of the dynamic susceptibility. In this section we will briefly discuss some details of its solution.

A. Iteration scheme

We begin by writing down the complete set of equations for the calculation of \( \chi^T(q) \) in a well-ordered form,

\[
\chi^T(q) = n_0 \sum_{\alpha \beta} G^{\alpha \beta}_0(q) + n_0^{1/2} \sum_{\alpha} G^{\alpha \beta}_0(q) J^{\beta \gamma}_F(q) f^{21}_{\alpha \beta}(q) + w^{21}_{21}(q),
\]

\[
G^{\alpha \beta}_0(q) = \left[ 1 - \frac{1}{4} g^{\alpha \beta}_F T J_{\gamma \delta}^{-1} \right] \rho^{\alpha \beta} g^{\gamma \delta}_0(q), \quad (54)
\]

\[
w^{21}_{21}(q) = \left[ 1 - \frac{1}{4} J \rho_{\alpha \beta} T J_{\gamma \delta}^{-1} \right] \rho^{\alpha \beta} f^{21}_{\alpha \beta}(q), \quad (55)
\]

\[
f^{\alpha \gamma}_{\alpha \beta}(q) = \left[ 1 - \frac{1}{2} J q \right] \rho^{\alpha \beta} \left[ f^{\alpha \gamma}_{\alpha \beta} + f^{\delta \gamma}_{\alpha \beta} \right], \quad (56)
\]

\[
f^{\delta \gamma}_{0 \alpha \beta}(q) = \frac{i}{(2\pi)^4} \int d^4 p G^{\alpha \beta}_0(-p + q/2) G^{\gamma}_{\delta \beta}(p + q/2), \quad (57)
\]

FIG. 6: Iteration scheme. See text for more details.

We see from the above equations that the functions \( f^{\alpha \gamma}_{0 \alpha \beta}(q) \) are all we need in order to calculate the dynamic susceptibility \( \chi^T(q) \). However, determination of these functions is not a trivial task, since they are contained implicitly on the right hand side of Eq. (57). We will solve these integral equations self-consistently via the following iteration procedure: We start with \( G^{\alpha \beta}_0 = g^{\alpha \beta}_0 \) (i.e. \( \Sigma^{\alpha \beta}_0(q) = 0 \)), and calculate \( f^{\alpha \gamma}_{\alpha \beta} \). The result is used to evaluate \( f^{\delta \gamma}_{0 \alpha \beta} \) from which new \( G^{\alpha \beta}_0 \) are obtained. With these \( G^{\alpha \beta}_0 \) we again calculate \( f^{\alpha \gamma}_{0 \alpha \beta} \) and the calculation is repeated until self-consistency is established. The procedure is illustrated schematically in the diagram in Fig. 6. Note that technically the iteration cycle has similarities with a calculation made by Götte and Lücke who considered density excitations in superfluid \(^4\text{He} \) using Mori’s formalism.

Obviously, we need the ‘bare’ quasiparticle propagators \( g^{\alpha \beta}_0(q) \) (i.e. \( \omega^\alpha_0 \) and the strengths \( A^{\alpha \beta}(\vec{q}) \)) and the interactions \( I(q) \) and \( J(q) \) in order to calculate \( \chi^T(q) \). For the sake of simplicity, we will treat them as independent parameters of the model. Neglecting the connection between the input quantities has some consequences. For instance, if one changes only the ‘bare’ spectrum \( \omega^0_\vec{q} \) and keeps the interactions fixed, one arrives effectively at a different physical system. In other words, the result of the iteration depends on the ‘bare’ spectrum. That is the reason why we need some criteria like high-momentum scattering (see Sec. VIB) in order to choose a suitable input spectrum for our calculation.
We will use the resulting one-quasiparticle spectrum \( \omega_q \), which is given by Eq. (11), as a consistency check: a solution is consistent, if after some number of iteration steps the renormalized spectrum does not change any more.

### B. Calculation of \( f_{0\alpha\beta}^{\delta\gamma}(q) \)

In order to facilitate our iteration scheme we want to carry out the integration over energy in Eq. (57) analytically.

According to Eqs. (24) and (38) we can split \( f_{0\alpha\beta}^{\delta\gamma}(q) \) into three terms:

\[
f_{0\alpha\beta}^{\delta\gamma}(q) = f_{0}^{1,1}(q) + f_{0}^{1,m}(q) + f_{0}^{m,m}(q).
\]

For the sake of simplicity we have suppressed the greek indices on the right hand side of the above expression. We find (recall that \( p = (\vec{p}, \epsilon) \) and \( q = (\vec{q}, \omega) \))

\[
f_{0}^{1,1}(q) = i \int \frac{d^3p}{(2\pi)^3} \int \frac{d\epsilon}{2\pi} \left[ A_{\alpha}^{\delta}(\vec{p})M_{\alpha\beta}(q - p)\Theta(2\Delta - \epsilon) - \frac{A_{\alpha}^{\delta}(\vec{q} - \vec{p})\Theta(2\Delta - \epsilon)}{\omega - \epsilon - \omega_0 + ARe\Sigma^*(p) + i\eta} \right]
\]

(60)

for the single-quasiparticle-single-quasiparticle term,

\[
f_{0}^{1,m}(q) = i \int \frac{d^3p}{(2\pi)^3} \int \frac{d\epsilon}{2\pi} \left[ A_{\alpha}^{\delta}(\vec{p})M_{\alpha\beta}^{\delta}(q - p)\Theta(2\Delta - \epsilon) + \frac{M_{\alpha}^{\delta}(p)A_{\beta}^{\gamma}(q - p)\Theta(2\Delta - \epsilon + \omega)}{\omega - \epsilon - \omega_0 + ARe\Sigma^*(q - p) + i\eta} \right]
\]

(61)

for the single-quasiparticle-continuum contribution and finally

\[
f_{0}^{m,m}(q) = i \int \frac{d^3p}{(2\pi)^3} \int \frac{d\epsilon}{2\pi} M_{\alpha}^{\beta}(p)M_{\beta\gamma}(q - p)
\]

(62)

for the continuum-continuum part coming from the product of two single-quasiparticle propagators. Here, we have introduced the auxiliary function

\[
M_{\alpha}^{\beta}(q) = G_{\alpha}^{\beta}(q)\Theta(\omega - 2\Delta).
\]

Note, that the imaginary part of \( M_{\alpha}^{\beta} \) is given by Eq. (40).

In order to carry out the energy integrals in Eqs. (59)-(62) we first make an analytic continuation of the integrands into the region of imaginary energies and then perform a contour integration. We are dealing with retarded propagators, so the contour should run along the real energy axis and be closed by a large arc in the lower half plane. Since the Green’s functions behaves like \( \omega^{-1} \) for \( |\omega| \to \infty \), Jordan’s lemma ensures that the contribution from the arc at infinity vanishes and we can evaluate the integral along the real axis by using of the theorem of residues.

Apart from \( f_{0}^{m,m}(q) \), which is analytical in the whole energy plane, all other terms in \( f_{0\alpha\beta}^{\delta\gamma} \) have single poles in the lower half plane. After calculating the corresponding residues we get for the imaginary part of \( f_{0\alpha\beta}^{\delta\gamma} \)

\[
\text{Im}\ f_{0\alpha\beta}^{\delta\gamma}(q) = -\pi \int \frac{d^3q}{(2\pi)^3} \left[ \{Z_{\alpha}^{\delta}(\vec{p})Z_{\beta}^{\gamma}(\vec{q} - \vec{p})\delta(\omega - \omega_{\vec{p}} - \omega_{\vec{q} - \vec{p}})\Theta(2\Delta - \omega_{\vec{p}})\Theta(2\Delta - (\omega - \omega_{\vec{p}})) + Z_{\alpha}^{\delta}(\vec{p})M_{\alpha\beta}^{\gamma}(q - \vec{p}, \omega - \omega_{\vec{p}})\Theta(2\Delta - \omega_{\vec{p}}) + ImM_{\alpha}^{\delta}(\vec{p}, \omega - \omega_{\vec{p}})Z_{\beta}^{\gamma}(\vec{q} - \vec{p})\Theta(2\Delta - \omega_{\vec{q} - \vec{p}})\} \right]
\]

(63)

through the causality relation

\[
\text{Re} f_{0\alpha\beta}^{\delta\gamma}(\vec{q}, \omega) = -\frac{1}{\pi} P \int \frac{d\epsilon}{\omega - \epsilon} \frac{\text{Im} f_{0\alpha\beta}^{\delta\gamma}(\vec{q}, \epsilon)}{\omega - \epsilon},
\]

(64)

where \( P \) denotes a Cauchy principal value. Since a calculation of the expression (64) requires less numerical effort than the direct method based on Eqs. (59)-(62), we will use it in our numerics.
VI. NUMERICAL RESULTS

Our calculation scheme contains several parameters: the condensate density $n_0$, the matrix functions $I$, $P$, and $A$, and the free quasiparticle spectrum $\omega_0^q$. For the condensate fraction we take $n_0 = 0.1n$, where $n$ is the density of the liquid. This assumption is in agreement with the condensate density extracted from experimental data\cite{5} and supported by Path Integral Monte Carlo calculations\cite{3,4}.

In a recent paper\cite{5}, we have presented first numerical results for $S(\vec{q}, \omega)$ obtained in a simplified version of the calculation with a momentum independent self energy of the quasiparticles and constant interactions between them. Since such an approximation led to some inconsistencies in the calculated spectra, in the present work we have removed this restriction for the self energy. However, for the sake of simplicity, we still treat the interaction functions as momentum and index independent, i.e.

$$I_{\alpha\beta}^q(\vec{q}) = g_4, \quad J_{\alpha\beta}^q(\vec{q}) = g_3. \quad (65)$$

Here, $g_4$ and $g_3$ are phenomenological constants. Similarly, we assume that the renormalization functions $A_{\alpha\beta}^q(\vec{q})$’s are momentum independent and equal in all channels (i.e. $A_{\alpha\beta}^q(\vec{q}) = A$ for $\alpha, \beta = 1, 2$). Obviously, this is not in line with the standard choices made to make a contact with ZRS-like models from the microscopic theory (see discussion in Sec. III A). However, under these assumptions, the elements of the Beliaev-Green’s matrix function are identical. If we now carry out summations over greek indices in our expressions, we are able to obtain a scheme of ZRS type.

In each iteration step, we have evaluated the dynamic structure factor for 56 $|\vec{q}|$-values and 501 $\omega$-values. As mentioned in Sec. V A, we have used the resulting spectrum $\omega^q$ as a consistency check: a solution was consistent, if after a certain number of iteration steps the renormalized spectrum did not change any more. Depending on the input parameters 10-50 steps were necessary to obtain a consistent solution.

A. Pitaevskii singularities

Let us first consider some general features of the results within a specific example with the Landau spectrum as the ‘bare’ quasiparticle spectrum $\omega_0^q$.

Results for the renormalized single-quasiparticle spectrum $\omega^q$, which is defined by Eq. (41), are shown in Fig. 7. $\omega^q$ is characterized by an maximum at the energy $\Delta_M = 9.6K$, a minimum at $\Delta_M = 7.0K$ and an endpoint at $(2\Delta_M, 2\Delta_M)$, where $\Delta_M$ is the wavevector of the roton minimum. At higher momentum transfers the renormalized spectrum differ qualitatively from the ‘bare’ spectrum. It bends toward $2\Delta_M$ due to quasiparticle decay. Since the density of states is high near the local extrema of the spectrum, we expect to observe a structure in the continuum part of $S(\vec{q}, \omega)$, whose origin is associated with the roton-roton, roton-maxon and maxon-maxon pair excitations. They are as well due to quasiparticle decay as discussed by Pitaevskii. Naively, one could expect to also observe features stemming from the plateau near the endpoint. But excitations associated to this part of the dispersion curve have a vanishing weight $Z^0_\alpha$ (the dashed-dotted line in Fig. 7) and corresponding singularities will not appear in the pair excitation spectrum.

In Fig. 8 we show results of the same calculation for $S(\vec{q}, \omega)$ at $q = 23 \text{ nm}^{-1}$. The dynamic structure factor consists of a sharp peak lying at the renormalized single-quasiparticle energy $\omega^q$ and a continuum, which is not featureless at all. As expected, we observe peaks at energies $2\Delta_R$, $\Delta_R + \Delta_M$ and $2\Delta_M$, respectively. Moreover, there is structure, which we cannot assign to particular regions of the single-quasiparticle excitation spectrum. We believe this to be a numerical defect. However, it has not been eliminated, since it is not important for the following discussion.

As mentioned above, we do not take phonons into account in our calculation. This results in a gap between the sharp peak and the continuum in $S(\vec{q}, \omega)$, For the same reason, there is no mechanism in the model, which would change the width of the sharp peak below the decay threshold.

B. Landau vs. Feynman spectrum

In this section, we want to compare results for $S(\vec{q}, \omega)$, which differ only in the ‘bare’ spectrum $\omega_0^q$ from each other (Fig. 7 and 10). All other input parameters are the same. They were chosen to reproduce the observed dynamic structure factor at $q = 23 \text{ nm}^{-1}$ in the case
The results at $q = 32 \text{ nm}^{-1}$ are presented in Fig. 11. In case of the Landau spectrum (left figure), we observe two peaks in the calculated $S(\vec{q}, \omega)$. The first one is due to Pitaevskii's singularities. Its position agrees with the experimental one to a good accuracy, however its strength does not fit the measured one any more. We will come back to this feature later. The continuum is dominated by a peak centered at $\omega \approx 35 \text{ K}$. It turns out, that this is the Landau energy of an excitation corresponding to the wavevector $q = 32 \text{ nm}^{-1}$ and the peak can be interpreted as quasifree peak. However, it appears at energy 25 K smaller than the observed one.

In case of the Feynman spectrum we still observe the shift of the whole structure to higher energies. But as expected, now the quasifree peak is qualitatively better described. Note, that now the shift is not the same for both peaks. The position of the quasifree peak is determined by the 'bare' spectrum, while the first peak (due to Pitaevskii singularities) comes from the renormalized one. So, its position should depend on other input parameters, i.e. vertex and renormalization functions.

As we see, neither the Landau spectrum nor the Feynman spectrum appears to be a good candidate for the 'bare' quasiparticle dispersion relation, if one wants to describe $S(\vec{q}, \omega)$ in a wide region of momentum transfers. While the Landau spectrum is better in the kinematic region, where the Pitaevskii's singularities play the dominant role, the Feynman spectrum is more suited for the quasifree region. Since our goal is a description of both regions, we decided to modify the 'bare' spectrum. In the following we use a phenomenological spectrum given by the dashed-dotted curve in Fig. 11. The phonon-maxon-roton part of the new $\omega^q$ agrees with the Landau spectrum (solid line), but it approaches the Feynman energy (dashed line) much faster above the roton minimum.

Apart from the Pitaevskii's singularities and the quasifree peak, in case of the Feynman spectrum there is an indication for a third peak lying between them (Fig. 10). It corresponds to the third experimental peak observed at $\omega \approx 39 \text{ K}$. But its strength is much to small compared with experiment. We will discuss this issue in more detail below.

C. $S(\vec{q}, \omega)$ with 'new' quasiparticles

The effects of the modified 'bare' quasiparticle spectrum on $S(\vec{q}, \omega)$ are shown in Fig. 12. In this calculation, we used

$$g_3 = 0.3 \text{ Knm}^{3/2}, \quad g_4 = 0.19 \text{ Knm}^3, \quad A = 0.4$$

and the Gaussian resolution function discussed in the previous section. As expected, the results at $q = 32 \text{ nm}^{-1}$ small.

of the Landau 'bare' quasiparticle spectrum as well as possible. The values are as follows:

$$g_3 = 0.5 \text{ Knm}^{3/2}, \quad g_4 = -0.04 \text{ Knm}^3, \quad A = 0.25.$$  \hspace{1cm} (66)

To include experimental resolution we have convoluted the calculated $S(\vec{q}, \omega)$ with a Gaussian function. The standard deviation of the Gaussian was taken to be $2.46 \text{ K}$ in agreement with the experimental resolution obtained by Fák and Bossy.

In Fig. 8 results for $S(\vec{q}, \omega)$ at $q = 23 \text{ nm}^{-1}$ are shown in comparison to experiment. We see that, indeed, in the case of the Landau 'bare' spectrum (left figure), the calculated results describe the two peak structure present in experimental data well. The lower energy peak corresponds to single-quasiparticle excitations. The higher energy structure comes from the Pitaevskii singularities discussed in the previous section. They have merged into a broad peak due to the convolution with a Gaussian. The theoretical and experimental strengths of the peaks agree to a reasonable accuracy. However, the calculated peaks appear at somewhat different energies as compared to the experimental data.

The results in case of the Feynman spectrum are much worse. We still observe a two peak structure, but the peaks are shifted to higher energies. Moreover, the strength of the single-quasiparticle peak is too small in relation to that of the second one. The shift in the energies indicates that the input parameters were too small to force the spectrum down to the experimental one. Actually, one can try to find some parameters, which lead to better results with the Feynman spectrum. But the stronger the vertex functions, the smaller the difference between the potential and kinetic energy of quasiparticles and the worse the approximation about locality of the vertices.
are now much better than in the case of the Landau spectrum. First of all, we see that the quasifree peak is sitting at the right position. Moreover, weights of the dominant peaks agree to a better accuracy with experiment. There is also evidence for the third peak observed in experiment. But its intensity is still much too small. However, the results at \( q = 23 \text{ nm}^{-1} \) and \( q = 28 \text{ nm}^{-1} \) are not satisfactory. In both cases the qualitative structure of \( S(\vec{q}, \omega) \) is still reasonable, but the agreement with the experiment is now much worse than at \( q = 32 \text{ nm}^{-1} \).

From the analysis of the results we are led to the conclusion, that it is difficult to describe \( S(\vec{q}, \omega) \) in a wide momentum region in the framework of ZRS-like models with momentum independent input parameters. We will remove this restriction consistently during further refinement of the calculation.

If the above conclusion was true, we should be able to find another set of parameters, which leads to better results for \( S(\vec{q}, \omega) \) at \( q = 23 \text{ nm}^{-1} \) or \( q = 28 \text{ nm}^{-1} \). Indeed, we have found such parameters, which lead to reasonable results in the region of smaller momenta. In Fig. 13, we present \( S(\vec{q}, \omega) \) calculated with

\[
g_3 = 0.5 \text{ Kmn}^{3/2}, \quad g_4 = -0.08 \text{ Kmn}^{3} \quad \text{and} \quad A = 0.265. \tag{68}
\]

Now, \( S(\vec{q}, \omega) \) at \( q = 23 \text{ nm}^{-1} \) is described quite well. However, if we compare Fig. 13 with the results of the previous section obtained with the Landau spectrum, we see, that the modification of the spectrum results in an unreasonable plateau at higher energies. This again points to a possible momentum dependence of the interaction parameters. Although somewhat worse than at \( q = 23 \text{ nm}^{-1} \), the calculated spectrum at \( q = 28 \text{ nm}^{-1} \) is still reasonable compared to the experiment in this special case of input parameters. And the results at \( q = 32 \text{ nm}^{-1} \), which are now worse than in the previous case, seem to confirm our conclusion that input parameters must be momentum dependent.

From the input parameters reported in (67) and (68)
FIG. 11: Our ‘free’ quasiparticle spectrum (dotted-dashed line): we modify the Landau curve (solid line) in the region above the roton minimum such that it approaches Feynman spectrum (dashed line) much faster.

an interesting feature of the irreducible four-point vertex function \( g_4 \) follows. We have achieved the best fit to the data at intermediate momenta for a negative \( g_4 \). But at high momenta, \( g_4 \) has to be positive in order to describe \( S(\vec{q}, \omega) \) properly. Thus, the effective interaction between quasiparticles changes its character from an attraction at intermediate momenta to a repulsion at higher ones. We will come back to this feature in forthcoming work.

As we know from Eq. (31), there are three contributions to \( S(\vec{q}, \omega) \), which come from the single-quasiparticle, interference and two-quasiparticle terms. We will refer to them as \( S^{(1)} \), \( S^{(int)} \) and \( S^{(2)} \), respectively. The energy integrated strengths of these contributions are reported in Table I. There are two important features shown in the table. First, \( S^{(int)} \) reduces the strength of the sharp single-quasiparticle peak at \( q = 23 \text{ nm}^{-1} \) and of the continuum at \( q = 32 \text{ nm}^{-1} \). Secondly, and more important, in all cases the structure factor is dominated by the two-particle contribution \( S^{(2)} \). Thus the expression

\[
S(\vec{q}, \omega) \propto \text{Im}G(\vec{q}, \omega),
\]

which was used in the literature (e.g. Ref. 3) in order to calculate \( S(\vec{q}, \omega) \) within ZSR-type models, cannot describe the data in the momentum region under consideration, since the most relevant term is neglected.

D. Comparisons with other calculations

In this section, we want to compare our results with those obtained by other methods. We will limit ourselves to the work of Götze and Lücke and of Manousakis and Pandharipande. All theoretical results are compared to the experimental data of Fäk and Bossy.

Götze and Lücke presented a detailed analysis of \( S(\vec{q}, \omega) \) for superfluid \(^4\text{He} \) at \( T = 0 \) within the memory function formalism. Their results at two selected momenta are presented in Fig. 14. In order to make comparisons with experiment we have convoluted the calculated spectra with the Gaussian resolution function discussed in Sec. VII.

In Fig. 15 we show \( S(\vec{q}, \omega) \) calculated by Manousakis and Pandharipande, who used correlated-basis-function methods at \( T = 0 \). Again, the theoretical spectra are convoluted with the above mentioned Gaussian resolution function.

In order to facilitate comparison of the different methods our best results for the dynamic structure factor are plotted again in Fig. 16. Recall, that each plot corresponds to different parameter sets in order to simulate...
FIG. 13: \( S(\vec{q}, \omega) \) calculated from the modified Landau spectrum, but with different interaction parameters: \( g_3 = 0.5 \) Knm\(^{3/2}\), \( g_4 = -0.08 \) Knm\(^3\) and \( A = 0.265 \). They were chosen to give a reasonable fit to the experimental data at \( q = 23 \) nm\(^{-1}\).

Table I: Energy integrated contributions to \( S(\vec{q}, \omega) \) from the single-quasiparticle, interference and two-quasiparticle terms at different momentum transfers. The contributions at \( q = 23 \) nm\(^{-1}\) and \( q = 28 \) nm\(^{-1}\) have been obtained with \( g_3 = 0.5 \) Knm\(^{3/2}\), \( g_4 = -0.08 \) Knm\(^3\) and \( A = 0.265 \). For \( q = 32 \) nm\(^{-1}\), we used \( g_3 = 0.3 \) Knm\(^{3/2}\), \( g_4 = 0.19 \) Knm\(^3\) and \( A = 0.4 \). The dynamic structure factor at \( q = 28 \) nm\(^{-1}\) and \( q = 32 \) nm\(^{-1}\) contains only a structured continuum. At these momenta, there is no sharp peak in \( S(\vec{q}, \omega) \), since the strength \( Z_\beta^\alpha \) given by Eq. (43) vanishes.

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VII. CONCLUSIONS

In this paper, we presented a calculation of the dynamic structure factor of superfluid \(^4\)He in the intermediate and high momentum transfer region within a model based on the Gavoret-Nozières\(^6\) microscopic theory. After the introduction of quasiparticles, we obtained an RPA-like expression for the density-density correlation function in a model, which has similarities to the phenomenological field theory of Zawadowski, Ruvalds and Solana\(^6\), but treats the condensate explicitly. We evaluated \( S(\vec{q}, \omega) \) numerically for the special case of momentum independent interactions between the quasiparticles. Our results suggest the following conclusions:

(i) The quasiparticles, that were introduced here, can be interpreted as helium atoms renormalized by the two-particle irreducible part of the self energy. Quasifree scattering may be used to determine the high energy part of the ‘bare’ quasiparticle spectrum appropriately.

(ii) \( S(\vec{q}, \omega) \) consists of three terms: one- and two-quasiparticle excitations and an interference term, \( S^{(1)} \), \( S^{(2)} \) and \( S^{(int)} \), respectively. All terms have the same pole structure and appear to be equally important in the momentum region at and above the roton minimum. Thus the expression \( S(\vec{q}, \omega) \propto \text{Im} G(\vec{q}, \omega) \) often used in literature in order to calculate the dynamic structure factor in ZRS-type models neglects important terms. In the absence of the condensate only the \( S^{(2)} \) term remains.

(iii) A model which employs momentum independent interactions cannot account quantitatively for the neutron scattering data in a wide momentum region.

(iv) The two-quasiparticle interaction \( g_4 \) should be attractive at intermediate momenta and repulsive at higher momentum transfers.

(v) As is seen from the comparison with other calculations, our model provides an alternative description of the experimental data. However, no method describes qualitatively the data at \( |\vec{q}| \geq 30 \) nm\(^{-1}\). This may indicate a lack of understanding of the underlying physics.
FIG. 14: Calculation of $S(\vec{q}, \omega)$ by Götze and Lücke\cite{gotze1992} using the memory function formalism at two selected momenta compared to experiment. The calculated spectra have been convoluted with a Gaussian resolution function as discussed in Sec. VIA.

FIG. 15: Calculation of $S(\vec{q}, \omega)$ by Manousakis and Phandaripande\cite{manousakis1994} using correlated basis function methods. See caption of Fig. 14 for more details.

FIG. 16: Our best results for $S(\vec{q}, \omega)$ at two selected momenta. The case $q = 23$ nm$^{-1}$ corresponds to $g_3 = 0.5$ Knm$^{3/2}$, $g_4 = -0.08$ Knm$^3$ and $A = 0.265$. For $q = 32$ nm$^{-1}$, we have used $g_3 = 0.3$ Knm$^{3/2}$, $g_4 = 0.19$ Knm$^3$ and $A = 0.4$.

We now turn to a somewhat more detailed discussion of the point (iii). At present, we do not know very well $g_3$ and $g_4$ as functions of $\vec{q}$. Thus for the sake of simplicity we assumed, that they are weakly momentum dependent and can be approximated by constants. The same holds for the residues $A^\beta$. For the chosen parameters, we evaluated $S(\vec{q}, \omega)$ at 56 values of $|\vec{q}|$. Our results show that it is difficult to describe $S(\vec{q}, \omega)$ in a wide momentum transfer region within a model with constant parameters $g_3$, $g_4$ and $A$. To avoid this problem, we have 'simulated' a momentum dependence by calculating the structure factor with different parameter sets. For each set, we picked out from the 56 spectra those with reasonably good agreement with experiment. In this way, we got...
sets of parameters, that led to good results in different momentum intervals.

Clearly, we have made progress towards the development of a quasiparticle model, which treats condensate and non-condensate terms in $S(\vec{q}, \omega)$ on the same footing. However, the numerical calculation needs further refinement which will be addressed in future work.

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REFERENCES

* michael.weyrauch@ptb.de; http://www.ptb.de/english/org/q/q1/q102/he4-team.htm

1 A. Griffin, *Excitations in a Bose-Condensed Liquid* (Cambridge University Press, Cambridge, 1993).
2 H. R. Glyde, *Excitations in Liquid and Solid Helium* (Clarendon Press, Oxford, 1994).
3 H. R. Glyde and A. Griffin, Phys. Rev. Lett. 65, 1454 (1990).
4 J. Gavoret and P. Nozières, Ann. Phys. 28, 349 (1964).
5 L. P. Pitaevskii, Sov. Phys. JETP 36, 830 (1959).
6 A. Zawadowski, J. Ruvalds, and J. Solana, Phys. Rev. A 5, 399 (1972).
7 R. Hastings and J. Halley, Phys. Rev. A 10, 2488 (1974).
8 F. Pistolesi, Phys. Rev. Lett. 81, 397 (1998).
9 S. T. Beliaev, Sov. Phys. JETP 34, 289 (1958).
10 N. N. Bogoliubov, J. Phys. USSR 11, 23 (1947).
11 L. D. Landau, J. Phys. U.S.S.R. 11, 91 (1947).
12 R. Feynman, Phys. Rev. 94, 262 (1954).
13 K. Fukushima and F. Iseki, Phys. Rev. B 38, 4448 (1988).
14 K. J. Juge and A. Griffin, J. Low Temp. Phys. 97, 105 (1994).
15 G. D. Mahan, *Many-Particle Physics* (Plenum, New York, 1990).
16 B. Fáčik and J. Bossy, J. Low Temp. Phys. 112, 1 (1998).
17 W. Götze and M. Lücke, Phys. Rev. B 13, 3822 (1976).
18 W. M. Snow, Y. Wang, and P. E. Sokol, Europhys. Lett. 19, 403 (1992).
19 D. M. Ceperley and E. L. Pollock, Phys. Rev. Lett. 56, 351 (1986).
20 D. M. Ceperley and E. L. Pollock, Can. J. Phys. 65, 1416 (1987).
21 J. Szwabiński and M. Weyrauch, J. Low Temp. Phys. 121 (2000).
22 J. Szwabiński and M. Weyrauch (2001), to be published.
23 E. Manousakis and V. R. Pandharipande, Phys. Rev. B 30, 5062 (1984).
24 E. Manousakis and V. R. Pandharipande, Phys. Rev. B 33, 150 (1986).