Sum rules for density and particle excitations in a superfluid of charged bosons

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Abstract. We derive and discuss sets of sum rules relating to the density fluctuation operator and to the single-particle creation and annihilation operators in a superfluid of charged bosons. The physical interpretation of the particle–particle and particle–density sum rules hinges on the single-particle excitation spectrum at long wavelengths having a gap equal to the plasma frequency in the presence of the Bose–Einstein condensate. This spectral property is shown to follow from the Hugenholtz–Pines relation for the chemical potential in terms of the half-diagonal two-body density matrix. Data on this density matrix are obtained by quantum Monte Carlo methods and are used to check the self-consistency between the Hugenholtz–Pines relation and the value of the chemical potential calculated from the ground-state energy. We also tabulate the contributions from the plasmon and from multiparticle excitations to various matrix elements and sum rules at long wavelengths.

1. Introduction

The fluid of point-like spinless charged bosons embedded in a uniform neutralizing background has drawn some attention in the literature as a model in quantum statistical mechanics with possible relevance to superconductors [1] and to systems of astrophysical interest [2, 3]. Early evaluations of the ground-state energy and the spectrum of elementary excitations in the high-density limit [4, 5] have been followed by variational calculations using Jastrow wavefunctions [6, 7, 8] and by quantum Monte Carlo (QMC) studies of ground-state properties [9, 10, 11, 12] over a density range extending down to Wigner crystallization. Studies of dielectric screening properties have been carried out in the framework of local field factor theories [13, 14] beyond the random-phase approximation analysis given by Hore and Frankel [15]. A first attempt to apply the sum rule approach to charged Bose fluids has recently led to the derivation of two rigorous upper bounds on the plasmon dispersion relation [16].

Sum rules have often been employed in the literature to explore various dynamic features of quantum many-body systems from a microscopic point of view. From the density–density sum rules in charged Fermi fluids it has been shown that the plasmon is the only relevant long-wavelength excitation [17, 18]. In neutral systems (e.g. ⁴He) a similar analysis was first carried out for the long-wavelength phononic excitation by Feynman [19]. In Bose condensed systems broken symmetry leads to a more complex picture, in which density and single-particle excitations are coupled. A number of mixed particle–density sum rules exist which have no analogue in non-condensed systems. A complete discussion in the case of ⁴He has been given by Stringari [20], who also determined the infrared divergences of

various physical quantities (e.g. the momentum distribution). We shall see below that the charged Bose fluid presents a rather different scenario, since the long-range nature of the Coulomb interactions leads to a gap in the single-particle excitation spectrum and to sharper infrared divergences.

The main purpose of this work is to give a thorough presentation of the results which can be obtained from the sum rule approach for the charged Bose fluid and to contrast them with those applying to the corresponding neutral fluid. The sum rules that we discuss provide rigorous relationships among different physical quantities, their derivation being based only on the basic commutation relations. Their interpretation requires that in the long-wavelength limit the single-particle excitation spectrum coincides with the density excitation spectrum, i.e. with the plasmonic collective excitation. While at high density this has been shown to be correct to leading perturbative order [4], a general proof applying to the fluid at arbitrary coupling strength is given below.

At an intuitive level a justification for the above result is provided by Feynman's argument [19] which, though referring to ⁴He in its original formulation, is completely general since it depends only on the symmetry of the wavefunction. The argument notices that the lowest-lying excited states are those which involve large groups of atoms or long wavelengths and that rearrangements of the atoms among themselves do not change the wavefunction because of the Bose statistics. Therefore to leading order the lowest excited states in a Bose fluid are the density waves, i.e. the phononic excitation in the neutral fluid and the plasmon in the charged fluid. The same conclusion can also be reached from the argument of Gavoret and Nozières [21], stating that in the presence of a condensate the single-particle and the collective excitations have the same spectrum apart from a factor. In fact the $q = 0$ and $q = -k$ terms in the density fluctuation operator $\rho_k = \sum_q a_q^\dagger a_{q+k}$ describe single-particle excitations with a macroscopic coefficient, their form being $\sqrt{Nn_0}(a_k + a_{-k}^\dagger)$.

The above-mentioned gap in the single-particle excitation spectrum, together with the hypothesis of non-interacting excitations, allows a description of the relevant long-wavelength physics via the so-called quantum hydrodynamics (QH). This approach is based on an effective free-boson Hamiltonian, the bosons representing the elementary excitations. A detailed discussion is given in an appendix, where it is also shown that QH allows one to compute independently all the infrared divergences that we derive from the sum rule approach. A complete summary of our main results in the long-wavelength limit can be found in table 3 below.

2. Density–density sum rules

In the following we consider a system of N charged bosons embedded in a uniform neutralizing background, which can be described by the Hamiltonian

$$H = \sum_k \frac{k^2}{2m} a_k^\dagger a_k + \frac{1}{2V} \sum_{\substack{pq \\ k \neq 0}} v_k a_{q+k}^\dagger a_{p-k}^\dagger a_p a_q \tag{2.1}$$

where V is the volume, a_k and $a_k^\dagger$ are the single-particle operators and $\rho_k = \sum_q a_q^\dagger a_{q+k}$ is the density operator. As usual $v_k = 4\pi e^2/k^2$ and $\varepsilon_k = k^2/2m$ represent the interaction potential and the kinetic energy coefficients. Further, ρ is the average density, ω_{pl} the plasma frequency, n_0 the fraction of particles in the $k = 0$ state and $\langle \ldots \rangle$ indicates an average over the ground state of the system. We also recall the useful relations $\omega_{pl}^2 = 2\rho v_k \varepsilon_k$ and

$\langle a_0 \rangle = \langle a_0^\dagger \rangle = \sqrt{n_0 N}$.

The density–density response function $\chi(k, \omega)$ describes the density response of the fluid to an external scalar potential, its imaginary part being related to correlations between density fluctuations through the fluctuation-dissipation theorem. The sum rule approach to the study of $\chi(k, \omega)$ is based on the observation that its spectral moments are equivalent via Fourier transformation to time derivatives at $t = 0$, which can be computed as commutators with the Hamiltonian. Since ρ_k is quadratic in the single-particle operators a_k there is no difference between bosons and fermions, the dominant role being played by the long-range nature of the Coulomb potential. The frequency moments of $\mathrm{Im}\,\chi(k, \omega)$ are defined through

$$m_j(k) = -\frac{2}{\pi} \int_0^\infty \mathrm{Im}\,\chi(k, \omega)\omega^j \, \mathrm{d}\omega = \frac{2}{V} \sum_{|n\rangle} \omega_n^j |\langle n|\rho_k|0\rangle|^2 \tag{2.2}$$

where $|0\rangle$ is the ground state and $|n\rangle$ are the excited states. The above-mentioned property and the Kramers–Kronig relations lead to the following results (see for instance [18]):

$$m_{-1}(k) = -\chi(k, 0) = \frac{1}{v_k} - \frac{1}{\rho^2 K_T v_k^2} + \mathrm{O}(k^6) \tag{2.3}$$

$$m_0(k) = \frac{1}{V} \langle \rho_k^\dagger \rho_k \rangle = 2\rho S(k) \tag{2.4}$$

$$m_1(k) = \frac{1}{V} \langle [\rho_k^\dagger, [H, \rho_k]] \rangle = 2\rho \frac{k^2}{2m} \tag{2.5}$$

$$m_2(k) = \frac{1}{V} \langle [\rho_k^\dagger, H][\rho_k, H] \rangle = -\frac{1}{V} \sum_{ij} k_i k_j \sum_{p,q} \frac{p_i}{m} \frac{q_j}{m} \langle a_{p+k/2}^\dagger a_{p-k/2} a_{q-k/2}^\dagger a_{q+k/2} \rangle \tag{2.6}$$

and

$$m_3(k) = \frac{1}{V} \langle [[[\rho_k^\dagger, H], H], [H, \rho_k]] \rangle = 2\rho\varepsilon_k \left(\varepsilon_k^2 + 4\varepsilon_k \langle \mathrm{KE} \rangle + \omega_{pl}^2 (1 - G^{PV}(k)) \right)$$

$$= 2\rho\varepsilon_k \left(\omega_{pl}^2 + 4\varepsilon_k \left(\langle \mathrm{KE} \rangle - \frac{2}{15} \langle \mathrm{PE} \rangle \right) \right) + \mathrm{O}(k^6). \tag{2.7}$$

Here K_T is the isothermal compressibility, $\langle \mathrm{KE} \rangle$ and $\langle \mathrm{PE} \rangle$ the average kinetic and potential energies, $S(k)$ the structure factor and $G^{PV}(k)$ a local field factor defined by

$$G^{PV}(k) = \frac{1}{\rho} \int \frac{\mathrm{d}^3 q}{(2\pi)^3} \frac{(\boldsymbol{k} \cdot \boldsymbol{q})^2}{q^2 k^2} (S(\boldsymbol{q}) - S(\boldsymbol{k} - \boldsymbol{q})). \tag{2.8}$$

Moments higher than the third are infinite since $\mathrm{Im}\,\chi(k, \omega) \propto k^2 \omega^{-11/2}$ at small k and large ω, as in the case of charged fermions [22].

Pines and Nozières [17] have shown that the plasmon is the dominant excitation to leading order in k in the charged fermion fluid. Their argument is based on the m_{-1}- and m_1-sum rules and on some physical assumptions concerning the asymptotics of electron–hole pair excitations. In appendix A we give an alternative argument based only on m_{-1}, m_1 and m_3 without any other assumption. The result is

$$\lim_{k \to 0} \frac{\mathrm{Im}\,\chi(k, \omega)}{k^2/2m} = -\frac{2\rho}{\omega_{pl}} \left(\delta(\omega - \omega_{pl}) - \delta(\omega + \omega_{pl}) \right) \tag{2.9}$$

or, with an arbitrary choice of the phase,

$$\langle n|\rho_k|0\rangle \simeq \sqrt{\frac{Nk^2}{2m\omega_{pl}}}. \tag{2.10}$$

This proves that the plasmon collective excitation exhausts all the density–density sum rules to order k^2, while plasmon dispersion and multiplasmon and multiparticle excitations [23] contribute to order k^4. In contrast, in the corresponding neutral systems the phononic and multiparticle contributions to the third moment are both of order k^4 [20].

For the sake of completeness we report some upper bounds on plasmon dispersion which can be derived from the previous sum rules [20, 24, 16], namely

$$\omega_k^{(min)} \leqslant \frac{m_0(k)}{m_{-1}(k)} \leqslant \sqrt{\frac{m_1(k)}{m_{-1}(k)}} \leqslant \frac{m_1(k)}{m_0(k)} \leqslant \cdots. \tag{2.11}$$

A variety of other upper bounds which also contain m_2 can easily be obtained as discussed e.g. in [20]. However, they provide useful information only if supported by independent evaluations of m_2, e.g. through Monte Carlo simulations [24].

3. Particle–particle sum rules

In this section the single-particle analogues of the density–density sum rules are discussed. Such sum rules exist also in the fermionic case, but significant differences arise because of the statistics. While there is no physical field coupling directly to single-particle excitations, the following discussion could be formulated in terms of a single-particle response to a fictitious gauge-breaking field, but this would bring no significant advantage. Use of the grand-canonical Hamiltonian $H_\mu = H - \mu N$ is anyway needed since single-particle operators do not conserve the particle number.

The relevant sum rules are the following:

$$\langle [a_{k^\dagger}, a_k] \rangle = \sum_{|n\rangle} \left(|\langle n|a_k|0\rangle|^2 - |\langle n|a_k^\dagger|0\rangle|^2 \right) = -1 \tag{3.1}$$

$$\langle 0|a_k^\dagger a_k|0\rangle = \sum_{|n\rangle} |\langle n|a_k|0\rangle|^2 = n(k) \tag{3.2}$$

$$\langle [a_k^\dagger, [H_\mu, a_k]] \rangle = \sum_{|n\rangle} \omega_n \left(|\langle n|a_k|0\rangle|^2 + |\langle n|a_k^\dagger|0\rangle|^2 \right) = \frac{k^2}{2m} - \mu + \frac{1}{V} \sum_{q \neq 0} n(|q+k|)v(q) \tag{3.3}$$

and

$$\langle a_k^\dagger[H_\mu, a_k] \rangle = \sum_{|n\rangle} \omega_n |\langle n|a_k|0\rangle|^2 = \left(\mu - \frac{k^2}{2m} \right) n(k) - \frac{1}{V} \sum_{q \neq 0} n(k, q)v(q). \tag{3.4}$$

Here $n(k)$ denotes the momentum distribution and the quantity

$$n(k, q) = \langle a_k^\dagger \rho_q a_{k-q} \rangle \tag{3.5}$$

is the two-body momentum distribution.

Equations (3.1), (3.2) and (3.3) represent the basic commutation relation, the definition of the ground-state momentum distribution and the energy-weighted sum rule, respectively. The first one shows that divergent contributions to the matrix elements, if present, are equal in $|\langle n|a_k|0\rangle|$ and $|\langle n|a_k^\dagger|0\rangle|$. Considering that in a Bose condensed system $n(k = 0) = Nn_0$ and that (as we shall explicitly demonstrate in section 5 below) the leading contributions arise at energy ω_{pl}, equation (3.3) shows that there is indeed a divergence in the limit $k \to 0$, i.e.

$$n(k) \simeq \frac{1}{2\omega_{pl}} n_0 \rho v_k = \frac{1}{4} \frac{n_0 \omega_{pl}}{\varepsilon_k}. \tag{3.6}$$

Using the relation

$$\int \frac{d^3 q}{(2\pi)^3} \frac{1}{q^2 (q-k)^2} = \frac{1}{8k} \tag{3.7}$$

the subleading divergent contribution to the energy-weighted sum rule can now be determine

$$\langle [a_k^\dagger, [H_\mu, a_k]] \rangle \xrightarrow[k \to 0]{} n_0 \rho v(k) + \frac{4\pi e^2}{16} \frac{n_0 m \omega_{pl}}{k}. \tag{3.8}$$

By the same divergence cancellation argument from equation (3.1) this leads to a determination of the subleading divergent contribution to the momentum distribution, with the result

$$n(k) = \frac{1}{4} \frac{n_0 \omega_{pl}}{\varepsilon_k} + \frac{4\pi e^2}{32} \frac{n_0 m \omega_{pl}}{k}. \tag{3.9}$$

The limiting result (3.9), which is recovered independently by QH arguments in appendix B, will be confirmed by the particle–density sum rules to be discussed in the following section. The present derivation clearly shows how the combined effects of the Bose condensate and of the singular nature of the Coulomb potential at small k affect the momentum distribution. This divergent behaviour has been found to be consistent with QMC data in [12]. It is also consistent with the rigorous lower bound imposed by the indetermination principle [25]:

$$n(k) \geqslant \frac{n_0}{4S(k)} - \frac{1}{2} \tag{3.10}$$

where $S(k) \to \varepsilon_k / \omega_{pl}$ for $k \to 0$.

Finally, equation (3.4) will be used in section 5 to prove that the single-particle excitations start at the plasma frequency in the long-wavelength limit.

4. Particle–density sum rules

The sum rules presented in this section are peculiar to Bose condensed systems. They are based on the fact that expectation values of the form $\langle \rho_k a_{-k} \rangle$ can be non-vanishing in the presence of broken phase symmetry. A naive explanation can be found in the fact that an operator $a_k^\dagger$ at $k = 0$ is equivalent to the C-number $\sqrt{N n_0}$. As shown in [20] in the case of a neutral Bose superfluid the particle–density sum rules allow one to relate the density–density sum rules to the particle–particle ones.

4.1. The Bogoliubov sum rule

Explicit evaluation of the commutator $[\rho_k, a_{-k}]$ yields

$$\langle [\rho_k, a_{-k}] \rangle = \sum_n [\langle n|\rho_k^\dagger|0\rangle \langle n|a_{-k}|0\rangle - \langle n|a_{-k}^\dagger|0\rangle \langle n|\rho_k|0\rangle] = -\sqrt{N n_0}. \tag{4.1}$$

If $|n\rangle$ is the plasmon state $\rho_k|0\rangle$, then the matrix elements $\langle n|\rho_k|0\rangle$ are of order k (see equation (2.10)), but otherwise they are of order k^2 or lower. Therefore, if $\langle n|a_k^\dagger|0\rangle$ does not contain divergences stronger than k^{-1} the plasmon state exhausts this sum rule and we have

$$\langle n|a_k - a_k^\dagger|0\rangle = -\sqrt{\frac{n_0 \omega_{pl}}{k^2/2m}}. \tag{4.2}$$

4.2. The particle–density f-sum rule

Expanding $\langle[[\rho_k, H_\mu], a_{-k}]\rangle$ and using the relation $[V, \rho_k] = 0$ one obtains [26]

$$\langle[[\rho_k, H_\mu], a_{-k}]\rangle = \sum_{|n\rangle} \omega_n(\langle 0|\rho_k|n\rangle\langle n|a_{-k}|0\rangle + \langle 0|a_{-k}|n\rangle\langle n|\rho_k|0\rangle) = \sqrt{Nn_0}\,\frac{k^2}{2m}. \tag{4.3}$$

This equation is exact at any k and may be called the particle–density f-sum rule.

The same considerations as in the previous subsection lead to

$$\langle n|a_k + a_k^\dagger|0\rangle \propto k. \tag{4.4}$$

Comparing with equation (4.2) we get

$$\langle n|a_k|0\rangle = -\langle n|a_k^\dagger|0\rangle = -\frac{1}{2}\sqrt{\frac{n_0\omega_{pl}}{k^2/2m}} \tag{4.5}$$

which is consistent with equation (3.6) and has the advantage of fixing the relative phase of the ρ_k- and a_k-operators.

4.3. The particle–density polarizability

In this subsection we discuss the analogue of the compressibility sum rule for the mixed polarizability within the framework of generalized linear response theory.

The relevant physical process is the change in the number of Bose condensed particles induced by a change in the chemical potential. The perturbing Hamiltonian is

$$H' = \int d^3r\,\delta\mu(r)\,\rho(r) \tag{4.6}$$

and the static particle–density response function $\chi_{a\rho}(k)$ is defined by

$$\delta\langle a_k\rangle = \chi_{a\rho}(k)\,\delta\mu(k). \tag{4.7}$$

Since $\langle a_0\rangle = \sqrt{Nn_0}$ we have

$$\chi_{a\rho}(k \to 0) = \frac{\delta\sqrt{Nn_0}}{\delta\mu}. \tag{4.8}$$

In the same limit the density–density response function χ relates the variation of the chemical potential to a density modulation. Recalling the long-wavelength expansion given in equation (2.3), we have

$$\delta\rho = \chi\,\delta\mu = -\frac{1}{v_k}\,\delta\mu. \tag{4.9}$$

Recovering the microscopic expression for $\chi_{a\rho}$ and using the above relations we obtain

$$\chi_{a\rho}(k \to 0) = \sum_{|n\rangle} \frac{\langle 0|\rho_k^\dagger|n\rangle\langle n|a_k|0\rangle + \langle 0|a_k|n\rangle\langle n|\rho_k|0\rangle}{\omega_n} = -\sqrt{Nn_0}\,\frac{k^2/2m}{n_0\omega_{pl}^2}\,\frac{\partial(n_0\rho)}{\partial\rho}. \tag{4.10}$$

The particle–density polarizability vanishes in the $k \to 0$ limit because the perturbation Hamiltonian H' does not modify the background charge density. The corresponding osmotic compressibility also vanishes. In the neutral system this effect is absent and $\chi_{a\rho}$ is finite at $k = 0$ [20]. In contrast, the derivative $\partial n_0\rho/\partial\rho$ does not depend on whether the background is held fixed, as in this case, or is modulated in order to guarantee charge neutrality, as in usual thermodynamic derivatives.

We finally remark that in the charged Bose fluid the condensate fraction increases with density [4, 12]. Therefore the derivative in equation (4.10) is positive, as in the weakly interacting Bose gas, while it is negative in ^{4}He [20].

4.4. The two-body momentum distribution

Ristig and Clark [27] have parametrized the long-range behaviour of the two-body density matrix $\rho_2(r_1, i_2; r_1', r_2')$ at $i_2 = r_2'$ with a function $F_1(r_1 - i_2)$ as

$$\lim_{r_1' \to \infty} \rho_2(r_1, i_2; r_1', i_2) = n_0 \rho^2 (1 + F_1(|r_1 - i_2|)) \tag{4.11}$$

with $F_1(r \to \infty) = 0$. The two-body density matrix is the Fourier transform of the two-body momentum distribution $n(k, q)$:

$$n(k, q) = \frac{1}{V} \int \rho_2(r_1, i_2; r_1', i_2) e^{-iq \cdot (r_1' - r_1)} e^{-ik \cdot (r_1 - i_2)} \, dr_1 \, di_2 \, dr_1' \tag{4.12}$$

(see equation (3.5)). The Fourier transform of $F_1(r)$

$$F_1(k) = \rho \int F_1(r) e^{ik \cdot r} \, dr \tag{4.13}$$

is related to the $q = k$ and $q = 0$ components of $n(k, q)$ through the relations

$$n(0, k) = \sqrt{Nn_0} \langle \rho_k a_{-k} \rangle = Nn_0 F_1(k) \tag{4.14}$$

and

$$n(k, k) = \sqrt{Nn_0} \langle a_k^\dagger \rho_k \rangle = Nn_0 F_1(k). \tag{4.15}$$

In the case of ^{4}He Ristig and Clark [27] have shown that $\lim_{k \to 0} F_1(k) = -1/2$. Their proof is based on the following symmetry and clustering properties of the one- and two-body density matrices:

$$\lim_{|r_1 - r_1'| \to \infty} \rho_1(r_1, r_1') = \rho n_0 \tag{4.16}$$

$$\rho_2(r_1, i_2; r_1', i_2) = \rho_2(r_1', i_2; r_1, i_2) \tag{4.17}$$

$$\int \rho_2(r_1, i_2; r_1', i_2) \, di_2 = (N - 1)\rho_1(r_1, r_1') \tag{4.18}$$

and

$$\lim_{|r_1 - r_1'| \to \infty} \rho_2(r_1, i_2; r_1', i_2) = n_0 \rho^2 [1 + F_1(|r_1 - i_2|) + F_1(|r_1' - i_2|)]. \tag{4.19}$$

The only non-trivial relation is the last one, giving the behaviour of ρ_2 for large separation between r_1 and r_1'. It has been obtained by recalling the definition (4.11) of F_1 and the symmetry property (4.17). Three-body correlations can be neglected to leading order in the particle–particle separation.

Expanding $\int \rho_2(r_1, i_2; r_1', i_2) \, di_2$ at large $|r_1 - r_1'|$, once via equations (4.18) and (4.16) and once via equation (4.19), we obtain

$$-n_0 \rho = 2n_0 \rho^2 \int F_1(r) \, dr \tag{4.20}$$

which can be written as $F_1(k = 0) = -1/2$ or, equivalently,

$$\lim_{k \to 0} \langle a_k^\dagger \rho_k \rangle = \lim_{k \to 0} \langle \rho_k a_{-k} \rangle = -\frac{\sqrt{Nn_0}}{2}. \tag{4.21}$$

The same conclusion can be independently recovered by appropriately expanding the QH matrix elements in $\langle \rho_k a_{-k} \rangle$.

5. Single-particle excited states at long wavelength

The single-particle excited state $|P_k\rangle$ is defined by

$$|P_k\rangle = \frac{1}{\sqrt{n(k)}} a_k |0\rangle. \tag{5.1}$$

Its average energy $\varepsilon_P(k) = \langle P_k|H_\mu|P_k\rangle/\langle P_k|P_k\rangle$ can be evaluated by using the sum rule in equation (3.4), with the result

$$\varepsilon_P(k) = \sum_{|n\rangle} \omega_n |\langle n|a_k|0\rangle|^2 \Big/ \sum_{|n\rangle} |\langle n|a_k|0\rangle|^2 = \left(\mu - \frac{k^2}{2m}\right) - \frac{1}{Vn(k)} \sum_{q\neq 0} n(k,q)v(q). \tag{5.2}$$

In the $k \to 0$ limit it is necessary to consider separately the $q = k$ term in the sum in equation (5.2), which is singular because the a_{q-k}-operator in $n(k,q)$ acts on the condensate. Namely, we write

$$\frac{1}{Vn(k)} \sum_{q\neq 0} n(k,q)v(q) = \frac{1}{Vn(k)} \sum_{\substack{q\neq 0 \\ q\neq k}} n(k,q)v(q) + \frac{1}{Vn(k)} n(k,k)v(k). \tag{5.3}$$

The first contribution is regular at small k, yielding

$$\frac{1}{VNn_0} \sum_{q\neq 0} n(0,q)v(q) = \int \frac{d^3q}{(2\pi)^3} \, v(q)F_1(q) \tag{5.4}$$

where $F_1(q)$ is defined by equations (4.14) and (4.15). The second term in equation (5.3) can be evaluated in the $k \to 0$ limit as

$$\lim_{k\to 0} \frac{1}{V} \frac{1}{n(k)} n(k,k)v(k) = \lim_{k\to 0} \frac{1}{V} \frac{4\varepsilon_k}{n_0\omega_{pl}} Nn_0 F_1(k)v_k = -\omega_{pl} \tag{5.5}$$

where the relations $F_1(k=0) = -1/2$ and $n(k \to 0) \simeq 4\varepsilon_k/n_o\omega_{pl}$ have been used. Therefore,

$$\lim_{k\to 0} \varepsilon_P(k) = \omega_{pl} + \mu - \int \frac{d^3q}{(2\pi)^3} \, v(q)F_1(q). \tag{5.6}$$

We have thus proved that the relation $\lim_{k\to 0} \varepsilon_P(k) = \omega_{pl}$ is equivalent to the relation of Hugenholtz and Pines [28],

$$\mu = \int \frac{d^3q}{(2\pi)^3} \, v(q)F_1(q). \tag{5.7}$$

This relation is tested numerically by QMC methods immediately below.

6. Monte Carlo study of $F_1(k)$

In this section the function $F_1(k)$ is investigated by QMC simulations and equation (5.7) is verified numerically by comparing the integral on its right-hand side with the value of the chemical potential obtained from QMC results for the ground-state energy [12]. The Fourier transform of $F_1(k)$ is given by

$$\lim_{r_1'\to\infty} \rho_2(r_1, i_2; r_1', i_2) = n_0\rho^2(1 + F_1(|r_1 - i_2|)) \tag{6.1}$$

(see equation (4.11)). We have performed both variational Monte Carlo (VMC) and diffusion Monte Carlo (DMC) simulations for various numbers of particles, ranging from 32 to 200. A separate analysis has been made using real-space and reciprocal-space estimators.

6.1. Real-space results

The estimator is

$$f(|\mathbf{r}_1 - \mathbf{i}_2|) = \frac{1}{V}\frac{1}{\rho^2}\int_V d^3\mathbf{r}'_1 \; \rho_2(\mathbf{r}_1, \mathbf{i}_2; \mathbf{r}'_1, \mathbf{i}_2) = \frac{1}{V}\int_V d^3\mathbf{r}'_1 \; \left\langle \frac{\Psi(\mathbf{r}'_1, \mathbf{i}_2, \ldots)}{\Psi(\mathbf{r}_1, \mathbf{i}_2, \ldots)} \right\rangle \qquad (6.2)$$

which equals $n_0(1 + F_1(|\mathbf{r}_1 - \mathbf{i}_2|))$ in the thermodynamic limit. Finite-size corrections arise mainly from the regions where $\mathbf{r}'_1 \simeq \mathbf{i}_2$ or $\mathbf{r}'_1 \simeq \mathbf{r}_1$, and these are of relative importance $1/N$.
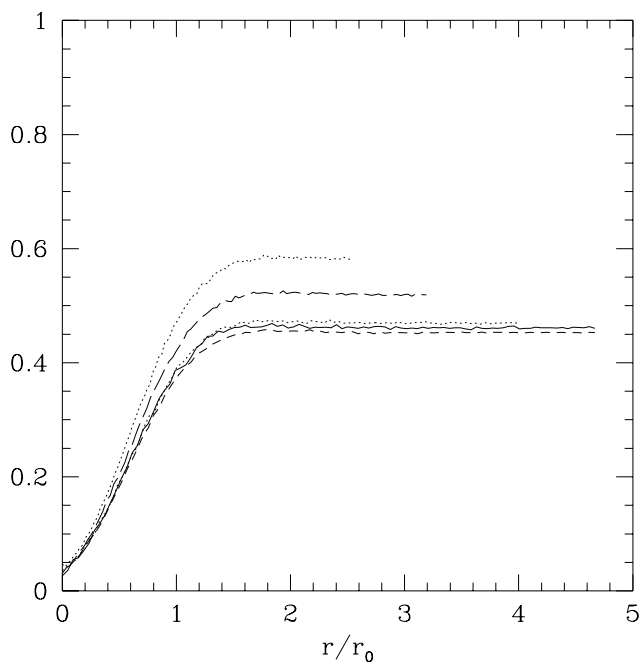

Figure 1. The function $f(r) = n_0(1 + F_1(r))$ at $r_s = 10$ as a function of r/r_0, where the mean interparticle distance r_0 is given by $(4\pi\rho/3)^{-1/3}$. VMC results with $N = 32, 64, 125$ and 200 are shown, from top to bottom. The full curve is from a DMC calculation at $N = 200$.

Table 1. Computed values of I_1 and I_2 from real-space estimators. The digits in parentheses represent the statistical error bar in the last decimal place. No size extrapolation has been made. Energies and frequencies are expressed in rydbergs.

r_s	N	I_1	I_2	μ	ω_{pl}
10	64	−0.52(2)	−0.162(3)	−0.1557	0.1095
10	125	−0.46(4)	−0.153(4)	−0.1557	0.1095
10	200	−0.48(2)	−0.153(2)	−0.1557	0.1095
10(DMC)	200	−0.48(2)	−0.151(2)	−0.1557	0.1095
1	200	−0.46(4)	−0.93(3)	−0.977	3.46
0.1	200	−0.45(4)	−5.2(1)	−5.62	109.5

Figure 1 shows the function $f(r)$ at $r_s = 10$ for $N = 32, 64, 125$ and 200. The size effect which is apparent in the data in figure 1 can be greatly reduced by dividing each
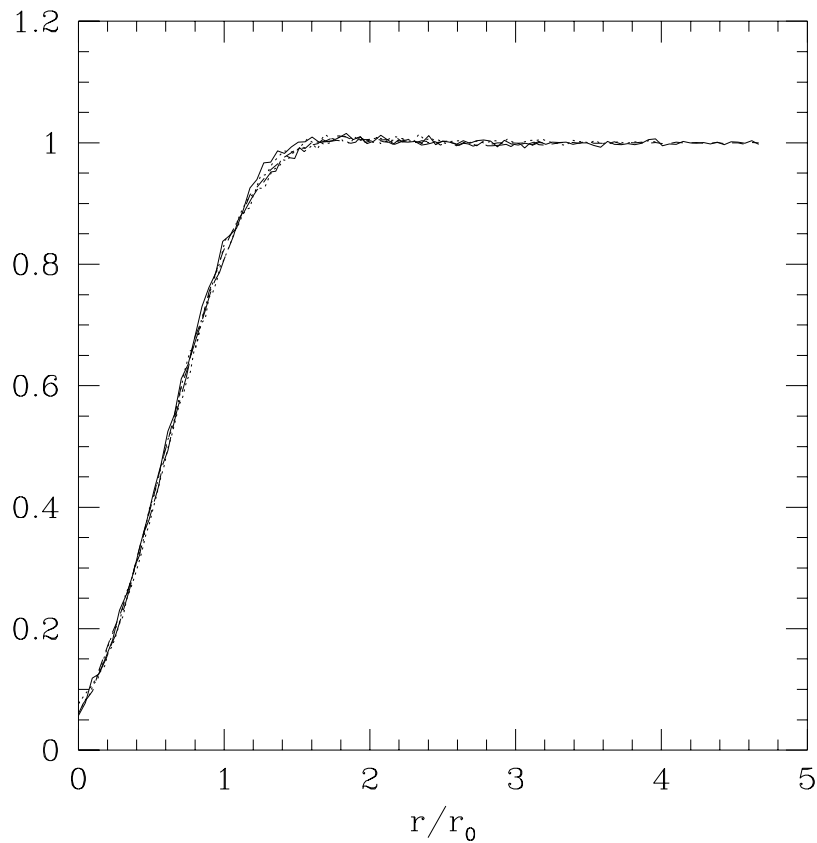
Figure 2. The same curves as in figure 1, after division by their large-r limit.

Table 2. Computed values of I_2 from reciprocal-space estimators. Energies and frequencies are expressed in rydbergs.

| r_s	N	I_2	μ	ω_{pl}
10	64	-0.1546	-0.1557	0.1095
10	125	-0.1604	-0.1557	0.1095
10	200	-0.1565	-0.1557	0.1095
10(DMC)	200	-0.1558	-0.1557	0.1095
1	200	-0.917	-0.977	3.46

curve by its value at large r, as is shown in figure 2. These curves are then integrated to determine the values of the integrals

$$I_1 = \rho \int_V F_1(r) \, \mathrm{d}^3 r = F_1(k = 0) \tag{6.3}$$

and

$$I_2 = \rho \int_V F_1(r) v(r) \, \mathrm{d}^3 r = \int \frac{\mathrm{d}^3 k}{(2\pi)^3} \, F_1(k) v(k). \tag{6.4}$$

According to the discussion in section 5 these ought to be equal to $-1/2$ and to the chemical potential μ, respectively. The results are shown in table 1 together with the chemical potential as obtained from interpolation of QMC data on the ground-state energy [12]. The table also reports the plasma frequency, showing that it is much larger than the remaining differences between μ and I_2 and thus confirming that $\varepsilon_P(k)$ goes to ω_{pl} for $k \to 0$ as shown in equation (5.6).
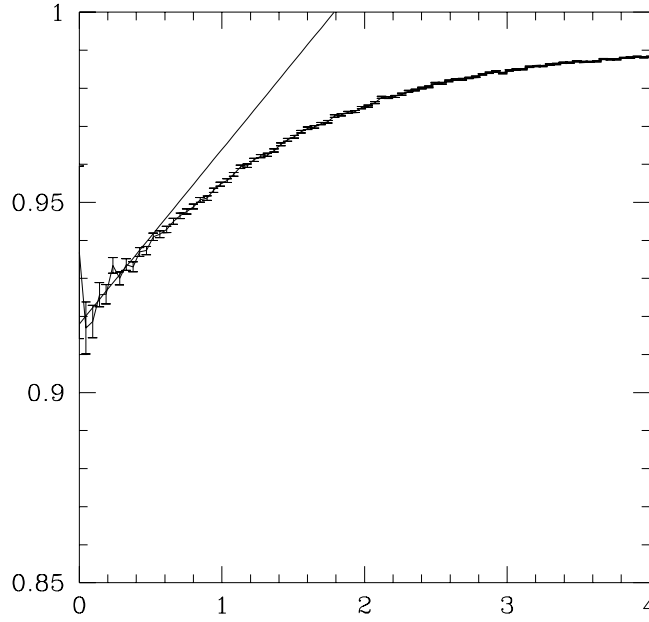
Figure 3. $F_1(r)$ at $r_s = 0.1$ as a function of r/r_0 from VMC data with $N = 200$. Also shown is the asymptotic behaviour given by the cusp condition in equation (6.5).

We also remark that good agreement has been found with the appropriate cusp condition

$$\left.\frac{\mathrm{d}}{\mathrm{d}r} F_1(r)\right|_{r=0} = \frac{1}{2a_0} F_1(r = 0) \tag{6.5}$$

as is shown in figure 3 for $r_s = 0.1$. As usual, the cusp condition is relevant only at large densities, where $F_1(r = 0) \neq 0$.

6.2. Reciprocal-space results

The estimator used is

$$f(k) = \frac{1}{V}\frac{1}{\rho^2}\int_V \mathrm{d}^3 r_1'\, \mathrm{e}^{\mathrm{i}k\cdot(r_1 - i_2)}\rho_2(r_1, i_2; r_1', i_2) = \frac{1}{V}\int_V \mathrm{d}^3 r_1' \left\langle \mathrm{e}^{\mathrm{i}k\cdot(r_1 - i_2)} \frac{\Psi(r_1', i_2, \ldots)}{\Psi(r_1, i_2, \ldots)}\right\rangle \tag{6.6}$$

which equals $n_0(F_1(k) + N\delta_{k0})$ in the thermodynamic limit. The condensate fraction is obtained from the relation $f(k = 0) = N n_0$.

Figure 4 shows the resulting DMC estimate of $F_1(k)$, which is clearly consistent with the theoretical limit $F_1(k \to 0) = -1/2$. Integration over k leads to significant averaging out
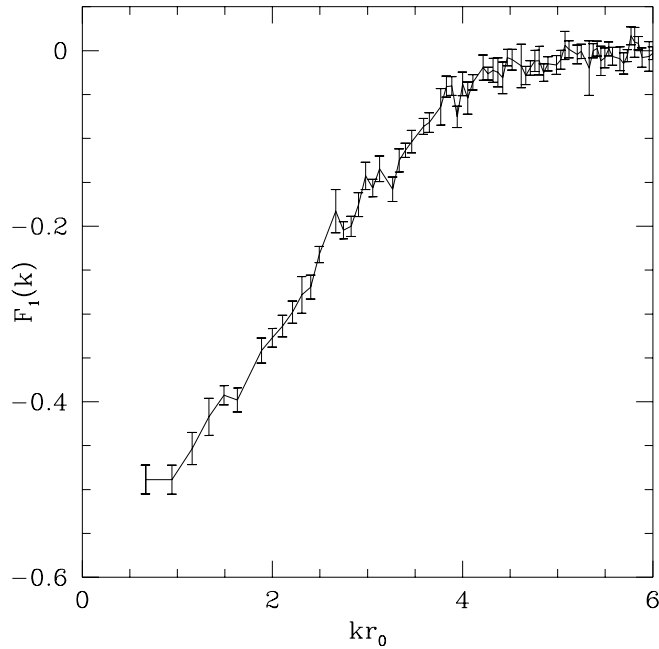
Figure 4. The function $F_1(k)$ versus kr_0 at $r_s = 10$ from DMC data with $N = 200$.

of the errors and to a very precise estimate of the integral I_2 at intermediate density. These data are reported in table 2. This kind of computation is more difficult at high densities because the momentum distribution is very narrow and only a few sampling wave vectors fall into the region where it is significantly different from zero. Strong size effects have also been observed in this regime. Therefore the result at $r_s = 1$ in table 2 is less reliable than those at $r_s = 10$. It has not been possible to obtain reliable results at $r_s = 0.1$.

7. Conclusions

As a summary of the main results of our analysis we present in table 3 a tabulation of the contributions from the plasmon excitation and from multiparticle excitations to the various matrix elements and sum rules at long wavelengths. The notation '$\leqslant k^2$' means 'of order k^n with $n \geqslant 2$'. We have marked with an asterisk those results which arise from exact cancellation at leading order and with a bullet those results which are identical for charged and neutral bosons. These latter ones are the f-sum rule, the commutation relation sum rule and the Bogoliubov sum rule.

Acknowledgments

Table 3. Leading and subleading contributions to various matrix elements and sum rules in the limit $k \to 0$. The single-plasmon and the multiparticle contributions are given separately.

	Plasmon	Multiparticle	
$\langle n|\rho_k|0\rangle = \langle n|\rho_k^\dagger|0\rangle$	$\sqrt{\dfrac{Nk^2}{2m\omega_{pl}}} \propto k$	$\propto k^2$	
$\langle n|a_k|0\rangle$	$-\sqrt{n_0\dfrac{\omega_{pl}}{4\varepsilon_k}} \propto \dfrac{1}{k}$	$\sqrt{\dfrac{n_0}{N}}\dfrac{m\omega_{pl}}{2|q||k-q|} \propto \dfrac{1}{\sqrt{k}}$	
$\langle n|a_k^\dagger|0\rangle$	$\sqrt{n_0\dfrac{\omega_{pl}}{4\varepsilon_k}} \propto \dfrac{1}{k}$	$\sqrt{\dfrac{n_0}{N}}\dfrac{m\omega_{pl}}{2|q||k-q|} \propto \dfrac{1}{\sqrt{k}}$	
ω_{n0}	ω_{pl}	$2\omega_{pl}$	
$\sum_n |\langle n|\rho_k|0\rangle|^2\omega_n^{-1}$	$N\varepsilon_k\omega_{pl}^{-2}$	$\propto k^4$	
$\sum_n |\langle n|\rho_k|0\rangle|^2$	$N\varepsilon_k\omega_{pl}^{-1}$	$\propto k^4$	
$\sum_n |\langle n|\rho_k|0\rangle|^2\omega_n$	$N\varepsilon_k$	$\propto k^4$	•
$\sum_n |\langle n|\rho_k|0\rangle|^2\omega_n^2$	$N\varepsilon_k\omega_{pl}$	$\propto k^4$	
$\sum_n |\langle n|\rho_k|0\rangle|^2\omega_n^3$	$N\varepsilon_k\omega_{pl}^2$	$\propto k^4$	
$\sum_n \left[|\langle n|a_k|0\rangle|^2 + |\langle n|a_k^\dagger|0\rangle|^2\right]\omega_n^{-1}$	$n_0 m/k^2$	$m^2 n_0\omega_{pl}/64\rho k$	
$\sum_n |\langle n|a_k|0\rangle|^2$	$n_0 m\omega_{pl}/2k^2$	$m^2 n_0\omega_{pl}^2/64\rho k$	
$\sum_n \left[|\langle n|a_k|0\rangle|^2 - |\langle n|a_k^\dagger|0\rangle|^2\right]$	$\leqslant$constant (∗)	$\leqslant$constant (∗)	•
$\sum_n \left[|\langle n|a_k|0\rangle|^2 + |\langle n|a_k^\dagger|0\rangle|^2\right]\omega_n$	$n_0 m\omega_{pl}^2/k^2$	$m^2 n_0\omega_{pl}^3/16\rho k$	
$\sum_n |\langle n|a_k|0\rangle|^2\omega_n$	$n_0 m\omega_{pl}^2/2k^2$	$m^2 n_0\omega_{pl}^3/32\rho k$	
$\sum_n \langle n|\rho_k|0\rangle\langle n|a_k + a_k^\dagger|0\rangle/\omega_n$	$\leqslant k^2$ (∗)	$\leqslant k^2$ (∗)	
$\sum_n \langle n|\rho_k|0\rangle\langle n|a_k - a_k^\dagger|0\rangle$	$-\sqrt{Nn_0}$	$\leqslant k^2$ (∗)	•
$\sum_n \langle n|\rho_k|0\rangle\langle n|a_k|0\rangle$	$-\sqrt{Nn_0}/2$	$\propto k^{3/2}$	
$\sum_n \langle n|\rho_k|0\rangle\langle n|a_k + a_k^\dagger|0\rangle\omega_n$	$\leqslant k^2$ (∗)	$\propto k^{3/2}$	
$\sum_n \langle n|\rho_k|0\rangle\langle n|a_k|0\rangle\omega_n$	$\sqrt{Nn_0}\omega_{pl}/2$	$\propto k^{3/2}$	

Appendix A. Asymptotics of density–density matrix elements

In this appendix we give a rigorous proof of the fact that the plasmon excitation exhausts the density–density sum rules to leading order in k. Our derivation is based only on the m_{-1}-, m_1- and m_3-sum rules and is therefore valid for both bosons and fermions.

We define $f(\omega)$ as the leading contribution to the density–density spectral weight in the limit $k \to 0$,

$$f(\omega) = -\lim_{k \to 0} v_k \, \text{Im} \, \chi(k, \omega). \tag{A.1}$$

Equations (2.5), (2.7) and (2.3) become

$$\frac{2}{\pi} \int_0^\infty \omega^{-1} f(\omega) \, d\omega = 1 \tag{A.2}$$

$$\frac{2}{\pi} \int_0^\infty f(\omega) \, d\omega = \omega_{pl}^2 \tag{A.3}$$

and

$$\frac{2}{\pi} \int_0^\infty \omega^3 f(\omega) \, d\omega = \omega_{pl}^4. \tag{A.4}$$

We next make use of Schwartz's lemma, stating that

$$\left(\int g(x)h(x) \, dx \right)^2 \leqslant \int g^2(x) \, dx \int h^2(x) \, dx \tag{A.5}$$

for two arbitrary functions $g(x)$ and $h(x)$, with the equality holding if and only if there is a constant λ such that $g(x) = \lambda h(x)$ almost everywhere. By substituting $g(\omega) = \sqrt{\omega^3 f(\omega)}$ and $h(\omega) = \sqrt{\omega^{-1} f(\omega)}$ into equation (A.5) we see from equations (A.2)–(A.4) that the equality holds in equation (A.5). Therefore $\sqrt{\omega^3 f(\omega)} = \lambda \sqrt{\omega^{-1} f(\omega)}$ or $\omega^4 f(\omega) = \lambda f(\omega)$.

We conclude that $f(\omega)$ must be proportional to a delta function, whose position and weight can be determined by inserting $f(\omega) = A \, \delta(\omega - \omega_0)$ in the previous relations. A contribution for $\omega < 0$ is then obtained by recalling that $\mathrm{Im}\, \chi(k, -\omega) = -\,\mathrm{Im}\, \chi(k, \omega)$. The final result

$$\lim_{k \to 0} v_k \, \mathrm{Im}\, \chi(k, \omega) = -\omega_{pl} \left(\delta(\omega - \omega_{pl}) - \delta(\omega + \omega_{pl}) \right) \tag{A.6}$$

coincides with equation (2.9) in the main text.

Appendix B. Quantum hydrodynamics

In this appendix we discuss in some detail the QH approach to the charged boson problem and show that one can independently recover from it all of the results that we have obtained from sum rule arguments. A similar approach for the neutral boson fluid was sketched in [29].

As discussed in the introduction, QH is based on the assumption of non-interacting elementary excitations, which can be described as fluctuations of the superfluid phase operator $\phi(r)$. This is defined by the relation $\Psi(r) = \sqrt{n_0} \exp\{i\phi(r)\}$ and will be considered as a small parameter. By expanding the particle operator $\Psi(r)$ in powers of $\phi(r)$ we obtain

$$\Psi(r) = \sqrt{n_0} e^{i\phi(r)} \simeq \sqrt{n_0} \left(1 + i\phi(r) - \frac{1}{2}\phi^2(r) + O(\phi^3) \right) \tag{B.1}$$

which can be Fourier transformed to give

$$a_k = \sqrt{n_0 N} \delta_{k0} + i\sqrt{n_0} \Phi_k - \frac{1}{2} \frac{\sqrt{n_0}}{\sqrt{N}} \sum_q \Phi_q \Phi_{k-q}. \tag{B.2}$$

The Hamiltonian can be written as

$$H = \int \rho \, d^3 r \, \frac{1}{2m} (\nabla \phi(r))^2 + \frac{1}{2}\rho^2 \int d^3 r \, d^3 r' \, \rho(r)\rho(r') \frac{e^2}{|r - r'|}$$

$$= \sum_k \frac{k^2}{2m} \Phi_{-k}\Phi_k + \frac{1}{2V} \sum_k v_k \rho_k \rho_{-k}. \tag{B.3}$$

The assumption of non-interacting elementary excitations is equivalent to the *ansatz*

$$H = \sum_k \omega_k \left(c_k^\dagger c_k + \frac{1}{2} \right). \tag{B.4}$$

The operators $c_k^\dagger$ and c_k can be expanded in terms of the phase and density fluctuation operators $c_k = \alpha_k \Phi_k + \beta_k \rho_k$, the result being

$$H = \sum_k \left(\omega_k |\alpha_k|^2 \Phi_k^\dagger \Phi_k + \omega_k |\beta_k|^2 \rho_k^\dagger \rho_k + \cdots \right) \tag{B.5}$$

where the dots indicate mixed terms describing couplings between phase and density fluctuations. They are supposed to vanish in the hydrodynamic regime. The present approximation is therefore equivalent to the statement that $[\Phi_k, \rho_k]$ is a *C*-number.

By equating corresponding terms we obtain

$$|\alpha_k| = \sqrt{\frac{k^2/2m}{\omega_k}} \tag{B.6}$$

$$|\beta_k| = \sqrt{\frac{\rho v_k}{2\omega_k}} \tag{B.7}$$

and, with straightforward algebra,

$$\Phi_k = \frac{c_k - c_{-k}^\dagger}{2\alpha_k} = \frac{i}{2} \sqrt{\frac{\omega_k}{k^2/2m}} (c_k - c_{-k}^\dagger) \tag{B.8}$$

and

$$\rho_k = \frac{c_k + c_{-k}^\dagger}{2\beta_k} = \frac{1}{2} \sqrt{\frac{2\omega_k}{\rho v_k}} (c_k + c_{-k}^\dagger). \tag{B.9}$$

Here, the phases have been chosen in accord with equation (2.10).

We finally expand the single-particle operators a_k in terms of c_k and $c_k^\dagger$:

$$a_k = \sqrt{N n_0}\, \delta_{k0} + \sqrt{n_0} \sqrt{\frac{\omega_k}{\varepsilon_k}} \frac{c_k - c_{-k}^\dagger}{2}$$
$$+ \frac{\sqrt{n_0}}{2\sqrt{N}} \sum_q \sqrt{\frac{\omega_q}{q^2/2m}} \sqrt{\frac{\omega_{k-q}}{(k-q)^2/2m}} \frac{c_q - c_{-q}^\dagger}{2} \frac{c_{k-q} - c_{q-k}^\dagger}{2} + \cdots. \tag{B.10}$$

This formula allows one to reduce expectation values between states of the interacting system to the trivial matrix elements $c_k|0\rangle = 0$ and $\langle 0|c_k c_k^\dagger|0\rangle = 1$.

Since we are interested in infrared divergences the details at finite and large k are immaterial, and in particular we can safely assume that $\omega_k = \omega_{pl}$. If $|k, \omega_{pl}\rangle = c_k^\dagger|0\rangle$ is the state of momentum k and energy ω_{pl} with one plasmon excited, we have

$$\langle k, \omega_{pl}|a_k|0\rangle = -\sqrt{\frac{n_0 \omega_{pl}}{4\varepsilon_k}} \tag{B.11}$$

and

$$\langle k, \omega_{pl}|a_k^\dagger|0\rangle = \sqrt{\frac{n_0 \omega_{pl}}{4\varepsilon_k}}. \tag{B.12}$$

Considering now two-plasmon terms we find

$$\langle k, 2\omega_{pl}, q|a_k|0\rangle = \sqrt{\frac{n_0}{N}} \frac{m \omega_{pl}}{2|q||k-q|} \tag{B.13}$$

and

$$\langle \boldsymbol{k}, 2\omega_{pl}, \boldsymbol{q}|a_{\boldsymbol{k}}^{\dagger}|0\rangle = \sqrt{\frac{n_0}{N}} \frac{m\omega_{pl}}{2|\boldsymbol{q}||\boldsymbol{k}-\boldsymbol{q}|} \tag{B.14}$$

where $|\boldsymbol{k}, 2\omega_{pl}, \boldsymbol{q}\rangle = c_{\boldsymbol{k}-\boldsymbol{q}}^{\dagger}c_{\boldsymbol{q}}|0\rangle$ is the state of total momentum $\boldsymbol{k}$ and energy $2\omega_{pl}$ with two plasmons excited, with momentum $\boldsymbol{q}$ and $\boldsymbol{k}-\boldsymbol{q}$ respectively. A factor of 2 has come from the fact that $|\boldsymbol{k}, 2\omega_{pl}, \boldsymbol{q}\rangle = |\boldsymbol{k}, 2\omega_{pl}, \boldsymbol{k}-\boldsymbol{q}\rangle$.

The momentum distribution can be straightforwardly evaluated as

$$
\begin{aligned}
n(k) &= \langle 0|a_{\boldsymbol{k}}^{\dagger}a_{\boldsymbol{k}}|0\rangle \\
&= n_0 \frac{\omega_{pl}}{4k^2/2m} - 2\frac{n_0}{64N}\sum_{\boldsymbol{q}} \frac{\omega_{pl}}{q^2/2m}\frac{\omega_{pl}}{(\boldsymbol{k}-\boldsymbol{q})^2/2m} \\
&= n_0 \frac{\omega_{pl}}{4\varepsilon_k} + \frac{m^2 n_0 \omega_{pl}^2}{64\rho\,k} + \cdots.
\end{aligned} \tag{B.15}
$$

The last term has been expanded using equation (3.7).

Divergent contributions to the other sum rules can be similarly evaluated, the results being in complete agreement with those obtained in the main text. We finally remark that, while the leading k^{-1} divergent contributions to $\langle n|a_{\boldsymbol{k}}|0\rangle$ arise from single-plasmon states, the subleading $k^{-1/2}$ contributions arise from double-plasmon states. Other (non-hydrodynamic) contributions are expected to be finite or zero in the $k \to 0$ limit.

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