Sum rules for density and particle excitations in Bose superfluids

S. Stringari
Dipartimento di Fisica, Università di Trento, I-38050 Povo, Italy
(Received 29 January 1992)

Various sum rules for the density and particle operators are derived and discussed. We investigate in detail the properties of the particle state, the natural counterpart of the Feynman state describing collective density excitations. An explicit expression for the energy of the particle state is derived in terms of the interatomic potential, the two-body half-diagonal density, and the momentum distribution. Sum rules accounting for the coupling between particle and density excitations are also derived and the role of the Bose-Einstein condensation explicitly pointed out. Finally we discuss the separate contribution to the various sum rules arising from one-phonon and multiparticle excitations.

I. INTRODUCTION

The theoretical investigation of the elementary excitations (phonons, maxons, and rotons) of superfluid ^{4}He has been the object of extensive and systematic work following the pioneering papers by Landau.[1,2] In most theoretical approaches the microscopic description of the elementary modes is given in terms of density excitations starting from the Bijl-Feynman proposal[3,4]

$$|F\rangle=\frac{1}{\sqrt{NS(q)}}\rho_{\mathbf{q}}|0\rangle \; , \tag{1.1}$$

later improved to include back-flow corrections and coupling with two or more density excitation states (see, for example, Refs. 5–9). In Eq. (1.1) $S(q)$ is the usual static form factor ensuring the normalization of the state. At low momenta the Feynman state (1.1) yields exactly the energy of the phonon state. Conversely, at higher q it gives a rather poor description of the maxon-roton states due to the role of multiparticle excitations that are sizably excited by the *density* operator ρ_q.

A natural alternative to the density picture is provided by the *particle* choice

$$|P\rangle=\frac{1}{\sqrt{n(q)}}a_{-\mathbf{q}}|0\rangle \; , \tag{1.2}$$

where $a_{\mathbf{q}}$ is the particle annihilation operator and $n(q)$ is the momentum distribution of the system.

Different from the Feynman state—whose properties have been extensively investigated in the literature—much less is known, from a microscopic point of view, about the particle state (1.2), except in the limit of the dilute Bose gas (Bogoliubov limit[10]), where $|F\rangle$ and $|P\rangle$ coincide with the exact solution of the many-body problem. The coupling between these states, due to the Bose Einstein condensation, is at the origin of rather fundamental features exhibited by the density and particle Green's functions[11–13] that are known to share the same poles corresponding, at low q, to the phonon branch.[13]

The purpose of this work is to discuss in a systematic way various sum rules for the density and particle operators. Some of them permit us to calculate the energy of the particle state (1.2) as well as its coupling with the Feynman state (1.1) as a function of q. They consequently contain useful information on the *particle* nature of the elementary excitations in Bose superfluids and can be used to derive rigorous upper bounds for the energy of the elementary excitations.

The paper is organized as follows. In Sec. II we provide a brief summary of sum rules for the density operator. These results are also used to derive a nontrivial lower bound for the compressibility sum rule at zero temperature.

In Sec. III we present a detailed study of various sum rules for the particle operators a_q and $a_q^\dagger$ and provide an investigation of the energy of the particle state (1.2). In Sec. IV we investigate crossed sum rules for the density and particle operators. These sum rules are peculiar of Bose superfluids and permit us to study the coupling between density and particle excitations due to the occurrence of the Bose condensate. In Sec. V we discuss in a systematic way the contributions to the different sum rules arising from one-phonon and multiparticle states in the low-momentum region.

II. SUM RULES FOR THE DENSITY OPERATOR

Sum rules for the density operator $\rho_{\mathbf{q}}$ have been extensively studied in quantum liquids (see for example Refs. 6 and 14–16). In this section we present a short summary of the main results. The positive-energy-weighted sum rules will be used at the end of the section to provide a useful rigorous lower bound for the compressibility sum rule (inverse-energy-weighted sum rule) at zero temperature.

Let us consider the density spectral function

$$\begin{aligned}A_{\rho^\dagger,\rho}(q,\omega)&=\int dt\, e^{i\omega(t-t')}\langle[\rho_{\mathbf{q}}^\dagger(t),\rho_{\mathbf{q}}(t')]\rangle\\&=\frac{1}{Z}\sum_{m,n}(e^{-\beta E_m}-e^{-\beta E_n})\langle m|\rho_{\mathbf{q}}^\dagger|n\rangle\langle n|\rho_{\mathbf{q}}|m\rangle\delta(\omega-E_n+E_m)\;,\end{aligned}\tag{2.1}$$

where $Z=\sum_n e^{-\beta E_n}$ is the partition function, $|n\rangle$ and E_n are eigenstates and eigenvalues of the Hamiltonian of the system, and $\rho_{\mathbf{q}}=\sum_k a^\dagger_{\mathbf{k}+\mathbf{q}} a_{\mathbf{k}}$ is the usual density operator.

The spectral function is related to the retarded Green's function through the well-known dispersion relation:

$$G^R(q,\omega)=\int_{-\infty}^{+\infty}\frac{A(x)}{\omega-x} . \tag{2.2}$$

On the other hand the dynamic structure function $S(q,\omega)$, measured in inelastic neutron scattering, is related to the spectral function through the equation

$$S(q,\omega)=\frac{A_{\rho^\dagger,\rho}(q,\omega)}{1-e^{-\beta\omega}} . \tag{2.3}$$

By using Eq. (2.3) and the completeness relationship $\sum_n |n\rangle\langle n|=1$ one can easily find compact expressions for the moments

$$m_p(q)=\int_{-\infty}^{\infty}\omega^p S(q,\omega)d\omega \tag{2.4}$$

of $S(q,\omega)$ that can be consequently calculated, avoiding the much more difficult problem of evaluating the complete ω dependence of the dynamic structure function. One finds

$$m_0(q)=\int_{-\infty}^{+\infty}\frac{1}{1-e^{-\beta\omega}}A_{\rho^\dagger,\rho}(q,\omega)d\omega=\langle\rho^\dagger_{\mathbf{q}}\rho_{\mathbf{q}}\rangle , \tag{2.5}$$

$$m_1(q)=\tfrac{1}{2}\int_{-\infty}^{+\infty}\omega A_{\rho^\dagger,\rho}(q,\omega)d\omega=\tfrac{1}{2}\langle[\rho^\dagger_{\mathbf{q}},[H,\rho_{\mathbf{q}}]]\rangle , \tag{2.6}$$

$$m_2(q)=\int_{-\infty}^{+\infty}\frac{\omega^2}{1-e^{-\beta\omega}}A_{\rho^\dagger,\rho}(q,\omega)d\omega =\langle[\rho^\dagger_{\mathbf{q}},H][H,\rho_{\mathbf{q}}]\rangle , \tag{2.7}$$

$$m_3(q)=\tfrac{1}{2}\int_{-\infty}^{+\infty}\omega^3 A_{\rho^\dagger,\rho}(q,\omega)d\omega =\tfrac{1}{2}\langle[[[\rho^\dagger_{\mathbf{q}},H],H],[H,\rho_{\mathbf{q}}]]\rangle . \tag{2.8}$$

Note that at $T=0$ one can write

$$S(q,\omega)=\sum_n |\langle n|\rho_{\mathbf{q}}|0\rangle|^2\delta(\omega-\omega_{n0}) , \tag{2.9}$$

where $\omega_{n0}=E_n-E_0$ and hence

$$m_p(q)=\int_0^\infty \omega^p S(q,\omega)d\omega=\sum_n \omega^p_{n0}|\langle n|\rho_{\mathbf{q}}|0\rangle|^2 . \tag{2.10}$$

In principle, the moments m_p can be determined experimentally by explicit integration of the dynamic structure function $S(q,\omega)$, measured via inelastic neutron scattering.[17] In practice, the inaccuracy of experimental data at high ω makes the determination of the high-frequency moments difficult. Contrariwise, the occurrence of the collective phonon-maxon-roton branch, typical of superfluid ^{4}He, makes the low-frequency region much easier to control.

By explicitly carrying out the commutators entering Eqs. (2.5)–(2.8) with the general Hamiltonian ($\hbar=1$),

$$H=\sum_i\frac{1}{2m}p_i^2+\sum_{i<j}V(|\mathbf{r}_i-\mathbf{r}_j|) =\sum_k\frac{1}{2m}k^2a^\dagger_{\mathbf{k}}a_{\mathbf{k}}+\tfrac{1}{2}\sum_{\mathbf{k},\mathbf{p},\mathbf{q}}V(q)a^\dagger_{\mathbf{k}+\mathbf{q}}a^\dagger_{\mathbf{p}-\mathbf{q}}a_{\mathbf{p}}a_{\mathbf{k}} , \tag{2.11}$$

where $V(q)=(1/V)\int d\mathbf{r}\, e^{i\mathbf{q}\cdot\mathbf{r}}V(r)$, one can find explicit expressions for the moments m_p. The main results are here briefly summarized.

The m_0 moment is proportional to the static structure function

$$m_0=\langle\rho^\dagger_{\mathbf{q}}\rho_{\mathbf{q}}\rangle=NS(q) , \tag{2.12}$$

which is related to the pair-correlation function $g(r)$,

$$\rho^2 g(|\mathbf{r}_1-\mathbf{r}_2|)=\rho^{(2)}(\mathbf{r}_1,\mathbf{r}_2;\mathbf{r}_1,\mathbf{r}_2) , \tag{2.13}$$

through the equation

$$S(q)-1=\int[g(r)-1]e^{-i\mathbf{q}\cdot\mathbf{r}}d\mathbf{r} . \tag{2.14}$$

The two-body density of Eq. (2.14) is defined by

$$\rho^{(2)}(\mathbf{r}_1,\mathbf{r}_2;\mathbf{r}'_1,\mathbf{r}'_2)=N(N-1)\int\Psi^*(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3,\ldots)\Psi(\mathbf{r}'_1,\mathbf{r}'_2,\mathbf{r}_3,\ldots)d\mathbf{r}_3\cdots d\mathbf{r}_N . \tag{2.15}$$

The comparison between theory and experiments has been extensively carried out at the level of the sum rule (2.12) (see for example Ref. 18 and references therein). In fact, on the one hand, neutron and x-ray scattering experiments provide a good determination of $S(q)$. On the other hand, the pair-correlation functions $g(r)$ is available with high accuracy starting from microscopic calculations of the ground-state wave function.[19]

The energy-weighted moment is fixed by the model independent f-sum rule:[20]

$$m_1(q)=\tfrac{1}{2}\langle[\rho^\dagger_{\mathbf{q}},[H,\rho_{\mathbf{q}}]]\rangle=N\frac{q^2}{2m} . \tag{2.16}$$

Result (2.16) simply follows from the velocity independence of the interatomic potential (2.11), which commutes with the density operator $[V,\rho_{\mathbf{q}}]=0$.

The m_2 moment is given by the sum rule[6,15]

$$m_2(q)=\langle[\rho^\dagger_{\mathbf{q}},H][H,\rho_{\mathbf{q}}]\rangle=N\left[\left[\frac{q^2}{2m}\right]^2[2-S(q)]+\frac{q^2}{m^2}D(q)\right] , \tag{2.17}$$

where

$$D(q)=\frac{1}{N}\int d\mathbf{r}_1 d\mathbf{r}_2\cos[q(z_1-z_2)]\nabla_1^z\nabla_2^z\rho^{(2)}(\mathbf{r}_1,\mathbf{r}_2;\mathbf{r}'_1,\mathbf{r}'_2)|_{\mathbf{r}_1=\mathbf{r}'_1,\mathbf{r}_2=\mathbf{r}'_2} \tag{2.18}$$

is the kinetic structure function. Here and in the following the wave vector $\mathbf{q}$ will be taken along the z direction. Differently from the static structure function $S(q)$, the determination of $D(q)$ requires the knowledge of off-diagonal components of the two-body density (2.15). Few microscopic calculations[6,21] are at present available for the function $D(q)$.

The cubic moment m_3 can also be easily calculated in terms of commutators. One finds the following result:[22]

$$m_3(q)=\tfrac{1}{2}\langle[[[\rho_{\mathbf{q}}^\dagger,H],H],[H,\rho_{\mathbf{q}}]]\rangle$$
$$=N\left[\left[\frac{q^2}{2m}\right]^3+\frac{q^4}{m^2}\langle E_K\rangle +\rho\frac{q^2}{2m^2}\int d\mathbf{s}(1-\cos qz)g(s)\nabla_z^2V(s)\right], \tag{2.19}$$

where $\langle E_K\rangle$ is the kinetic energy of the system. This sum rule has been extensively employed to investigate the role of multiparticle excitations[23] in superfluid ^{4}He and has also been used in the study of Fermi liquids [electrons (Refs. 24 and 25) and ^{3}He (Refs. 26 and 27)].

We point out that equations (2.12)–(2.19) rigorously hold for any value of q and that their determination requires only the knowledge of the two-body density matrix relative to the ground state. In particular only the structure functions $S(q)$ and $D(q)$ (in addition to the kinetic energy $\langle E_K\rangle$) are needed for their explicit evaluation.

In the last part of the section we use the sum rules m_0, m_1, m_2, and m_3 in order to get a rigorous constraint on the inverse-energy-weighted moment

$$m_{-1}(q)=\int_0^\infty \frac{1}{\omega}S(q,\omega)d\omega \tag{2.20}$$

at zero temperature. As previously anticipated the occurrence of a discretized collective branch in Bose systems makes the experimental determination of this moment, through the explicit integration of the dynamic structure function, considerably more precise than that of any positive moment due to the $1/\omega$ factor that suppresses the contributions arising from the high-frequency region. The experimental analysis of $m_{-1}(q)$ in superfluid ^{4}He was discussed by Cowley and Woods[17] who pointed out the occurrence of an important structure in the roton region (see Fig. 1). The m_{-1} sum rule is also known as the compressibility sum rule and in the long-wavelength limit reduces to

$$\lim_{q\to 0} m_{-1}(q)=\frac{N}{2mc^2}, \tag{2.21}$$

where c is the usual sound velocity. The interest in a better knowledge of $m_{-1}(q)$ is also related to its crucial role in the density-functional theory of inhomogeneous quantum systems (see, for example, Ref. 28 and references therein).

The m_{-1} moment is related to the static response to an external field coupled to the system through the density operator:

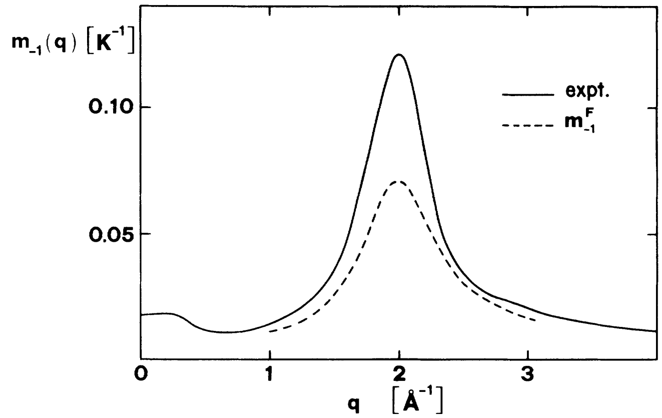

FIG. 1. Polarizability sum rule m_{-1} as a function of q. The solid line gives the experimental results from Ref. 17. The dashed line gives the Feynman lower bound (2.27).

$$H(\lambda)=H+\lambda\rho_{\mathbf{q}}^\dagger . \tag{2.22}$$

The density fluctuations induced by the external field λ then provide the static polarizability and hence the m_{-1} moment:

$$\lim_{\lambda\to 0}\frac{1}{\lambda}\langle\lambda|\rho_{\mathbf{q}}|\lambda\rangle=-2m_{-1}(q), \tag{2.23}$$

where $|\lambda\rangle$ is the ground state of $H(\lambda)$. Any restricted variational determination of the state $|\lambda\rangle$ starting from Hamiltonian (2.22) then provides a *lower bound* for the moment m_{-1}. The simplest basis to carry out such a calculation is given by the choice

$$|\lambda\rangle=|0\rangle+\alpha\rho_{\mathbf{q}}|0\rangle \tag{2.24}$$

accounting for the coupling between the ground state and the Feynman state

$$|F\rangle=\frac{1}{\sqrt{NS(q)}}\rho_{\mathbf{q}}|0\rangle . \tag{2.25}$$

The variational calculation yields the result[14]

$$m_{-1}(q)\ge m_{-1}^F(q) \tag{2.26}$$

with the Feynman lower bound given by

$$m_{-1}^F(q)=\frac{m_0(q)^2}{m_1(q)}=NS(q)^2\frac{2m}{q^2} . \tag{2.27}$$

This calculation is equivalent to assuming that the strength of the density operator is concentrated in a single collective mode exhausting the sum rules m_{-1}, m_0, and m_1. It is exact only in the low-q limit where $S(q)\to q/2mc$, and one finds

$$m_{-1}(q=0)=m_{-1}^F(q=0)=N\frac{1}{2mc^2} . \tag{2.28}$$

As discussed in Ref. 14, the Feynman approximation significantly underestimates the experimental value of m_{-1} in the maxon-roton region (see Fig. 1), since it does not provide any decoupling between its collective and multiparticle components. For the same reason the energy of the Feynman state (2.25),

$$\varepsilon_F=\frac{m_1}{m_0}=\frac{q^2}{2mS(q)}\ , \tag{2.29}$$

provides only a poor estimate of the energy of the collective state except in the low-q limit.

A natural improvement of the Feynman ansatz is given by the choice[6]

$$|\lambda\rangle=|0\rangle+\alpha\rho_{\mathbf{q}}|0\rangle+\beta(|[H,\rho_{\mathbf{q}}]-\varepsilon_F\rho_{\mathbf{q}})|0\rangle\ , \tag{2.30}$$

where α and β are parameters to be fixed in the variational calculation of the static polarizability. The combination of the operators entering the term in β ensures its orthogonality to the Feynman state $\rho_{\mathbf{q}}|0\rangle$. With respect to the Feynman ansatz (2.25), choice (2.30) enlarges the basis of the variational calculation and consequently yields a higher lower bound for m_{-1} (a similar ansatz was employed in Ref. 6 to lower the Feynman upper bound for the excitation energy). A straightforward calculation yields

$$m_{-1}(q)\geq\frac{m_{-1}^F(q)}{1-\Delta(q)/\varepsilon_b(q)}\ , \tag{2.31}$$

where

$$\varepsilon_b(q)=\frac{\langle b|H|b\rangle}{\langle b|b\rangle}=\frac{\left[\frac{m_3}{m_1}+\left[\frac{m_1}{m_0}\right]^2-2\frac{m_2}{m_0}\right]}{\left[\frac{m_2}{m_1}-\frac{m_1}{m_0}\right]}\ , \tag{2.32}$$

is the energy of the state $|b\rangle=([H,\rho_{\mathbf{q}}]-\varepsilon_F\rho_{\mathbf{q}})|0\rangle$ and the (positive) variance $\Delta(q)$ is defined by

$$\Delta(q)=\frac{m_2(q)}{m_1(q)}-\frac{m_1(q)}{m_0(q)}\ . \tag{2.33}$$

The explicit evaluation of the new lower bound requires the knowledge of the sum rules m_0, m_1, m_2, and m_3. At small q the ratio $\Delta(q)/\varepsilon_b(q)$ behaves like q^2 and the lower bound (2.31) approaches the exact $q=0$ result (2.28). At higher momenta one expects a significant improvement with respect to the Feynman lower bound.

III. SUM RULES FOR THE PARTICLE OPERATOR

The particle spectral function is defined, analogously to the density spectral function (2.1), by the equation

$$\begin{aligned}A_{a^\dagger,a}(q,\omega)&=\int dt\, e^{i\omega(t-t')}\langle[a_{\mathbf{q}}^\dagger(t),a_{\mathbf{q}}(t')]\rangle\\&=\frac{1}{Z}\sum_{m,n}(e^{-\beta E_m}-e^{-\beta E_n})\langle m|a_{\mathbf{q}}^\dagger|n\rangle\langle n|a_{\mathbf{q}}|m\rangle\delta(\omega-E_n+E_m),\end{aligned} \tag{3.1}$$

where E_m, E_n are eigenvalues of the grand canonical Hamiltonian

$$H'=H-\mu N\ . \tag{3.2}$$

The spectral function (3.1) is related to the particle Green's function through the general relation (2.2).

Several sum rules can be derived for the particle spectral function. Using the completeness relation for the eigenstates of the Hamiltonian one finds the following results for a system of interacting bosons:

$$\int_{-\infty}^{+\infty}A_{a^\dagger,a}(q,\omega)d\omega=\langle[a_{\mathbf{q}}^\dagger,a_{\mathbf{q}}]\rangle=-1\ , \tag{3.3}$$

$$\int_{-\infty}^{+\infty}\frac{1}{1-e^{-\beta\omega}}A_{a^\dagger,a}(q,\omega)d\omega=\langle a_{\mathbf{q}}^\dagger a_{\mathbf{q}}\rangle=n(q)\ , \tag{3.4}$$

$$\int_{-\infty}^{+\infty}\omega A_{a^\dagger,a}(q,\omega)d\omega=\langle[a_{\mathbf{q}}^\dagger,[H',a_{\mathbf{q}}]]=\frac{q^2}{2m}-\mu+NV(0)+\sum_{\mathbf{p}}n(|\mathbf{p}+\mathbf{q}|)V(p)\ , \tag{3.5}$$

$$\int_{-\infty}^{+\infty}\frac{\omega}{1-e^{-\beta\omega}}A_{a^\dagger,a}(q,\omega)d\omega=\langle a_{\mathbf{q}}^\dagger[H',a_{\mathbf{q}}]\rangle=\left[\mu-\frac{q^2}{2m}\right]n(q)-\sum_{\mathbf{p}}n(\mathbf{q},\mathbf{p})V(p)\ . \tag{3.6}$$

In the above equations $V(p)$ is the Fourier transform of the interaction potential [see Eq. (2.11)], $n(q)=\langle a_{\mathbf{q}}^\dagger a_{\mathbf{q}}\rangle$ is the momentum distribution of the system and

$$n(\mathbf{q},\mathbf{p})=\langle\rho_{\mathbf{p}}a_{\mathbf{q}-\mathbf{p}}^\dagger a_{\mathbf{q}}\rangle-n(q) \tag{3.7}$$

is the two-body momentum distribution recently investigated in Ref. 29. In terms of the off-diagonal two-body density (2.15) one can write

$$n(\mathbf{q},\mathbf{p})=\frac{1}{V}\int d\mathbf{r}_1d\mathbf{r}_2d\mathbf{r}_1'\rho^{(2)}(\mathbf{r}_1,\mathbf{r}_2;\mathbf{r}_1',\mathbf{r}_2)e^{-i\mathbf{q}\cdot(\mathbf{r}_1'-\mathbf{r}_1)}e^{-i\mathbf{p}\cdot(\mathbf{r}_1-\mathbf{r}_2)}\ . \tag{3.8}$$

Results (3.3)–(3.5) are well known in the literature (see for example Ref. 30). In particular result (3.3) follows from the

Bose commutation rule, while result (3.4) defines the momentum distribution of the system. Result (3.5) was first discussed by Wagner.[31] Conversely result (3.6) has never been discussed, to our knowledge, in the context of Bose superfluids.

The sum rules (3.4) and (3.6) have a particularly clear interpretation in the $T=0$ limit where the left-hand side can be written in the following way

$$\int_{-\infty}^{+\infty}\frac{1}{1-e^{-\beta\omega}}A_{a^\dagger,a}(q,\omega)d\omega=\int_0^{+\infty}A_{a^\dagger,a}(q,\omega)d\omega=\sum_n|\langle n|a_{-\mathbf{q}}|0\rangle|^2\,, \tag{3.9}$$

$$\int_{-\infty}^{+\infty}\frac{\omega}{1-e^{-\beta\omega}}A_{a^\dagger,a}(q,\omega)d\omega=\int_0^{+\infty}\omega A_{a^\dagger,a}(q,\omega)d\omega=\sum_n\omega_{n0}|\langle n|a_{-\mathbf{q}}|0\rangle|^2\,. \tag{3.10}$$

Equations (3.9) and (3.10) have a structure similar to the moments of the dynamic structure function [see Eq. (2.9)] with the particle operator $a_{-\mathbf{q}}$ replacing the density operator $\rho_{\mathbf{q}}$. In particular, the ratio

$$\varepsilon_P(q)=\frac{\sum_n\omega_{n0}|\langle n|a_{-\mathbf{q}}|0\rangle|^2}{\sum_n|\langle n|a_{-\mathbf{q}}|0\rangle|^2} \tag{3.11}$$

provides the energy $\varepsilon_P=\langle P|H'|P\rangle/\langle P|P\rangle$ of the particle state [see Eq. (1.2)]

$$|P\rangle=\frac{1}{\sqrt{n(q)}}a_{-\mathbf{q}}|0\rangle\,. \tag{3.12}$$

We refer to $|P\rangle$ as to the *particle* state to distinguish it from the *density* state $|F\rangle$ given by the Feynman ansatz (2.25). It is obtained by removing a particle with momentum $-\mathbf{q}$ from the ground state $|0\rangle$. It is worth noting that, in general, neither $|P\rangle$ nor $|F\rangle$ are exact eigenstates of the system.

Using Eqs. (3.4), (3.6), and (3.11), one finds the following expression for the energy of the particle state:

$$\varepsilon_P(q)=\mu-\frac{q^2}{2m}-\frac{W(q)}{n(q)}\,, \tag{3.13}$$

where

$$W(q)=\sum_p n(\mathbf{q},\mathbf{p})V(p)=\int d\mathbf{r}_1d\mathbf{r}_1'\rho^{(2)}(\mathbf{r}_1,0;\mathbf{r}_1',0)e^{-i\mathbf{q}\cdot(\mathbf{r}_1'-\mathbf{r}_1)}V(r_1) \tag{3.14}$$

and $\rho^{(2)}(\mathbf{r}_1,\mathbf{r}_2;\mathbf{r}_1',\mathbf{r}_2)$ is defined in Eq. (3.8). It is interesting to compare the energies ε_F and ε_P. In fact, in a Bose superfluid, due to the occurrence of the Bose condensate, the states $|F\rangle$ and $|P\rangle$ are not orthogonal and are both expected to have a significant overlap with the *exact* excited state of the system. The two states coincide with the exact solution only in the case of a weakly interacting Bose gas (Bogoliubov limit[10]). In a strongly interacting Bose liquid both Eqs. (2.29) and (3.13) provide rigorous upper bounds for the energy of the phonon-maxon-roton state. The interest in the comparison between ε_F and ε_P is also motivated by the recent debate[32,33] about the microscopic nature of the roton excitation following the availability of accurate experimental data from inelastic neutron scattering.[34] In fact, according to the suggestions of Ref. 33, the physical picture of the roton should be more particlelike than densitylike, the two descriptions being, however, coupled due to the presence of the Bose condensate. One then might expect ε_P to be smaller than ε_F in the roton region.

Differently from the Feynman energy (whose evaluation requires only the knowledge of the static structure function) the explicit calculation of the particle energy is more difficult and requires the knowledge of the two-body off-diagonal density entering the integral of Eq. (3.14). First microscopic results for this density are now becoming available.[29,35,36]

A useful comparison between the Feynman and particle energies nevertheless can be made avoiding the explicit calculation of $\rho^{(2)}$. To this purpose it is convenient to define the average particle energy in momentum space according to

$$\bar{\varepsilon}_P=\frac{\sum_{\mathbf{q}}n(q)\varepsilon_P(q)}{\sum_{\mathbf{q}}n(q)}\,. \tag{3.15}$$

This average is sensitive to the values of $\varepsilon_P(q)$ in the interval of momenta, where the quantity $q^2n(q)$ has a significant weight. This corresponds to the range $q=1$–3 Å^{-1} including the maxon and roton region. The average (3.15) can be explicitly calculated using the exact relations

$$\sum_{\mathbf{q}}n(q)=N\,,\qquad \sum_{\mathbf{p},\mathbf{q}}n(\mathbf{q},\mathbf{p})V(p)=2\langle V\rangle\,, \tag{3.16}$$

or, equivalently, the operator identity[37]

$$-\sum_{\mathbf{p}}a_{\mathbf{p}}^\dagger[H,a_{\mathbf{p}}]=E_K+2V\,, \tag{3.17}$$

where E_k and V are the kinetic- and potential-energy operators respectively. One finds

$$\bar{\varepsilon}_P=\mu-\langle E_K\rangle-2\langle V\rangle\,, \tag{3.18}$$

where $\langle E_K\rangle$ and $\langle V\rangle$ are the kinetic energy and the potential energy per particle relative to the ground state of the system. Result (3.18) was applied in a similar form by Koltun[38] to the study of nuclear knock-out reactions. At zero pressure, where $\mu=\langle E_K\rangle+\langle V\rangle$, Eq. (3.18) yields $\bar{\varepsilon}_P=-\langle V\rangle=21$–$22$ K in superfluid ^{4}He. It is instructive to compare the above value with the corresponding

Feynman average energy:

$$\bar{\varepsilon}_F=\frac{\sum_{\mathbf{q}} n(q)\varepsilon_F(q)}{\sum_{\mathbf{q}} n(q)} . \tag{3.19}$$

Using microscopic estimates for $S(q)$ and $n(q)$ we find $\bar{\varepsilon}_F=24-25$ K a value slightly higher than $\bar{\varepsilon}_P$.

A more direct comparison between the Feynman and particle states can be made in the low-q limit, where the Feynman energy (2.29) is known to reproduce rigorously the correct phonon dispersion law $\omega=cq$. Contrariwise, the low-q limit of Eq. (3.13) is less trivial. In Sec. V we discuss in a systematic way the phonon and multiparticle contributions to the various sum rules in the $q\to 0$ limit. The main results concerning the sum rules (3.9) and (3.10) are as follows.

(i) The non-energy-weighted sum rule (3.9) entering the denominator of Eq. (3.11) is dominated by the phonon contribution and diverges[13,39] as $1/q$,

$$n(q)=\frac{n_0mc}{2q} . \tag{3.20}$$

(ii) The energy-weighted sum rule (3.10) approaches a constant value and takes a contribution both from one-phonon and multiparticle excitations. Two important consequences follow from the above results.

(a) At $q=0$ the energy ε_P of the particle state must vanish. This implies [see Eq. (3.13)] the nontrivial relationship for the chemical potential

$$\mu=\lim_{q\to 0}\frac{W(q)}{n(q)} . \tag{3.21}$$

By introducing the function F_1 characterizing the long-range order of the two-body half-diagonal density (3.8) through the relation[29]

$$\lim_{r_1'\to\infty}\rho^{(2)}(\mathbf{r}_1,\mathbf{r}_2;\mathbf{r}_1',\mathbf{r}_2)=n_0\rho^2[1+F_1(|\mathbf{r}_1-\mathbf{r}_2|)] , \tag{3.22}$$

where $n_0=(1/N)\langle a_0^\dagger a_0\rangle$ is the condensate fraction, result (3.21) can be rewritten in the following way:[40]

$$\mu=\rho\int d\mathbf{r}[1+F_1(r)]V(r) . \tag{3.23}$$

Equation (3.23) represents a nontrivial result holding for any Bose system exhibiting Bose-Einstein condensation and interacting with central potentials. It is instructive to point out an analogy between Eq. (3.23) and the Hugenholtz and Pines[12] relation for the chemical potential. Both results turn out in fact to be connected with the absence of a gap in the excitation spectrum.

(b) A second important consequence of the above discussion is that the dispersion of ε_P is linear in q, with a slope larger than the velocity of sound c, due to the contribution arising from multiparticle excitations in the energy-weighted sum rule (3.10). An explicit result for the slope can be obtained exploiting the low-q behavior of Eq. (3.6). Using result (3.21) for the chemical potential we find

$$\lim_{q\to 0}\langle a_{\mathbf{q}}^\dagger[H,a_{\mathbf{q}}]\rangle=b$$

with

$$b=-\int d\mathbf{r}_1 d\mathbf{r}_1'\{\rho^{(2)}(\mathbf{r}_1,0;\mathbf{r}_1',0)-\rho\rho^{(1)}(r_1')[1+F_1(r_1)]\}V(r_1) \tag{3.24}$$

from which one gets

$$\varepsilon_P(q)_{q\to 0}=\frac{2qb}{n_0mc} \tag{3.25}$$

with $2b/n_0mc>c$. Clearly the occurrence in ε_P of a slope larger than the sound velocity, together with the fact that the average value of the particle energy $\bar{\varepsilon}_P$ is smaller than $\bar{\varepsilon}_F$, is compatible with a particle energy ε_P significantly lower than ε_F in the roton region.

To conclude this section we note that, in contrast with what happens in a dilute Bose gas where the operators $a_{\mathbf{q}}$ and $a_{\mathbf{q}}^\dagger$ (as well as the density operator $\rho_{\mathbf{q}}$) have an equivalent role in generating the elementary excitations of the system, because higher-energy excitations have a minor importance, in a strongly interacting system the role of such operators is highly asymmetric. In particular the state $a_{\mathbf{q}}^\dagger|0\rangle$ provides a much worse description of the elementary mode compared to the state $a_{\mathbf{q}}|0\rangle$, since adding a particle with momentum $\mathbf{q}$ to the system yields a violation of the core condition imposed by the repulsive component of the interatomic potential on the two-body density matrix. This is responsible for the occurrence of important high-energy components in the state $a_{\mathbf{q}}^\dagger|0\rangle$ as results from the explicit calculation of its average energy

$$\frac{\langle a_{\mathbf{q}}Ha_{\mathbf{q}}^\dagger\rangle}{\langle a_{\mathbf{q}}a_{\mathbf{q}}^\dagger\rangle}=\frac{\langle[a_{\mathbf{q}},[H,a_{\mathbf{q}}^\dagger]]\rangle-\langle a_{\mathbf{q}}^\dagger[H,a_{\mathbf{q}}]\rangle}{1+n(q)} . \tag{3.26}$$

The quantities at the numerator of Eq. (3.26) correspond to the energy weighted sum rules (3.5) and (3.6). However, while the second term, characterizing the energy of the state $a_{\mathbf{q}}|0\rangle$, is also well behaved in strongly interacting systems, the first term [see Eq. (3.5)] is dramatically affected by the short-range components of the potential.[29] This indicates that in liquid ^{4}He the Wagner sum rule (3.5) is not particularly useful in the study of the elementary excitations being dominated by multiparticle effects.

IV. SUM RULES FOR THE PARTICLE-DENSITY SPECTRAL FUNCTION

As anticipated in Sec. III, particle and density excitations are not decoupled in superfluid ^{4}He due to the existence of the Bose condensate. This property is explicitly revealed by the fact that the particle-density spectral function

$$\begin{aligned}A_{\rho,a}(q,\omega)&=\int dt\, e^{i\omega(t-t')}\langle[\rho_{\mathbf{q}}(t),a_{\mathbf{q}}(t')]\rangle\\&=\frac{1}{Z}\sum_{m,n}(e^{-\beta E_m}-e^{-\beta E_n})\langle m|\rho_{\mathbf{q}}|n\rangle\langle n|a_{\mathbf{q}}|m\rangle\delta(\omega-E_n+E_m)\end{aligned} \tag{4.1}$$

does not vanish in Bose superfluids. Many important properties of this function have already been investigated in the framework of the dielectric formalism (see, for example, Ref. 41). Similarly to the density and particle case (Secs. II and III, respectively) also for this spectral function one can derive useful sum rules:

$$\int_{-\infty}^{+\infty} A_{\rho,a}(q,\omega)d\omega=\langle[\rho_{\mathbf{q}},a_q]\rangle=-\sqrt{Nn_0(T)}\ , \tag{4.2}$$

$$\int_{-\infty}^{+\infty}\frac{1}{1-e^{-\beta\omega}}A_{\rho,a}(q,\omega)d\omega=\langle\rho_{\mathbf{q}}a_{\mathbf{q}}\rangle=\frac{1}{\sqrt{Nn_0(T)}}n(\mathbf{q},\mathbf{q})\ , \tag{4.3}$$

$$\int_{-\infty}^{+\infty}\omega A_{\rho,a}(q,\omega)d\omega=\langle[[\rho_{\mathbf{q}},H'],a_{\mathbf{q}}]\rangle=\sqrt{Nn_0(T)}\frac{q^2}{2m}\ , \tag{4.4}$$

$$\int_{-\infty}^{+\infty}\frac{\omega}{1-e^{-\beta\omega}}A_{\rho,a}(q,\omega)d\omega=\langle[\rho_{\mathbf{q}},H']a_{\mathbf{q}}\rangle=-\frac{q}{m\sqrt{Nn_0(T)}}\sum_{\mathbf{k}}(k^z+\tfrac{1}{2}q^z)n(\mathbf{k},\mathbf{q},\mathbf{q}), \tag{4.5}$$

where $n_0(T)=N_0/N$ is the condensate fraction. In the above equations $n(\mathbf{q},\mathbf{p})$ and $n(\mathbf{k},\mathbf{p},\mathbf{q})$ are the generalized momentum distribution functions defined by Eq. (3.7) and

$$n(\mathbf{k},\mathbf{p},\mathbf{q})=\langle a^\dagger_{\mathbf{k}+\mathbf{q}}a_{\mathbf{k}}a^\dagger_{\mathbf{p}-\mathbf{q}}a_{\mathbf{p}}\rangle-n(p)\ , \tag{4.6}$$

and we have used the Bogoliubov prescription $a_0^\dagger|0\rangle=a_0|0\rangle=\sqrt{Nn_0}|0\rangle$. Result (4.2) was employed by Hohenberg[42] to demonstrate that Bose-Einstein condensation cannot occur in *one* and *two*-dimensional systems at finite temperature and more recently by Pitaevskii and Stringari[43] to demonstrate the same result in *one*-dimensional systems at zero temperature. Results (4.3) and (4.5) depend explicitly on the two-body momentum distribution (3.8). In particular, the relevant matrix element of Eq. (4.3) can be written in the form (for $q\neq0$)

$$n(\mathbf{q},\mathbf{q})=Nn_0F_1(q)\ , \tag{4.7}$$

where $F_1(q)=\rho\int d\mathbf{r}\,e^{i\mathbf{q}\cdot\mathbf{r}}F_1(r)$ is the Fourier transform of the function $F_1(r)$ defined in Eq. (3.23) (see also Ref. 29). In the macroscopic limit $q\to0$ the function $F_1(q)$ approaches[29] the value $-\frac{1}{2}$. Result (4.4), which together with result (4.2) is implicitly contained in the high-frequency limit of the particle-density Green's function,[41] has recently been discussed in Ref. 44. Its validity is ensured by the velocity independence of the interaction potential, which commutes with the density operator $\rho_{\mathbf{q}}$. The same property yields the most famous f-sum rule (2.16).

Let us now discuss some interesting consequences of these particle-density sum rules. Result (4.3) permits us to calculate the overlap between the Feynman and the particle states discussed in Secs. II and III. In fact, using the definition of such states [Eqs. (2.25) and (3.12)] one can write

$$\langle F|P\rangle=\frac{1}{\sqrt{NS(q)n(q)}}\langle\rho^\dagger_{\mathbf{q}}a_{-\mathbf{q}}\rangle=\left[\frac{n_0}{S(q)n(q)}\right]^{1/2}F_1(q)\ . \tag{4.8}$$

It is worth noting that the overlap is complete when $q\to0$ [in fact, in this limit one has $S(q)=q/2mc$, $n(q)=n_0mc/2q$, and $F_1(0)=-\frac{1}{2}$]. This shows that the two states coincide in the $q\to0$ limit. Result (4.3) has also recently been used to provide an estimate of the residue

$$Z_{a^\dagger,a}(q)=|\langle\mathbf{q}|a_{-\mathbf{q}}|0\rangle|^2 \tag{4.9}$$

of the particle-particle Green's function in the collective (phonon-maxon-roton) branch of superfluid ^{4}He. In fact, assuming that the sum rule (4.3) is exhausted by the collective state, hereafter called $|\mathbf{q}\rangle$ (Feynman-type ansatz), one finds the following result:[44]

$$\langle\mathbf{q}|a^\dagger_{\mathbf{q}}|0\rangle=\left[\frac{n_0}{S(q)}\right]^{1/2}[1+F_1(q)]\ ,\qquad \langle\mathbf{q}|a_{-\mathbf{q}}|0\rangle=\left[\frac{n_0}{S(q)}\right]^{1/2}F_1(q)\ , \tag{4.10}$$

and hence

$$Z_{a^\dagger,a}(q)=n_0\frac{F_1(q)^2}{S(q)}\ . \tag{4.11}$$

In deriving Eqs. (4.10) and (4.11) we have assumed the density matrix element $\langle\mathbf{q}|\rho_{\mathbf{q}}|0\rangle$ to be real and positive. Estimate (4.11) for the residue $Z_{a^\dagger,a}(q)$ becomes rigorous in the $q\to0$ limit, where it reproduces the Gavoret-Nozieres result[13]

$$Z_{a^\dagger,a}(q\to0)=n_0\frac{mc}{2q}\ . \tag{4.12}$$

Furthermore (see Sec. 5), the next correction to the expansion (4.12) [term constant in q in $Z_{a^\dagger,a}(q)$] is also correctly given by Eq. (4.11). Even if at higher momenta result (4.11) is not rigorous because of the non-negligible role of multiparticle excitations, it can serve as a first description for the spectral function in the maxon-roton region. In particular, the bump predicted by Eq. (4.11) (see Fig. 2) in the roton region provides a suggestive explanation of the shoulder recently found in microscopic calculations of the momentum distribution in the same range of momenta (see Fig. 2 and Refs. 45–47). At $T=0$ the momentum distribution can, in fact, be written as $n(q)=\sum_n|\langle n|a_{-\mathbf{q}}|0\rangle|^2$, and hence the residue (4.9) corresponds to the "collective" contribution to $n(q)$.

Let us conclude our discussion of the sum rules

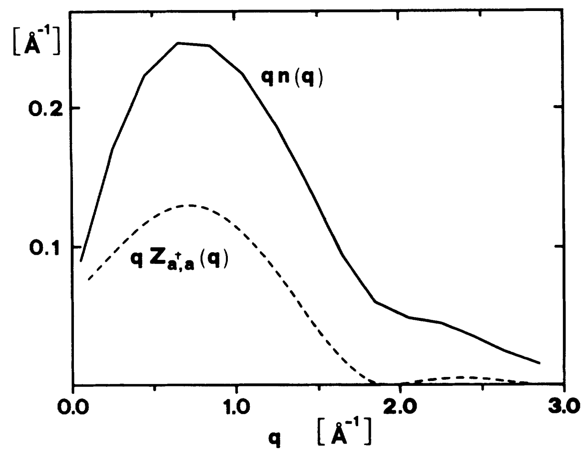

FIG. 2. Residue $Z_{a^\dagger,a}(q)$ of the particle-particle Green's function in the collective branch of superfluid ^{4}He. The residue was calculated using the estimate (4.11) with the values of $F_1(q)$ and $S(q)$ taken from Ref. 29.

(4.2)–(4.5) by noting that Eq. (4.5) plays a crucial role in the study of the coupling between the Feynman and particle states (2.25) and (3.12). In fact, if one optimizes the wave function for the excited state looking for a linear combination of the form

$$|\mathbf{q}\rangle=\alpha|F\rangle+\beta|P\rangle \ , \tag{4.13}$$

one explicitly needs the crossed term

$$\langle F|H'|P\rangle=\frac{1}{\sqrt{NS(q)n(q)}}\langle[\rho_{\mathbf{q}},H']a_{\mathbf{q}}\rangle \ . \tag{4.14}$$

The determination of the matrix element (4.14) requires, as shown by Eq. (4.5) the knowledge of the two-body off-diagonal density.

V. PHONON AND MULTIPARTICLE CONTRIBUTIONS AT LOW MOMENTUM

Because of the discretization of the collective phonon-maxon roton branch, it is interesting to distinguish between the contribution to the different sum rules discussed in this work arising from the collective and multiparticle states. This separation becomes explicit in the calculation of the sum rules at low q and zero temperature. Similar analysis have already been carried out for the density response of superfluid ^{4}He (Ref. 16) as well as for the density and spin-density response of normal ^{3}He (Refs. 16, 26, 27, and 48). The main results are listed in Table I, where we report the leading contributions to the matrix elements

$$(\rho_{\mathbf{q}})_{n0}\equiv\langle n|\rho_{\mathbf{q}}|0\rangle \ ,$$
$$(a_{\mathbf{q}})_{n0}\equiv\langle n|a_{\mathbf{q}}|0\rangle \ ,$$
$$(a^\dagger_{\mathbf{q}})_{n0}\equiv\langle n|a^\dagger_{\mathbf{q}}|0\rangle,$$

coming from one-phonon and multiparticle excitations. Some comment are in order here.

(a) The phase of the phonon states have been always chosen in order to have real and positive density matrix elements

$$(\rho_{\mathbf{q}})_{n0}=(\rho_{\mathbf{q}})_{0n}=\left[\frac{Nq}{2mc}\right]^{1/2}[1+O(q^2)] \ . \tag{5.1}$$

(b) The particle matrix elements relative to the phonon state have been parametrized in the following way:

$$\begin{aligned}(a_{\mathbf{q}})_{n0}&=(a^\dagger_{\mathbf{q}})_{0n}\\&=-\left[\frac{n_0mc}{2q}\right]^{1/2}\left[1+\frac{\alpha}{mc}q+O(q^2)\right] ,\\(a^\dagger_{\mathbf{q}})_{n0}&=(a_{\mathbf{q}})_{0n}\\&=\left[\frac{n_0mc}{2q}\right]^{1/2}\left[1-\frac{\alpha}{mc}q+O(q^2)\right] .\end{aligned} \tag{5.2}$$

The opposite signs in the leading terms in $1/\sqrt{q}$ of Eq. (5.2) are essential in order to satisfy the sum rule (4.2) [see also Eq. (5.11) below]. For the same reason the next corrections in Eqs. (5.2) have the same sign in order to ensure the exact cancellation of the term linear in q in the same sum rule (note that multiparticle states contribute to this sum rule only with terms in q^2).

The following conclusions can be drawn on the basis of the results of Table I.

(a) Regarding density-density sum rules, as already discussed in the literature,[16] the moments m_{-1}, m_0, m_1, and m_2 are dominated, at low q, by the phonon contribution. On the other hand, the m_3 moment is affected, to the leading order in q^4, also by multiparticle effects.

(b) Regarding particle-particle sum rules, the polarizability sum rule

$$\int_{-\infty}^{+\infty}\frac{1}{\omega}A_{a^\dagger,a}(q,\omega)=\sum_n[|(a_{\mathbf{q}})_{n0}|^2+|(a^\dagger_{\mathbf{q}})_{n0}|^2]/\omega_{n0} \tag{5.3}$$

is dominated, at low q, by the phonon contribution and exhibits the well known $1/q^2$ divergent behavior predicted by the Bogoliubov's inequality[49] (see also Ref. 31).

It is worth noting that the multiparticle contribution to this sum rule is not constant, as one would naively conclude by looking at the q dependence of the matrix elements and energies reported on the table. In fact, one can show that the energy integration of such contributions, limited at low ω by the phonon dispersion $\omega=cq$, gives rise to a divergent logarithmic contribution,[50–51] arising from two-phonon excitations.

(c) The momentum distribution sum rule (3.9)

$$n(q)=\sum_n|(a_{\mathbf{q}})_{n0}|^2 \tag{5.4}$$

is dominated by the $1/q$ phonon contribution [see Eq. (3.20)]. In the table we have explicitly also taken into account the constant term proportional to α arising from the phonon contribution. This term can be determined through the study of another sum rule [see Eq. (5.9) below and Ref. 40].

(d) The Bose commutation sum rule (3.3)

$$\langle [a_q^\dagger, a_q] \rangle = \sum_n [\,|(a_q)_{n0}|^2 - |(a_q^\dagger)_{n0}|^2] = -1 \qquad (5.5)$$

receives a contribution from both the phonon and multiparticle states. As we shall see, the multiparticle contribution plays a crucial rule in exhausting this sum rule.

(e) The energy-weighted sum rules (3.5), (3.6),

$$\langle [a_q^\dagger, [H', a_q]] \rangle = \sum_n [\,|(a_q)_{n0}|^2 + |(a_q^\dagger)_{n0}|^2]\omega_{n0} \,, \qquad (5.6)$$

and

$$\langle a_q^\dagger [H', a_q] \rangle = \sum_n |(a_q)_{n0}|^2 \omega_{n0} \qquad (5.7)$$

receive a contribution from both phonon and multiparticle excitations. In particular, the multiparticle contribution to the sum rule (5.6) is expected to be very large in the presence of strongly repulsive potentials (see discussion at the end of Sec. III and Ref. 31).

(f) Regarding particle-density sum rules, in addition to the various sum rules discussed in Sec. IV it is interesting to discuss the static polarizability

$$\int_{-\infty}^{+\infty} \frac{1}{\omega} A_{\rho,a}(q,\omega) d\omega = \sum_n [(\rho_q^\dagger)_{n0}(a_q)_{n0} + (a_q^\dagger)_{n0}(\rho_q)_{n0}]/\omega_{n0} \,. \qquad (5.8)$$

At low q this sum rule gives the fluctuations of the particle number in the condensate induced by changes of the total number of particles and can be consequently written in the following way:

$$\lim_{q\to 0} \int_{-\infty}^{+\infty} \frac{1}{\omega} A_{\rho,a}(q,\omega) d\omega = \sqrt{N n_0} \frac{1}{2mn_0 c^2} \frac{\partial(n_0\rho)}{\partial \rho} \,. \qquad (5.9)$$

As emerges from the table the sum rule (5.8) is dominated by the phonon contribution at low q. However, the divergent terms characterizing the particle matrix elements on the phonon state [see Eqs. (5.2)] cancel out in this sum rule which then turns out to be proportional to the next term in α. Comparison with Eq. (5.9) yields[40]

$$\alpha = -\frac{1}{2n_0} \frac{\partial(n_0\rho)}{\partial \rho} \,. \qquad (5.10)$$

(g) The Bogoliubov-Wagner-Hohenberg sum rule (4.2)

$$\langle [\rho_q, a_q] \rangle = \sum_n [(\rho_q^\dagger)_{n0}(a_q)_{n0} - (a_q^\dagger)_{n0}(\rho_q)_{n0}] = -\sqrt{N n_0} \qquad (5.11)$$

plays a crucial role in establishing the divergent behavior of the particle matrix elements (5.2) and fix, in particular, their relative signs. At low q it is exhausted by the phonon contribution.

TABLE I. Matrix elements, excitation energies and sum rule contributions from one-phonon and multiparticle excitations at $T=0$.

	Phonon	Multiparticle
$(\rho_0)_{n0} = (\rho_q^\dagger)_{n0}$	$\sqrt{Nq/2mc}$	q^2
$(a_q)_{n0}$	$-\sqrt{n_0 mc/2q}\,(1+\alpha q/mc)$	const
$(a_q^\dagger)_{n0}$	$+\sqrt{n_0 mc/2q}\,(1-\alpha q/mc)$	const
ω_{n0}	cq	const
$\sum_n \|(\rho_q)_{n0}\|^2/\omega_{n0}$	$N/2mc^2$	q^4
$\sum_n \|(\rho_q)_{n0}\|^2$	$Nq/2mc$	q^4
$\sum_n \|(\rho_q)_{n0}\|^2 \omega_{n0}$	$Nq^2/2m$	q^4
$\sum_n \|(\rho_q)_{n0}\|^2 \omega_{n0}^2$	$Nq^3 c/2m$	q^4
$\sum_n \|(\rho_q)_{n0}\|^2 \omega_{n0}^3$	$Nq^4 c^2/2m$	q^4
$\sum_n [\,\|(a_q)_{n0}\|^2 + \|(a_q^\dagger)_{n0}\|^2]/\omega_{n0}$	$n_0 m/q^2$	$\ln q$
$\sum_n \|(a_q)_{n0}\|^2$	$n_0 mc/2q + n_0\alpha$	const
$\sum_n [\,\|(a_q)_{n0}\|^2 - \|(a_q^\dagger)_{n0}\|^2]$	$n_0 2\alpha$	const
$\sum_n [\,\|(a_q)_{n0}\|^2 + (a_q^\dagger)_{n0}\|^2]\omega_{n0}$	$n_0 mc^2$	const
$\sum_n \|(a_q)_{n0}\|^2 \omega_{n0}$	$n_0 mc^2/2$	const
$\sum_n [(\rho_q^\dagger)_{n0}(a_q)_{n0} + (a_q^\dagger)_{n0}(\rho_q)_{n0}]/\omega_{n0}$	$-\sqrt{Nn_0}\,\alpha/mc^2$	q^2
$\sum_n [(\rho_q^\dagger)_{n0}(a_q)_{n0} - (a_q^\dagger)_{n0}(\rho_q)_{n0}]$	$-\sqrt{Nn_0}$	q^2
$\sum_n (\rho_q^\dagger)_{n0}(a_q)_{n0}$	$-\frac{1}{2}\sqrt{Nn_0}(1+\alpha q/mc)$	q^2
$\sum_n [(\rho_q^\dagger)_{n0}(a_q)_{n0} + (a_q^\dagger)_{n0}(\rho_q)_{n0}]\omega_{n0}$	$-\sqrt{Nn_0}\,\alpha q^2/m$	q^2
$\sum_n (\rho_q^\dagger)_{n0}(a_q)_{n0}\omega_{n0}$	$-\frac{1}{2}\sqrt{Nn_0}\,cq$	q^2

(h) The sum rule (4.3), (4.7),

$$\langle \rho_q a_q \rangle = \sum_n [(\rho_q^\dagger)_{n0}(a_q)_{n0}] = \sqrt{N n_0} F_1(q) \; , \tag{5.12}$$

is exhausted, up to terms linear in q, by the phonon contribution. This result permits to relate the low-q behavior of $F_1(q)$ to the parameter α. One finds for $q \to 0$,

$$F_1(q) + \frac{1}{2} = -\frac{\alpha}{2mc} q \; . \tag{5.13}$$

Results (5.9) and (5.13) are interesting because they link the slope of the function $F_1(q)$ at small q with the thermodynamic quantity $\partial(n_0\rho)/\partial\rho$:

$$\lim_{q\to 0} \frac{1}{q}[F_1(q)+\tfrac{1}{2}] = \frac{1}{4n_0 mc}\frac{\partial(n_0\rho)}{\partial\rho} \; . \tag{5.14}$$

Note the analogy between result (5.12) and the relationship between the slope in the static structure function $S(q)$ and the velocity of sound. The slope (5.12) is expected to be negative in superfluid ^{4}He because of the rather strong dependence of the condensate fraction n_0 on the density. A rough estimate based on theoretical[45,46] and experimental[52] results yields $\partial(n_0\rho)/\partial\rho = -0.3 - 0.2$ at low pressure. The negativity of the slope is clearly confirmed by recent microscopic calculations of $F_1(q)$. The fact that the slope is negative, and hence the coefficient α is positive, makes liquid ^{4}He very different from a weakly interacting Bose gas where $n_0 = 1$ and hence $\alpha = -\frac{1}{2}$. In particular, in a weakly interacting gas the sum rule (5.5) is entirely dominated by the phonon state. On the other hand, in liquid ^{4}He the phonon contribution to this model-independent sum rule (see the table) is of opposite sign, revealing the crucial role played by multiparticle excitations in exhausting the Bose commutation sum rule.

The results for the sum rule (5.11), compared with the expansion given in the table, permits us to write the expansion

$$Z_{a^\dagger,a}(q) = n_0\frac{mc}{2q} - \frac{1}{2}\frac{\partial(n_0\rho)}{\partial\rho} + O(q) \tag{5.15}$$

for the residue of the particle Green's function in the collective phonon branch by generalizing the Gavoret-Nozieres result (4.12).

VI. CONCLUSIONS

In this paper we have investigated in a systematic way different sum rules for the density and particle operators in Bose superfluids. Some of the new results are summarized here.

(1) An exact lower bound [Eq. (2.31)] for the compressibility sum rule has been derived improving the Feynman lower bound (2.27). The explicit determination of the improved lower bound requires the knowledge of the sum rules m_0, m_1, m_2, and m_3.

(2) In Sec. III we have introduced the particle state [Eq. (3.12)] and derived an expression for its energy. The comparison between this energy and the energy of the density state given by the Feynman ansatz (2.25) is expected to provide interesting insight on the *particle* and *density* nature of the elementary excitations of superfluid ^{4}He especially in the roton region. An explicit formula for the average of the particle energy in momentum space has been obtained in terms of the chemical potential and kinetic and potential energy. We have, furthermore, investigated the energy of the particle state in the low-q region and shown that the absence of the gap at $q = 0$ implies a nontrivial relationship for the chemical potential.

(3) In Sec. IV we have calculated the overlap between the particle and Feynman states in terms of the function F_1 characterizing the long-range order in the two-body off diagonal density.

(4) In Sec. V we have provided a systematic investigation of the q dependence of the relevant sum rules discussed in the work by explicitly distinguishing between one-phonon and multiparticle contributions.

Many of the formulas given in this work could become the starting point for a quantitative and systematic description of the dynamics of superfluid ^{4}He based on the sum-rule approach. In particular, the required microscopic ingredients are limited to the two-body density (diagonal and nondiagonal terms) of the ground state. Accurate and systematic calculations of this quantity are consequently expected to be quite useful for a more microscopic understanding of the *density* and *particle* nature of the elementary excitations in Bose superfluids.

ACKNOWLEDGMENTS

I am particularly indebted to S. Giorgini for his valuable collaboration. Useful discussions with J. Clark, F. Dalfovo, L. Pitaevskii, and G. Senger are also acknowledged. Financial support was provided by INFN.

[1]L. D. Landau, J. Phys. U.S.S.R. **5**, 71 (1941).

[2]L. D. Landau, J. Phys. U.S.S.R. **11**, 91 (1947).

[3]A. Bijl, Physica **8**, 655 (1940).

[4]R. P. Feynman, in *Progress in Low Temperature Physics*, edited by C. J. Gorter (North-Holland, Amsterdam, 1955), Vol. 1, Chap. 2.

[5]R. P. Feynman and M. Cohen, Phys. Rev. **102**, 1189 (1956).

[6]E. Feenberg, *Theory of Quantum Fluids* (Academic, New York, 1969).

[7]G. V. Chester, in *The Helium Liquids*, edited by J. C. M. Armitage and I. E. Farquhar (Academic, London, 1975), p. 33.

[8]C. E. Campbell, in *Progress in Liquid Physics*, edited by C. A. Croxton (Wiley, New York, 1978), p. 213.

[9]E. Manousakis and V. R. Pandharipande, Phys. Rev. B **33**, 150 (1986).

[10]N. N. Bogoliubov, J. Phys. U.S.S.R. **11**, 23 (1947).

[11]S. T. Beliaev, Zh. Eksp. Teor. Fiz. **34**, 417 (1958) [Sov. Phys. JETP **7**, 289 (1958)].

[12]N. Hugenholtz and D. Pines, Phys. Rev. **116**, 489 (1959).

[13]J. Gavoret and Ph. Nozieres, Ann. Phys. (N.Y.) **28**, 349 (1964).

[14]D. Hall and E. Feenberg, Ann. Phys. **63**, 335 (1971).
[15]C. W. Woo, in *The Physics of Liquid and Solid Helium,* edited by K. H. Bennemann and J. B. Ketterson (Wiley, New York, 1976), p. 349.
[16]D. Pines and Ph. Nozieres, *The Theory of Quantum Liquids* (Benjamin, New York, 1966), Vol. I; Ph. Nozieres and D. Pines, *The Theory of Quantum Liquids* (Addison-Wesley, 1990), Vol. II.
[17]R. A. Cowley and A. D. B. Woods, Can. J. Phys. **49**, 177 (1971); A. D. B. Woods and R. A. Cowley, Rep. Prog. Phys. **36**, 1135 (1973).
[18]H. Glyde and E. C. Svensson, in *Neutron Scattering in Condensed Matter Research,* edited by K. Skold and D. L. Price (Academic, New York, 1987), Vol. 23, Pt. B, Ch. 13.
[19]P. A. Whitlock, D. M. Ceperley, G. V. Chester, and M. H. Kalos, Phys. Rev. B **19**, 5598 (1979); M. H. Kalos, M. A. Lee, P. A. Whitlock, and G. V. Chester, *ibid.* **24**, 115 (1981).
[20]D. Pines and Ph. Nozieres, Phys. Rev. **109**, 741 (1958).
[21]E. L. Pollock and D. M. Ceperley, Phys. Rev. B **36**, 8343 (1987).
[22]R. D. Puff, Phys. Rev. A **137**, 406 (1965).
[23]D. Pines and C.-W. Woo, Phys. Rev. Lett. **24**, 1044 (1970).
[24]K. S. Singwi and M. P. Tosi, Solid State Phys. **36**, 177 (1981).
[25]D. Pines, in *Highlights of Condensed Matter Theory,* edited by F. Bassani, F. Fumi, and M. P. Tosi (North-Holland, Amsterdam, 1985), p. 580.
[26]E. Safier, and A. Widom, J. Low Temp. Phys. **6**, 397 (1972).
[27]F. Dalfovo and S. Stringari, Phys. Rev. Lett. **63**, 532 (1989).
[28]F. Dalfovo, J. Dupont-Roc, N. Pavloff, S. Stringari, and J. Treiner, Europhys. Lett. **16**, 205 (1991).
[29]M. L. Ristig and J. Clark, Phys. Rev. B **40**, 4355 (1989).
[30]A. Griffin, Phys. Rev. B **30**, 5057 (1984).
[31]H. Wagner, Z. Phys. **195**, 273 (1966).
[32]W. G. Stirling and H. R. Glyde, Phys. Rev. B **41**, 4224 (1990).
[33]H. R. Glyde and A. Griffin, Phys. Rev. Lett. **65**, 1454 (1990); H. R. Glyde, Phys. Rev. B **45**, 7321 (1992).
[34]E. F. Talbot, H. R. Glyde, W. G. Stirling, and E. C. Svensson, Phys. Rev. B **38**, 11 229 (1988).
[35]G. Senger (private communication).
[36]D. M. Ceperley, in *Momentum Distributions,* edited by R. N. Silver and P. E. Sokol (Plenum, New York, 1989), p. 71.
[37]A. L. Fetter and J. D. Walecka, *Quantum Theory of Many-Particle Systems* (McGraw-Hill, New York, 1971).
[38]D. Koltun, Phys. Rev. Lett. **28**, 182 (1972).
[39]L. Reatto and G. V. Chester, Phys. Rev. **155**, 88 (1967).
[40]S. Stringari, J. Low Temp. Phys. **84**, 279 (1991).
[41]V. K. Wong and H. Gould, Ann. Phys. (N.Y.) **83**, 252 (1974).
[42]P. C. Hohenberg, Phys. Rev. **158**, 383 (1967).
[43]L. Pitaevskii and S. Stringari, J. Low Temp. Phys. **85**, (1991).
[44]S. Giorgini and S. Stringari, Physica B **165-166**, 511 (1990).
[45]E. M. Manousakis, V. R. Pandharipande, and U. N. Usmani, Phys. Rev. B **31**, 7022 (1985).
[46]P. Whitlock and R. M. Panoff, Can. J. Phys. **65**, 1409 (1987).
[47]D. M. Ceperley and E. L. Pollock, Can. J. Phys. **65**, 1416 (1987).
[48]C. H. Aldrich, C. J. Pethick, and D. Pines, Phys. Rev. Lett. **37**, 845 (1976).
[49]N. N. Bogoliubov, Phys. Abhandl. SU **6**, 1 (1962).
[50]V. N. Popov and A. V. Seredniakov, Zh. Eksp. Teor. Fiz. **77**, 377 (1979) [Sov. Phys. JETP **50**, 193 (1979)].
[51]S. Giorgini, L. Pitaevskii, and S. Stringari, Phys. Rev. B (to be published).
[52]J. H. Root and E. C. Svensson, Physica B **169**, 505 (1991); W. M. Snow, Y. Wang, and P. E. Sokol (unpublished).