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LETTER TO THE EDITOR

Upper bounds on plasmon dispersion in the degenerate boson plasma

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Abstract. Sum-rule arguments are used to derive two rigorous upper bounds for the plasmon dispersion curve in a fluid of charged bosons at zero temperature. They are readily evaluated (i) at long wavelengths, to show that the leading dispersion coefficient is negative at all couplings, and (ii) at weak coupling, to obtain a simple analytic upper bound for the whole dispersion curve.

Recent work by three of us [1] dealing with the dielectric response of the degenerate fluid of charged bosons has emphasized that the compressibility, K, of the fluid, entering its static dielectric function at long wavelengths, is negative at all values of the Coulomb coupling strength $r_s > 0$. Here, r_s is the dimensionless length parameter r_0/a_0, where r_0 is related to the particle number density n by $r_0 = (4\pi n/3)^{-1/3}$ and a_o is the Bohr radius. The inequality $K < 0$ at $r_s > 0$ is a consequence of the fact that the contribution of correlations to the effective interaction between the particles is intrinsically attractive, and implies overscreening of a foreign charge and long-range attraction between foreign charges in a linear response regime. The inequality is confirmed by the low-r_s expansion of the ground-state energy given by Brueckner [2]. The available evidence on the ground state energy and the static dielectric response from microscopic calculations in the hypernetted-chain approximation [3] and from quantum Monte Carlo simulations by Ceperley and Alder [4], Sugiyama and coworkers [5] and Moroni (unpublished) explicitly confirms the inequality in a wide range of r_s.

As pointed out in [1], further consequence of the inequality $K < 0$ is that, on calculating the dynamic response of the fluid in an approximation that neglects the frequency dependence of the correlation potential, the plasmon dispersion curve ω_k is found to have a leading dispersion coefficient $d^2\omega_k/dk^2|_{k=0}$ which is negative at all values of $r_s > 0$. This implies that the dispersion curve goes through a minimum before approaching the free-particle recoil frequency $\epsilon_k = k^2/2m$ at large wavenumber k ($\hbar = 1$).

In this letter we show by a sum-rule argument for Bose fluids that the inequality $K < 0$ provides a rigorous upper bound $d^2\omega_k/dk^2|_{k=0} < 0$ on the leading dispersion coefficient (see (8)). We also present an easily calculable analytic formula providing an equally rigorous upper bound for the whole dispersion curve ω_k at small r_s (see (11)). At long wavelengths, this yields the weaker inequality $d^2\omega_k/dk^2|_{k=0} \leqslant 0$.

The sum-rule approach has been widely used in the literature to examine various dynamic properties of many-body systems (see the work of Stringari [6, 7] and references given therein). Of specific interest in the present context are the rigorous zero-temperature inequalities

$$\omega_0^2 \leqslant \frac{\langle [A^\dagger, [H, A]] \rangle}{\chi_{A^\dagger, A}} \tag{1}$$

and

$$\omega_0^2 \leqslant \frac{\langle [A^\dagger, [H, A]] \rangle \langle [B^\dagger, [H, B]] \rangle}{|\langle A^\dagger, [B] \rangle|^2} \tag{2}$$

for the energy ω_0 of the lowest state excited by the operators A and B, H being the Hamiltonian of the system. In the inequality (1), $\chi_{A^\dagger, A}$ is the static response relating to the operator A and the numerator expresses the energy-weighted sum rule. The inequality (2) is proven by combining (1) with the Bogoliubov inequality [8, 9]

$$\chi_{A^\dagger, A} \langle [B^\dagger, [H, B]] \rangle \geqslant |\langle [A^\dagger, B] \rangle|^2. \tag{3}$$

Clearly, (2) provides a less stringent upper bound on the excitation frequency.

For a Bose superfluid at zero temperature, choosing $A^\dagger = \rho_k$ where ρ_k is the density fluctuation operator, equation (1) yields the following inequality on the dispersion relation of the lowest collective excitation

$$\omega_k^2 \leqslant -\frac{nk^2}{m\chi(k, 0)} \tag{4}$$

where $\chi(k, 0)$ is the static linear density response function and we have used the f-sum rule, $\langle [\rho_k (H, \rho_{-k})] \rangle = nk^2/m$. Choosing $A^\dagger = \rho_k$ and $B = a_k - a_{-k}^\dagger$ where a_k and $a_{-k}^\dagger$ are the particle annihilation and creation operators, equation (2) yields the inequality [7]

$$\omega_k^2 \leqslant \frac{1}{\alpha}\epsilon_k \left(\epsilon_k - \mu + \frac{1}{(2\pi)^3} \int \mathrm{d}p \, v_p \big[n(p+k) + \bar{n}(p+k) \big] \right). \tag{5}$$

Here, v_p is the Fourier transform of the interaction potential, μ is the chemical potential, α is the fraction of particles in the zero-momentum condensate and

$$n(p) = \langle 0 | a_p^\dagger a_p | 0 \rangle = (2\pi)^3 \alpha n \delta(p) + n_1(p) \tag{6}$$

$$\bar{n}(p) = \tfrac{1}{2} \langle 0 | a_p^\dagger a_{-p}^\dagger + a_p a_{-p} | 0 \rangle = (2\pi)^3 \alpha n \delta(p) + \bar{n}_1(p) \tag{7}$$

where $n_1(p)$ and $\bar{n}_1(p)$ refer to the particles out of the condensate.

In applying equations (4) and (5) to the degenerate fluid of charged bosons neutralized by a uniform background we use $v_p = 4\pi e^2/p^2$ $(p \neq 0)$ and recall that the plasma frequency $\omega_{\mathrm{pl}} = (4\pi n e^2/m)^{1/2}$ at $k = 0$ is given by $\omega_{\mathrm{pl}} = (2n\epsilon_k v_k)^{1/2}$. From equation (4) we then obtain

$$\omega_k^2 \leqslant \omega_{\mathrm{pl}}^2 + \frac{k^2}{nmK} \tag{8}$$

in the long-wavelength limit $k \to 0$. This shows that the leading dispersion coefficient is necessarily negative at all $r_s > 0$.

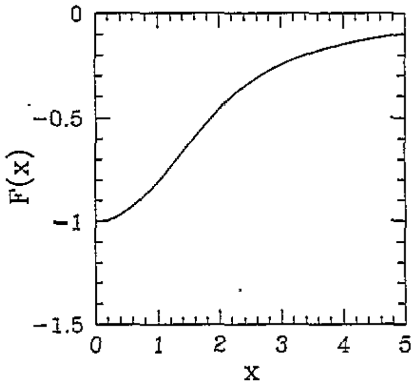

Figure 1. Graph of the function $F(x)$ defined in equation (12).

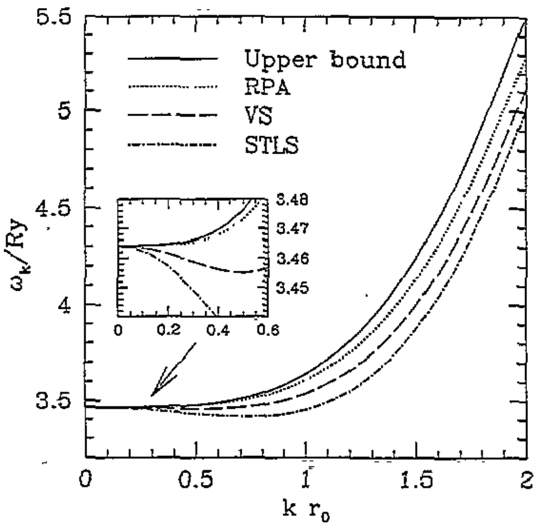

Figure 2. Plasmon dispersion relation at $r_s = 1$ in various approximations (from [1]), compared with the upper bound given by equation (11). The inset gives an enlarged view of the small-k region.

From equation (5), after changing the integration variable to $q = p + k$ and carrying out the angular integration, we have

$$\omega_k^2 \leqslant \omega_{\rm pl}^2 + \frac{1}{\alpha}\epsilon_k\left(\epsilon_k - \mu + \frac{e^2}{\pi}\int_0^\infty {\rm d}q\,\frac{q}{k}\,\ln\left|\frac{q+k}{q-k}\right|\left[n_1(q) + \bar{n}_1(q)\right]\right). \qquad (9)$$

This expression is readily evaluated in the small-coupling limit $r_s \to 0$, where all the quantities entering it are known from the early work of Foldy [10]. His results to lowest order in r_s are

$$2\left[n_1(q) + \bar{n}_1(q)\right] = \frac{\epsilon_q}{(\omega_{\rm pl}^2 + \epsilon_q^2)^{1/2}} - 1 \qquad (10)$$

and $\alpha = 1$. Using to the same order of accuracy the value of the chemical potential in the random phase approximation (RPA), $\mu = -Cr_s^{-3/4}$ Ryd with $C = (2/\pi)\int_0^\infty {\rm d}x(1 - (1 + 12/x^4)^{-1/2}) \approx 1.003\,848\,3$, we find

$$\omega_k^2 \leqslant \omega_{\rm pl}^2 + \epsilon_k^2 + \epsilon_k r_s^{-3/4}\left[F\left(kr_0 r_s^{-1/4}\right) + C\right] \qquad (11)$$

in Rydberg units. We have here introduced the function $F(x)$, which is defined by

$$F(x) = \frac{1}{\pi}\int_0^\infty {\rm d}y\,\frac{y}{x}\,\ln\left|\frac{y+x}{y-x}\right|\left[\left(1 + 12y^{-4}\right)^{-1/2} - 1\right]. \qquad (12)$$

The graph of this function is given in figure 1. In regard to the leading dispersion coefficient for the plasmon at long wavelengths from equation (11), it is readily seen that $F(x)$ tends to $-C$ for $x \to 0$. Hence, equation (11) yields

$$\left.{\rm d}^2\omega_k/{\rm d}k^2\right|_{k=0} \leqslant 0 \qquad (13)$$

as an upper bound.

The upper bound obtained in equation (11) for the plasmon dispersion curve is compared in figure 2 at $r_s = 1$ with the results given in [1] on the basis of approximate theories of dynamic screening, including the RPA and two forms of (frequency-independent) effective correlation potential. Of course, the effect of short-range correlations is to lower the excitation energy. We recall in particular that the curve marked VS is evaluated in an approximation which takes self-consistent account of the compressibility sum rule and yields very close agreement with the available evidence on the compressibility.

The result in equation (11) is valid only at weak coupling and it would be worth carrying the perturbative treatment of the charged boson fluid to the next order in r_s, where we expect that the upper bound would become more stringent. On the other hand, the VS results already provide a more stringent upper bound on the leading dispersion coefficient by virtue of equation (8). This is displayed on an enlarged scale in the inset in figure 2.

In summary, we have demonstrated a rigorous upper bound on the plasmon dispersion relation at small coupling and a more stringent upper bound on the leading dispersion coefficient at all couplings.

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